

CLEO 2017

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Laser Science to Photonic Applications

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 → **strongly-confined modes**
 - Highly dispersive
 - Highly nonlinear, Kerr-type response → **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**



Laser Science to Photonic Applications

Mathematical Framework

Perturbation Theory

Nonlinear frequency shift (perturbation theory)

Classic form:
$$\frac{\Delta\omega}{\omega_0} = -\frac{1}{2} \frac{\iiint_V (\Delta\bar{\epsilon}_r \mathbf{E}_0) \cdot \mathbf{E}_0^* dV}{\iiint_V \bar{\epsilon}_r \mathbf{E}_0 \cdot \mathbf{E}_0^* dV} \quad [\text{Bravo-Abad, JLT 25, 2539}]$$

Extended form:

$$\frac{\Delta\omega}{\omega_0} = - \frac{\iiint_V \mathbf{P}_{\text{NL}} \cdot \mathbf{E}_0^* dV - j \frac{1}{\omega_0} \iiint_V \mathbf{J}_{\text{NL}} \cdot \mathbf{E}_0^* dV}{\iiint_V \epsilon_0 \frac{\partial\{\omega\bar{\epsilon}_r\}}{\partial\omega} \mathbf{E}_0 \cdot \mathbf{E}_0^* dV + \iiint_V \mu_0 \mathbf{H}_0 \cdot \mathbf{H}_0^* dV + \iiint_V \frac{\partial\bar{\sigma}_{\text{Im}}^{(1)}}{\partial\omega} \mathbf{E}_0 \cdot \mathbf{E}_0^* dV}$$

[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 ($W_e \neq W_m$; next slide)

Energy density in media with complex conductivity

Poynting theorem in the time domain

$$\langle \mathcal{J}(t) \cdot \mathcal{E}(t) \rangle = \underbrace{\frac{1}{2} \bar{\sigma}_{\text{Re}}^{(1)} \mathbf{E}_0(\omega) \cdot \mathbf{E}_0^*(\omega)}_{\text{Power loss density}} + \underbrace{\frac{\partial}{\partial t} \left\{ \frac{1}{4} \frac{\partial \bar{\sigma}_{\text{Im}}^{(1)}}{\partial \omega} \mathbf{E}_0(\omega) \cdot \mathbf{E}_0^*(\omega) \right\}}_{\text{Stored energy density}}$$

Zero when
dispersion is
neglected

Energy density in media with complex conductivity

Poynting theorem in the time domain

$$\langle \mathcal{J}(t) \cdot \mathcal{E}(t) \rangle = \underbrace{\frac{1}{2} \bar{\sigma}_{\text{Re}}^{(1)} \mathbf{E}_0(\omega) \cdot \mathbf{E}_0^*(\omega)}_{\text{Power loss density}} + \underbrace{\frac{\partial}{\partial t} \left\{ \frac{1}{4} \frac{\partial \bar{\sigma}_{\text{Im}}^{(1)}}{\partial \omega} \mathbf{E}_0(\omega) \cdot \mathbf{E}_0^*(\omega) \right\}}_{\text{Stored energy density}}$$

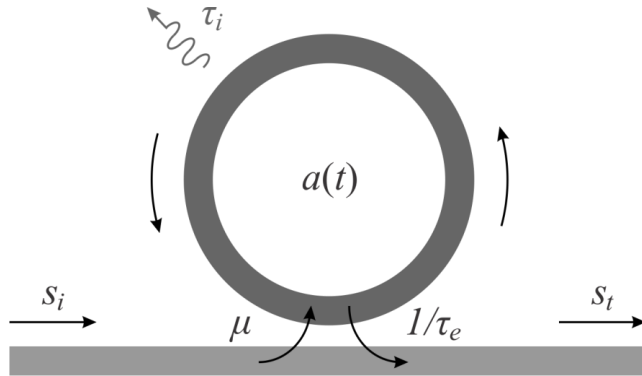
Zero when
dispersion is
neglected

Poynting theorem in the frequency domain

$$\begin{aligned} - \iiint_V \nabla \cdot \mathbf{S} dV &= \frac{1}{2} \iiint_V \bar{\sigma}_{\text{Re}}^{(1)} \mathbf{E}_0 \cdot \mathbf{E}_0^* dV - \\ &\quad - j \frac{1}{2} \omega_0 \iiint_V \varepsilon_0 \bar{\varepsilon}_r \mathbf{E}_0 \cdot \mathbf{E}_0^* dV + j \frac{1}{2} \omega_0 \iiint_V \mu_0 \mathbf{H}_0 \cdot \mathbf{H}_0^* dV + j \frac{1}{2} \iiint_V \bar{\sigma}_{\text{Im}}^{(1)} \mathbf{E}_0 \cdot \mathbf{E}_0^* dV \\ &= P_{\text{loss}} + j(-Q_E + Q_H + Q_J) \end{aligned}$$

- Reactive power \neq 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)



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

$$s_t = s_i + \mu a$$

$\alpha(t)$	cavity amplitude, $ a ^2 \equiv W_e + W_m + W_j$
ω_0	unperturbed resonance frequency
$\Delta\omega$	nonlinear frequency shift
τ	photon lifetime, $\tau = 2Q/\omega_0$
μ	coupling coefficient, $\mu = j\sqrt{2/\tau_e}$
$s(t)$	w/g mode amplitude, $ s ^2 \equiv P$

[Tsilipakos, JOSA B 31, 2014]

[Soljacic, PRE 5, 2002]

Steady-state response

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

$$\delta = \tau_i(\omega - \omega_0)$$

normalized detuning

$$\delta_{\text{th}} = -(1 + r_Q)\sqrt{3}$$

detuning threshold for BI

$$r_Q = Q_i/Q_e$$

quality factor ratio

$$p = P/P_0$$

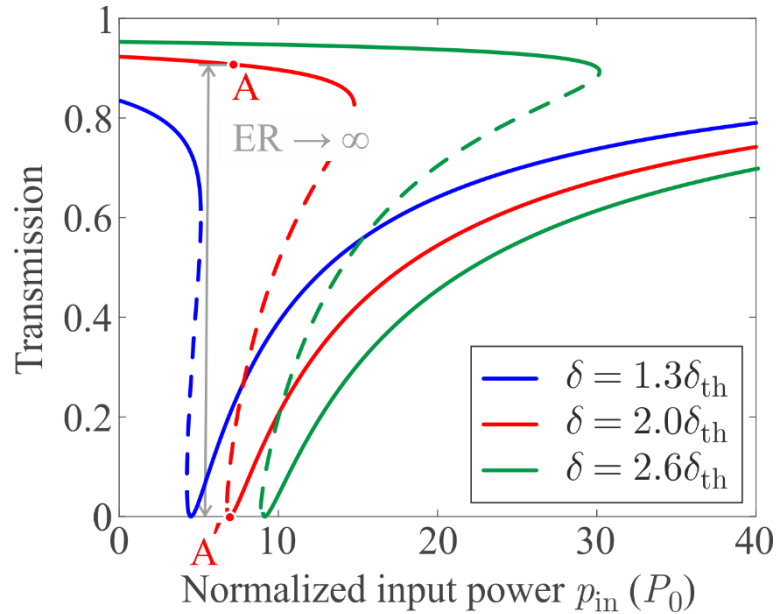
normalized power

$$P_0$$

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, $r_Q = 1$

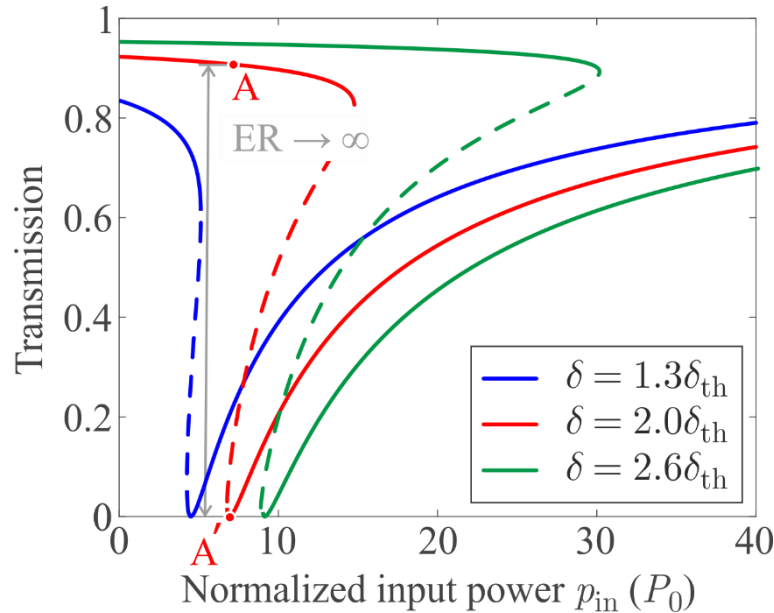
Application to optical bistability



Increase in $|\delta|$

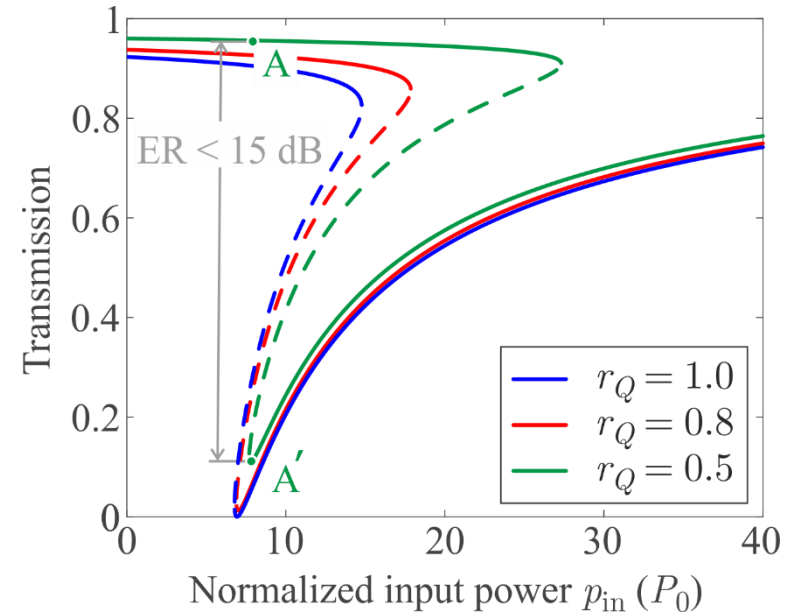
- ✗ Higher input power required
- ✓ Loop span increases
- ✓ Maximum transmission increases

Application to optical bistability



Increase in $|\delta|$

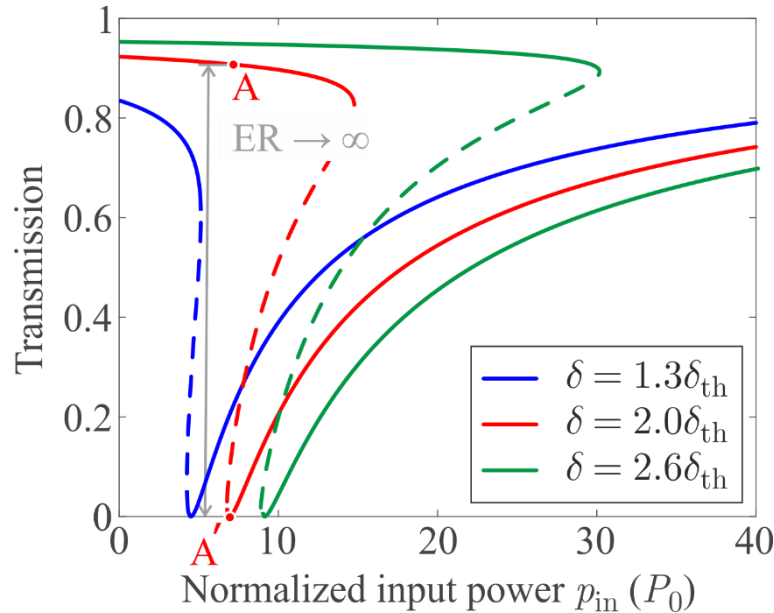
- ✗ Higher input power required
- ✓ Loop span increases
- ✓ Maximum transmission increases



Decreasing r_Q below 1

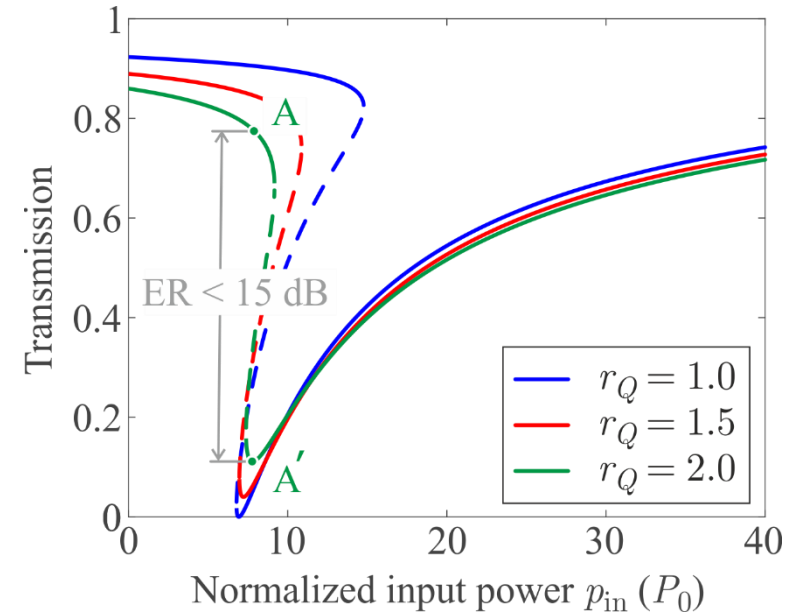
- ✗ Higher input power required
- ✗ T_{min} increases (loop elevation)
- ✓ Loop span increases (δ_{th} decreases)

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_{min} increases (loop elevation)
- ✓ Loop span increases (δ_{th} decreases)

Increasing r_Q above 1

- ✗ Higher input power required
- ✗ T_{min} increases (loop elevation)
- ✗ Loop span decreases (δ_{th} increases)



Laser Science to Photonic Applications

Graphene Properties

Far-Infrared regime (THz)

Linear Properties

$$\mathbf{J}_{s,\text{lin}} = \sigma_{\text{intra}}(\omega) \mathbf{E}_{0,\parallel}$$

- 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**

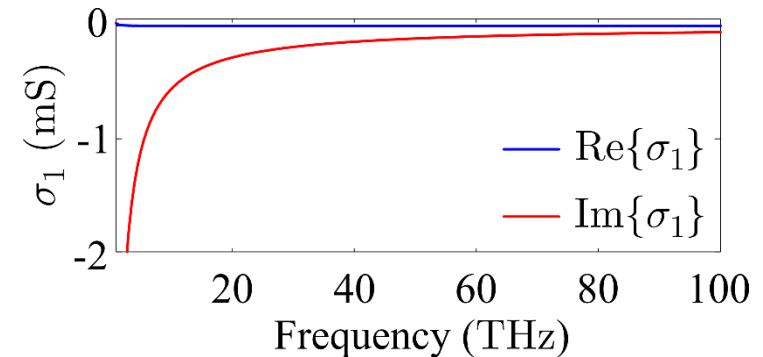
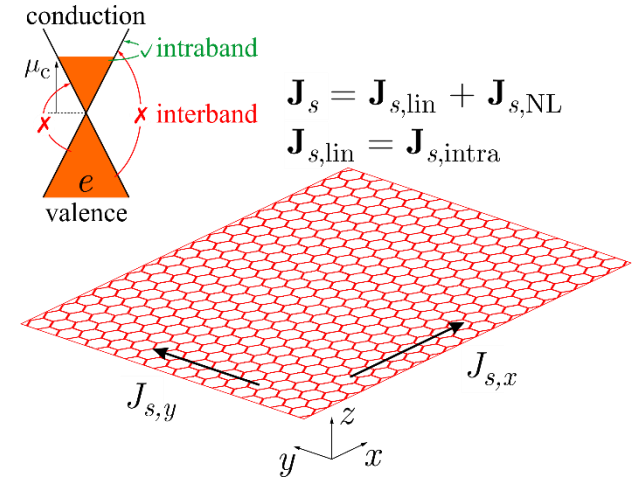
[Falkovsky, *Phys. Usp.* 178, 887]

Nonlinear Properties

$$\mathbf{J}_{s,\text{NL}} = \frac{\sigma_3(\omega)}{4} [2(\mathbf{E}_{0,\parallel} \cdot \mathbf{E}_{0,\parallel}^*) \mathbf{E}_{0,\parallel} + (\mathbf{E}_{0,\parallel} \cdot \mathbf{E}_{0,\parallel}) \mathbf{E}_{0,\parallel}^*]$$

- Kerr-type nonlinearity (purely imaginary σ_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**)

[Mikhailov, *J. Phys.: Condens. Matter* 20, 384204]



Near-Infrared regime (NIR)

Linear Properties

$$\mathbf{J}_{s,\text{lin}} = (\sigma_{\text{intra}}(\omega) + \sigma_{\text{inter}}(\omega))\mathbf{E}_{0,\parallel}$$

- 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]

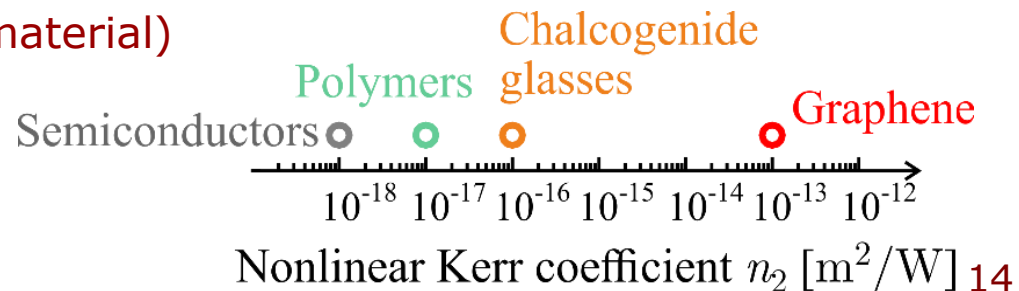
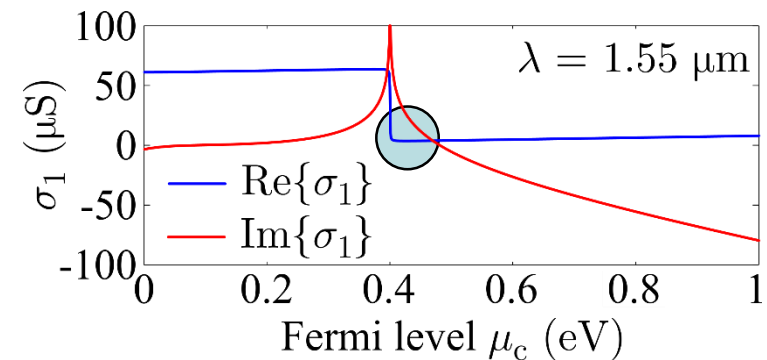
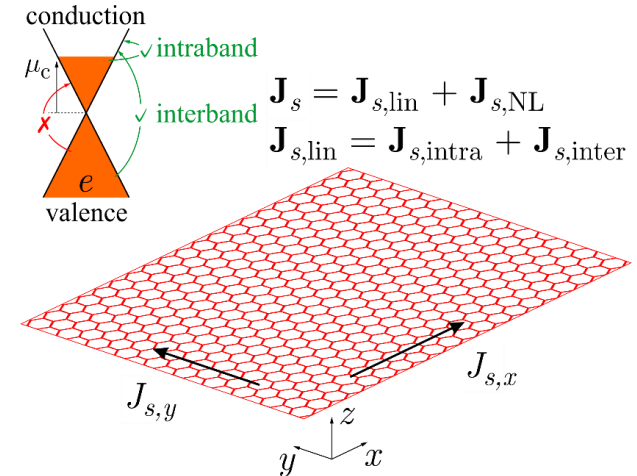
Nonlinear Properties

$$\mathbf{J}_{s,\text{NL}} = \frac{\sigma_3(\omega)}{4} [2(\mathbf{E}_{0,\parallel} \cdot \mathbf{E}_{0,\parallel}^*)\mathbf{E}_{0,\parallel} + (\mathbf{E}_{0,\parallel} \cdot \mathbf{E}_{0,\parallel})\mathbf{E}_{0,\parallel}^*]$$

- Kerr-type nonlinearity (purely imaginary σ_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]

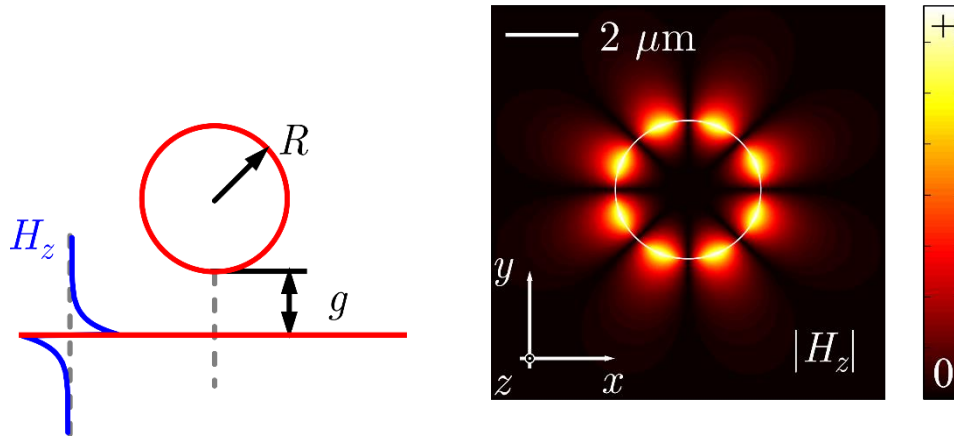




Laser Science to Photonic Applications

Resonant Structures

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

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

Characteristic Power

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

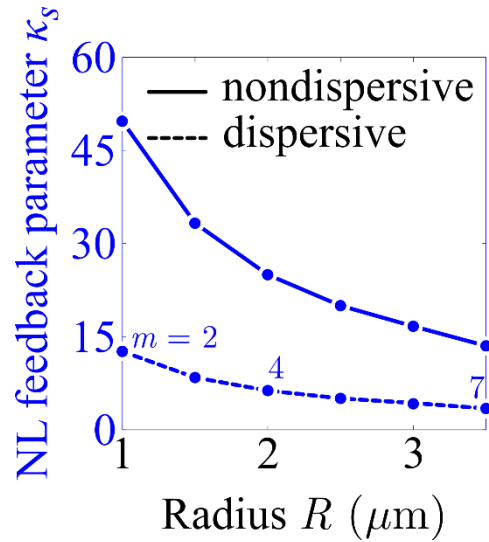
P_0 must be minimized for optimum performance

Nonlinear feedback parameter

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

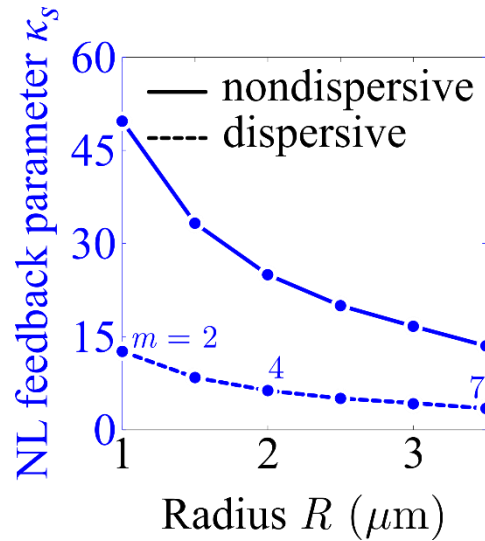
$$\kappa_s = \left(\frac{c_0}{\omega_0}\right)^3 \frac{\int_l \sigma_{3,\text{Im}} \left(2|\mathbf{E}_{0,\parallel}|^4 + |\mathbf{E}_{0,\parallel} \cdot \mathbf{E}_{0,\parallel}|^2\right) dl}{\left[\iint_S \varepsilon_r |\mathbf{E}_0|^2 dS + \iint_S \eta_0^2 |\mathbf{H}_0|^2 dS + \frac{1}{\varepsilon_0} \int_l \frac{\partial \sigma_{1,\text{Im}}}{\partial \omega} |\mathbf{E}_{0,\parallel}|^2 dl\right]^2 \sigma_{3,\text{Im}}^{\max}}$$

2D graphene-tube ring resonator (2)

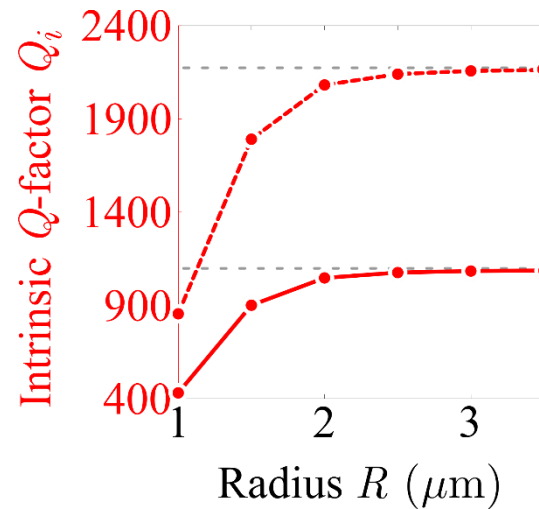


- $\kappa_s \propto 1/R$
- $\kappa_s^{\text{non}} \approx 4\kappa_s^{\text{disp}}$

2D graphene-tube ring resonator (2)

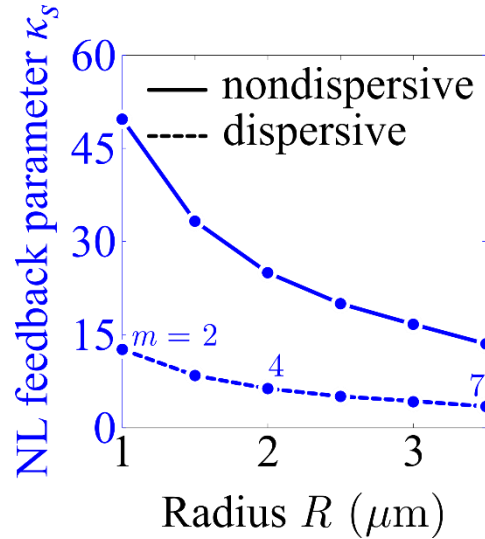


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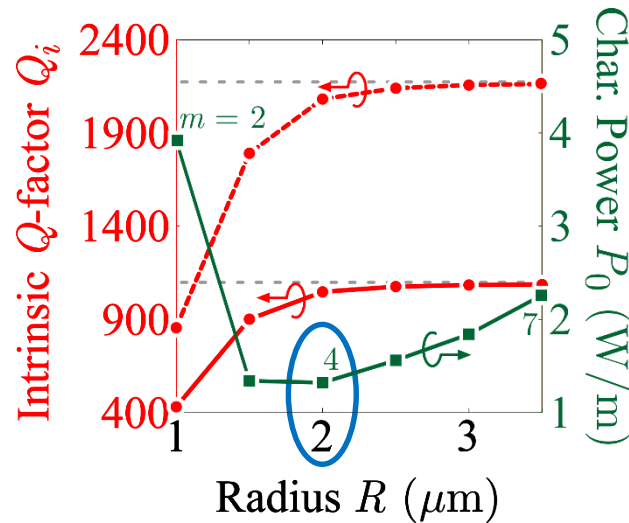


- $Q_i \propto R$
- $Q_i^{\text{disp}} \approx 2Q_i^{\text{non}}$

2D graphene-tube ring resonator (2)



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

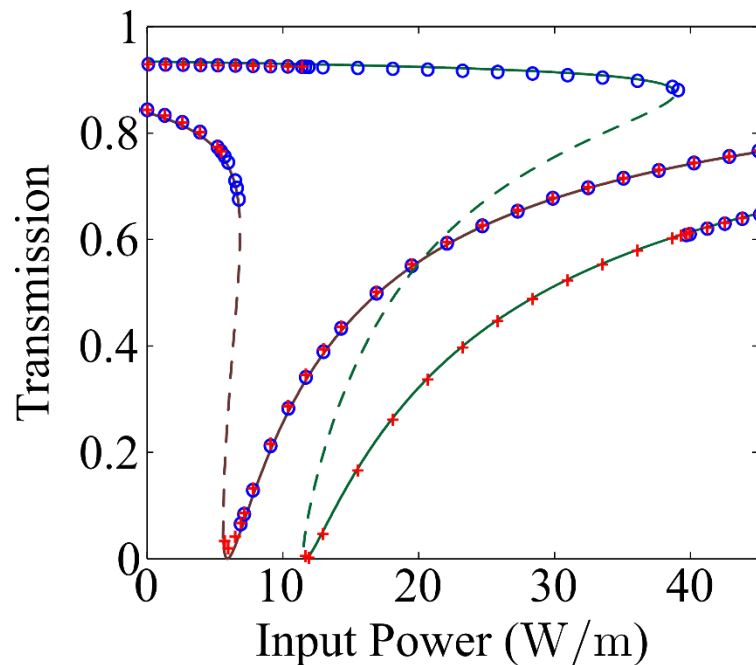


- $Q_i \propto R$
- $Q_i^{\text{disp}} \approx 2Q_i^{\text{non}}$

- $R = 2 \mu\text{m}$
- $g = 1.74 \mu\text{m}$
- $P_0 = 1.32 \text{ W/m}$
- $P_{0,\text{eq}}^{3\text{D}} \approx 20 \mu\text{W}$
- $f_0 = 10.021 \text{ THz}$

- 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 [$r_Q = 1$]

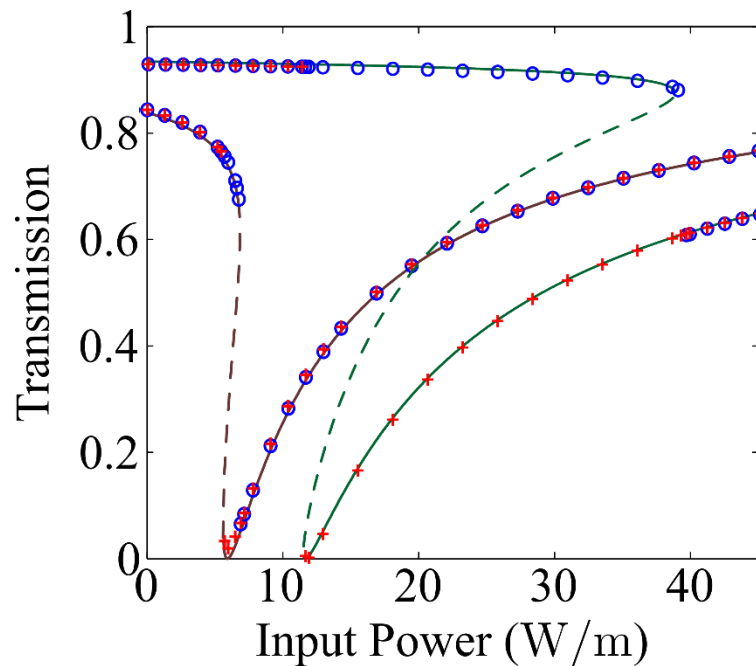
2D graphene-tube ring resonator (3)

CW case

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

- 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

2D graphene-tube ring resonator (3)

CW case

○ CMT

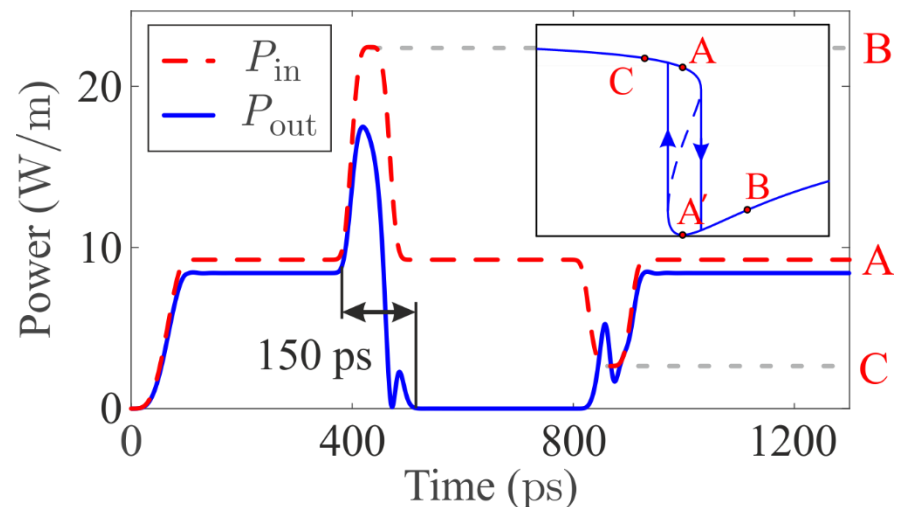
$$Q_i^{\text{disp}} \approx 2Q_i^{\text{non}} \Rightarrow \delta^{\text{disp}} = 2\delta^{\text{non}}$$

✓ Always include dispersion

○ NL-VFEM

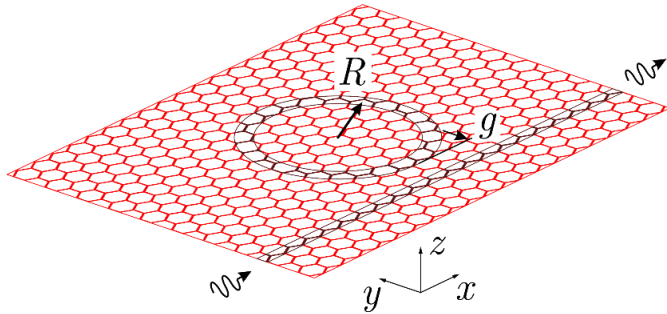
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✓ Excellent agreement between FEM and CMT

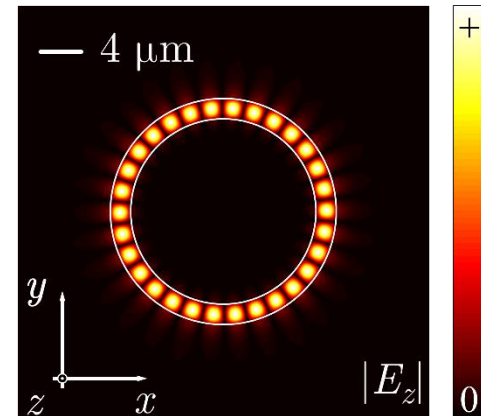
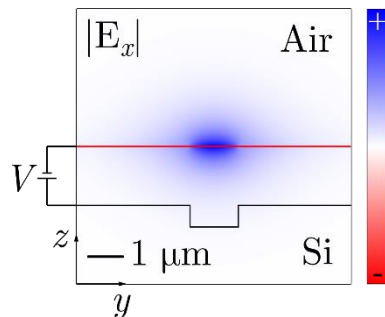
Dynamic memory implementation

3D graphene nanoribbon ring resonator

- graphene with conductivity σ'_1
- graphene with conductivity σ_1



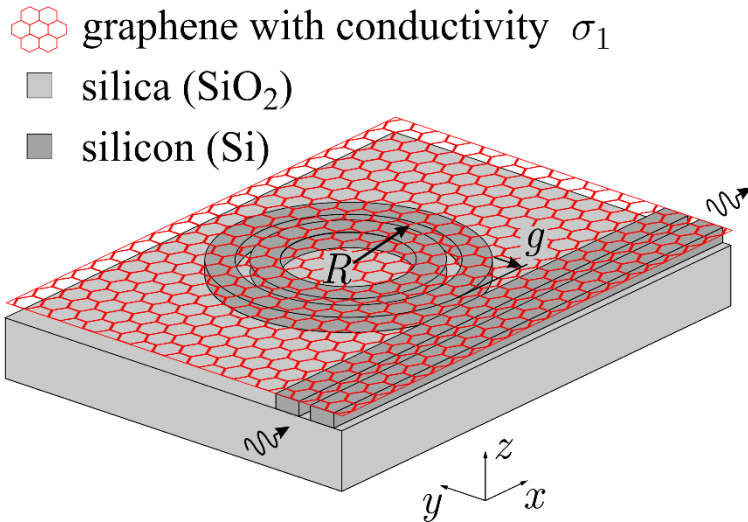
- Infinite graphene sheet
- Resonator/waveguide:
 - “Written” with $|\sigma_{1,\text{Im}}| < |\sigma'_{1,\text{Im}}|$
 - Uneven ground and/or voltage
- ✓ Surface Plasmon Polariton supported at THz



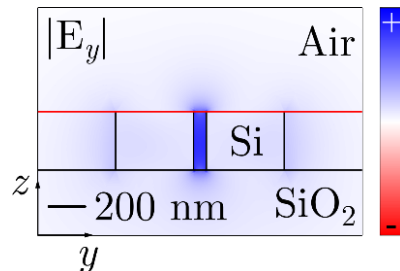
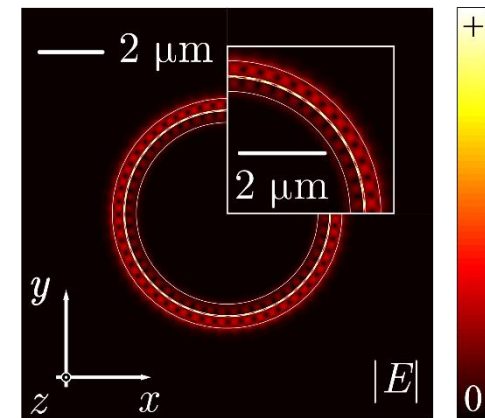
- $R = 10.1 \mu\text{m}$
- $g = 2.20 \mu\text{m}$
- $P_0 = 24 \mu\text{W}$
- $f_0 = 10 \text{ THz}$

- $Q_i^{\text{non}} = 1048$
- $Q_i^{\text{disp}} = 2080$
- $\kappa_s^{\text{non}} = 6.52$
- $\kappa_s^{\text{disp}} = 1.65$

3D silicon-slot ring resonator incorporating graphene



- Si-slot platform
 - High confinement
 - Major E -field component \parallel to graphene
- Infinite graphene sheet on top



- $R = 3.25 \mu\text{m}$

- $g = 150 \text{ nm}$

- $P_0^{\text{Kerr}} = 6.2 \text{ mW}$

- $\lambda_0 = 1.553 \mu\text{m}$

- $P_{0,s}^{\text{Kerr}} = 6.1 \text{ mW}$

- $P_{0,b}^{\text{Kerr}} = 1.6 \text{ W}$

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 (μ_c tuning)

Thank you!

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And... there is more

Back up material !

Energy density in media with complex conductivity (full proof)

- Poynting vector in time domain: $-\nabla \cdot \mathcal{S} = -\nabla \cdot (\mathcal{E} \times \mathcal{H}) = \mathcal{J} \cdot \mathcal{E} + \frac{\partial \mathcal{D}}{\partial t} \cdot \mathcal{E} + \frac{\partial \mathcal{B}}{\partial t} \cdot \mathcal{H}$
- Second and third terms correspond to stored energy. **What about the first term?**
- Slow varying envelope: $\mathcal{F} = \text{Re}\{\mathbf{F}_0 \exp(+j\omega_0 t)\} = (\mathbf{F}_0 + \mathbf{F}_0^*)/2$, $\mathcal{F} = \{\mathcal{E}, \mathcal{J}\}$
- Time averaging w.r.t. $T_0 = 2\pi/\omega_0$: $\langle \mathcal{J} \cdot \mathcal{E} \rangle = (\mathbf{E}_0^* \cdot \mathbf{J}_0 + \mathbf{E}_0 \cdot \mathbf{J}_0^*)/4$
- Fourier transform on the envelope: $\mathbf{J}_0(t) = \frac{1}{2\pi} \int \tilde{\mathbf{J}}_0(\omega) e^{j\omega t} d\omega$
- Apply Ohm's law to the "high" frequency: $\tilde{\mathbf{J}}_0(\omega) = \bar{\sigma}^{(1)}(\omega + \omega_0) \tilde{\mathbf{E}}_0(\omega)$
- Expand $\bar{\sigma}^{(1)}$ in Taylor series:
$$\begin{cases} \bar{\sigma}_{\text{Re}}^{(1)}(\omega + \omega_0) \approx \bar{\sigma}_{\text{Re}}^{(1)}(\omega_0) \\ \bar{\sigma}_{\text{Im}}^{(1)}(\omega + \omega_0) \approx \bar{\sigma}_{\text{Im}}^{(1)}(\omega_0) + \omega \left. \frac{\partial \bar{\sigma}_{\text{Im}}^{(1)}}{\partial \omega} \right|_{\omega=\omega_0} \end{cases}$$
- Inverse Fourier transform on the result

- Finally:

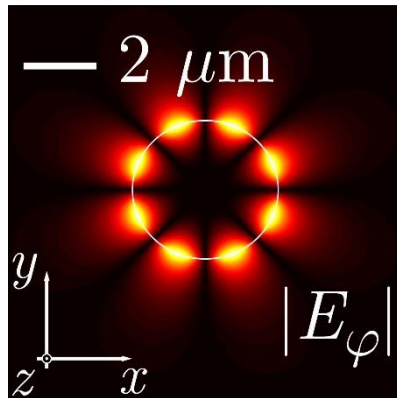
$$\langle \mathcal{J} \cdot \mathcal{E} \rangle = \underbrace{\frac{1}{2} \bar{\sigma}_{\text{Re}}^{(1)} \mathbf{E}_0 \cdot \mathbf{E}_0^*}_{\text{Power loss density}} + \underbrace{\frac{\partial}{\partial t} \left\{ \frac{1}{4} \frac{\partial \bar{\sigma}_{\text{Im}}^{(1)}}{\partial \omega} \mathbf{E}_0 \cdot \mathbf{E}_0^* \right\}}_{\text{Stored energy density}}$$

[Landau and Lifshitz,
Electrodynamics of continuous
media, Elsevier, 1984]

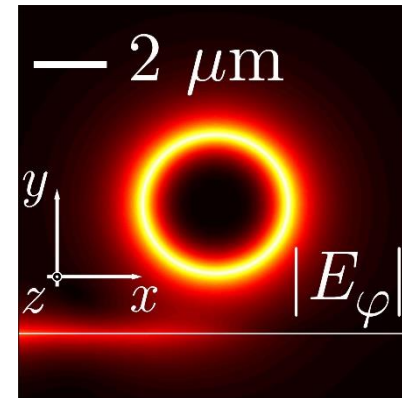
[Christopoulos, PRE 94,
062219]

Correct calculation of κ **FEM eigenvalue solution**

- Two degenerated counter-propagating modes
- Standing-wave pattern
- $\mathbf{E}(\rho, \varphi) = \mathbf{e}^+(\rho, \varphi) + \mathbf{e}^-(\rho, \varphi)$
- $\mathbf{H}(\rho, \varphi) = \mathbf{h}^+(\rho, \varphi) + \mathbf{h}^-(\rho, \varphi)$

**FEM propagation solution**

- One single mode propagating (counter)clockwise
- Traveling-wave pattern
- $\mathbf{E}(\rho, \varphi) = \mathbf{e}^+(\rho, \varphi)$
- $\mathbf{H}(\rho, \varphi) = \mathbf{h}^+(\rho, \varphi)$

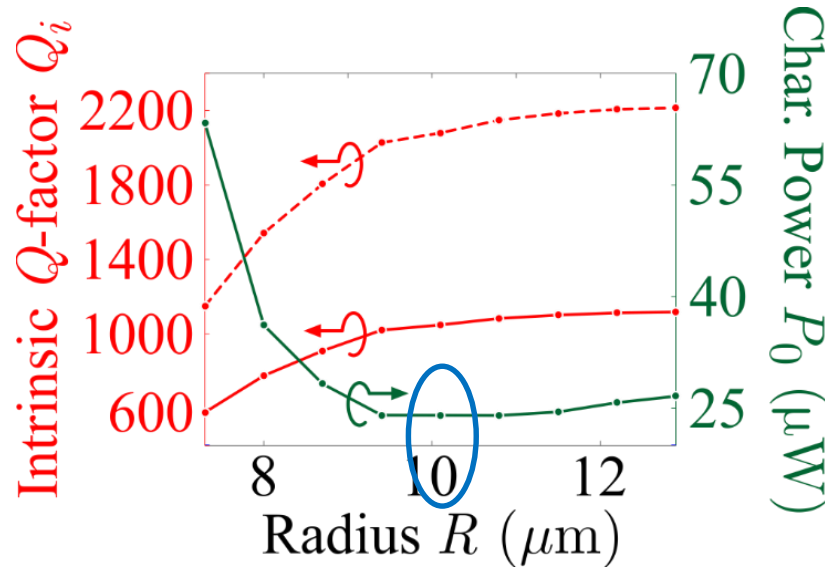
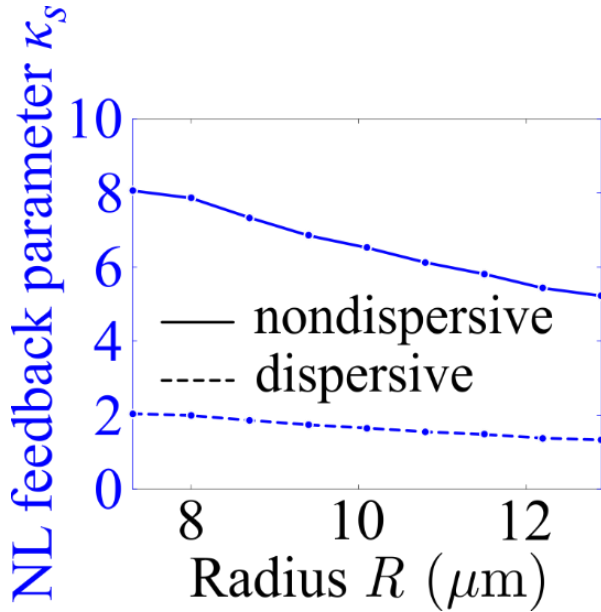


$$\mathbf{e}^{\pm}(\rho, \varphi) = [e_{\rho}(\rho)\hat{\mathbf{p}} \pm je_{\rho}(\rho)\hat{\boldsymbol{\phi}}]\exp\{\mp jm\varphi\}$$

$$\mathbf{h}^{\pm}(\rho, \varphi) = \mp h_z(\rho)\hat{\mathbf{z}}\exp\{\mp jm\varphi\}$$

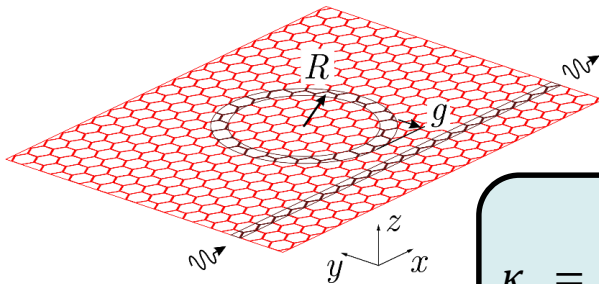
$$\frac{\kappa_s^{\text{prop}}}{\kappa_s^{\text{eig}}} = \frac{2}{3}$$

3D graphene nanoribbon ring resonator



- $R = 10.1 \mu\text{m}$
- $g = 2.20 \mu\text{m}$
- $P_0 = 24 \mu\text{W}$
- $f_0 = 10 \text{ THz}$

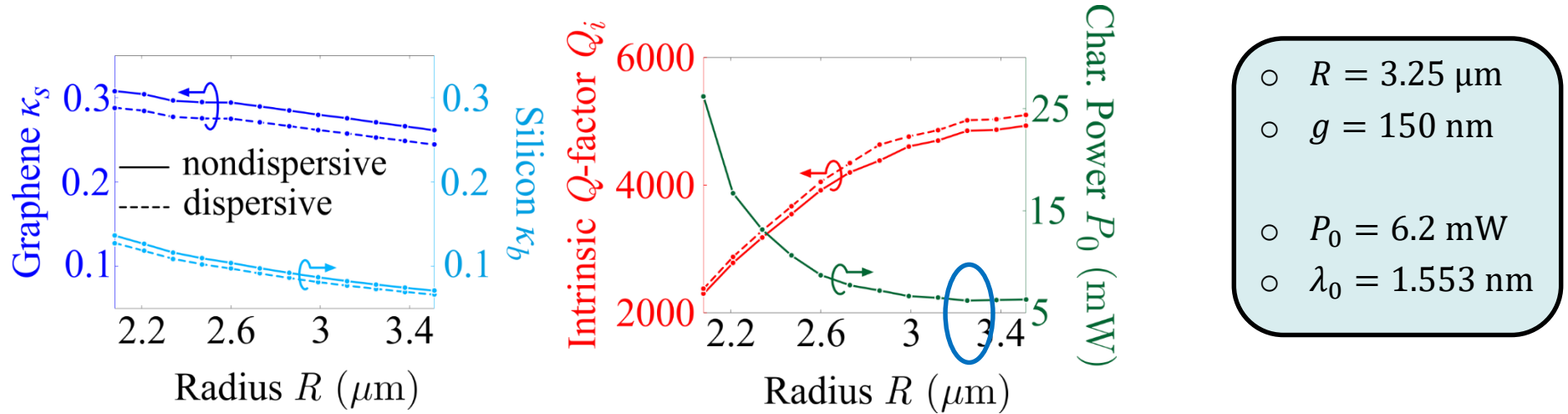
- graphene with conductivity σ_1'
- graphene with conductivity σ_1



Nonlinear feedback parameter

$$\kappa_s = \left(\frac{c_0}{\omega_0} \right)^4 \frac{\iint_S \sigma_3 \left(2|\mathbf{E}_{0,\parallel}|^4 + |\mathbf{E}_{0,\parallel} \cdot \mathbf{E}_{0,\parallel}|^2 \right) dS}{\left[\iiint_V \epsilon_r |\mathbf{E}_0|^2 dV + \iiint_V \eta_0^2 |\mathbf{H}_0|^2 dV + \frac{1}{\epsilon_0} \iint_S \frac{\partial \sigma_{1,\text{Im}}}{\partial \omega} |\mathbf{E}_{0,\parallel}|^2 dS \right]^2 \sigma_3^{\max}}$$

3D silicon-slot ring resonator incorporating graphene



Nonlinear feedback parameters

$$\kappa_s = \left(\frac{c_0}{\omega_0} \right)^4 \frac{\iint_S \sigma_3 \left(2|\mathbf{E}_{0,\parallel}|^4 + |\mathbf{E}_{0,\parallel} \cdot \mathbf{E}_{0,\parallel}|^2 \right) dS}{\left[\iiint_V \varepsilon_r |\mathbf{E}_0|^2 dV + \iiint_V \eta_0^2 |\mathbf{H}_0|^2 dV + \frac{1}{\varepsilon_0} \iint_S \frac{\partial \sigma_{1,\text{Im}}}{\partial \omega} |\mathbf{E}_{0,\parallel}|^2 dS \right]^2 \sigma_3^{\max}}$$

$$\kappa_b = \left(\frac{c_0}{\omega_0} \right)^3 \frac{\frac{1}{3} \iiint_V n^2 n_2 (2|\mathbf{E}_0|^4 + |\mathbf{E}_0 \cdot \mathbf{E}_0|^2) dV}{\left[\iiint_V \varepsilon_r |\mathbf{E}_0|^2 dV + \iiint_V \eta_0^2 |\mathbf{H}_0|^2 dV + \frac{1}{\varepsilon_0} \iint_S \frac{\partial \sigma_{1,\text{Im}}}{\partial \omega} |\mathbf{E}_{0,\parallel}|^2 dS \right]^2 n_2^{\max}}$$

