A strict framework for analyzing linear and nonlinear propagation in photonic and terahertz graphene waveguides

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Presentation Outline

- **Introduction**
  - Graphene and waveguides
  - Motivation & Objective

- **Graphene Properties**
  - Sheet/2D vs. equivalent Bulk/3D medium representation
  - Linear and nonlinear surface conductivity formulas
  - Electric biasing – Voltage controlled conductivity

- **Electromagnetic Modeling**
  - Linear analysis – FEM eigenmode solver
  - Nonlinear propagation – Perturbation method

- **Linear Regime Applications**
  - Absorption and phase modulation via voltage control

- **Nonlinear Propagation**
  - Optical: SOI-based & metal (plasmonic) waveguides
  - THz: Graphene Nano-Ribbons (GNR)

- **Conclusions & Outlook**
Graphene-comprising Waveguides

Introduction
Introduction

Graphene
- Carbon allotrope in 2D “honeycomb” lattice
- Sheet (monolayer), thickness ~0.34 nm
- High electric conductivity
- Spectrum: THz – optical (300 um – 0.3 um)
- Thermal conductivity, mechanical strength

Focus: Electronic Properties
- Zero-bandgap semiconductor
- Tunable conductivity → Doping or electric biasing
  - Chemical potential \( \mu_c \) (Fermi level)
  - Interband absorption: Vanishes for \( hf < 2\mu_c \)

Waveguides with In-Plane Graphene
- Optical: Perturbation
- THz: Plasmonic properties
- Normal-incidence: Absorbs 2.3% of red light
Motivation & Objective

**Graphene** – A “hot” material for waveguide applications
✓ Voltage-controlled conductivity
✓ Reports of high, even **giant** (?), Kerr-type nonlinearity

**Compared to photonics...**
✗ Theoretical framework relatively underdeveloped
✗ Various misconceptions & simplifications in modeling techniques
✗ Few device-oriented experiments
✗ Uncertainty about magnitude of nonlinearity

**Main Objective** – A strict framework for Maxwellian modeling
- Treat graphene as a **true sheet/2D** material
- Avoid the “**equivalent**” bulk/3D material representation
- Complete **tensorial representation** of surface conductivity
- Rigorous calculation of **NL parameter** $\gamma_{NL}$ (units: [W$^{-1}$m$^{-1}$])
- Waveguide **engineering** to enhance interaction with graphene
Electromagnetic Properties

Graphene
Sheet/2D vs. Bulk/3D

**Sheet/2D medium** → Zero thickness
- Linear & NL surface conductivity tensors:

\[
\bar{\sigma}_{s,\text{ref}}^{(1)} = \begin{bmatrix} \sigma_{s,xx} & 0 & \sigma_{s,xz} \\ 0 & 0 & 0 \\ \sigma_{s,zx} & 0 & \sigma_{s,zz} \end{bmatrix}, \quad \bar{\sigma}_{c} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}
\]

\[
\sigma_{s,jklm,\text{ref}}^{(3)} = \frac{1}{3} \left( \delta_{jk} \delta_{lm} + \delta_{jm} \delta_{kl} + \delta_{jl} \delta_{mk} \right), \quad j,k,l,m = \{x,z\}
\]

**Bulk/3D medium** → Thickness ~0.34 nm
- Equivalent susceptibility:

\[
\chi_{\text{eq}}^{(m)} = \frac{i \bar{\sigma}_{s}^{(m)}}{\omega \varepsilon_0 d_{\text{gr}}}
\]

- Tensor properties (anisotropy) inherited from \( \bar{\sigma}_{s}^{(m)} \)
- Equivalent linear and nonlinear index

\[
\varepsilon_{r,\text{eq}} = n_{0,\text{eq}}^2 = 1 + \frac{i \sigma_c}{\omega \varepsilon_0 d_{\text{gr}}}, \quad n_{2,\text{eq}} = \frac{3 \chi_{\text{eq}}^{(3)}}{4 \varepsilon_{r,\text{eq}} ^2} Z_0
\]
Linear surface conductivity
Simplest form of $\bar{\sigma}_s^{(1)} \rightarrow \sigma_c$ (complex; [Siemens])

- **Intraband** term: Dominant at THz
- **Interband** term: Dominant at optical
  - $\text{Re}\{\sigma_{c,\text{inter}}\}$ vanishes for $\mu_c > 0.5 \ h\!\!f$
  - $\text{Im}\{\sigma_{c,\text{inter}}\}$ peaks near $\mu_c = 0.5 \ h\!\!f$

\[
\sigma_{c,\text{intra}} = i \frac{e^2 \mu_c}{\pi \hbar^2 (\omega + i \tau^{-1}_a)} \times \mathcal{T} \left( \frac{\mu_c}{2 k_B T} \right)
\]

\[
\sigma_{c,\text{inter}} = i \frac{e^2}{4 \pi \hbar} \ln \left[ \frac{2 \mu_c - \hbar (\omega + i \tau^{-1}_b)}{2 \mu_c + \hbar (\omega + i \tau^{-1}_b)} \right]
\]

Nonlinear surface conductivity
Simplest form of $\bar{\sigma}_s^{(3)} \rightarrow \sigma_3$ (imaginary; [Sm²/V²])

- Optical: [Hendry et al., PRL, 2010]
Two Photon Absorption (TPA): $\text{Re}\{\sigma_3\} \rightarrow \text{No data!}$

\[
\sigma_{3,\text{opt}} = -i \frac{9 e^4 v_F^2}{32 \omega^4 \hbar^3}
\]

\[
\sigma_{3,\text{THz}} = -i \frac{3 e^4 v_F^2}{32 \omega^3 \hbar^2 \mu_c}
\]
Electric Biasing / Voltage Controlled Conductivity

Carrier surface density \( (n_s) \ vs. \ \mu_c \)
- Electrons and holes on graphene surface
- Example: \( n_s \sim 10^{12} \ \text{cm}^{-2} \) when \( \mu_c \sim 0.1 \ \text{eV} \)

\[
n_s(\mu_c) = \frac{\mu_c^2}{\pi \hbar^2 v_F^2}
\]

What happens when electric-biasing (voltage) is applied?
How does \( \mu_c \) (and thus \( \sigma_c \)) depend on \( V_{bias} \)?

Parallel-plate Capacitor Model: \( \Delta V_{bias} \rightarrow \Delta \sigma_c \)
- Plates: Graphene sheet and a conducting material (or two sheets)
- Filling dielectric: thickness \( d_y \) and rel. permittivity \( \varepsilon_{r,d} \)
  - Capacitance (parallel plate): \( C = \varepsilon_0 \varepsilon_{r,d} (L_z w_x)/d_y \)
  - Charge (on graphene sheets): \( Q = n_s (L_z w_x) |e| \)
  - Using \( C = Q/V_{bias} \) and \( n_s(\mu_c) \) expression ⇒

\[
\mu_c = \hbar v_F \sqrt{\pi \eta} \left| V_{bias} \right|, \quad \eta = \frac{\varepsilon_0 \varepsilon_{r,d}}{d_y |e|}
\]
Eigenmode Solver & Nonlinear Parameter Calculation

Electromagnetic Modeling for Numerical Simulations
Linear Analysis – FEM Eigenmode Solver

Solver: Waveguide eigenmodes (profile, $n_{\text{eff}}$ and $L_{\text{prop}}$) at given $\lambda$

Finite Element Modeling

- For 2D case, waveguide cross-section:
  - Bulk/3D materials: $\chi^{(1)}$ or $n_0$ → Per element face
  - Sheet/2D materials: $\sigma_s^{(1)}$ or $\sigma_c$ → Per mesh edge

Boundary Conditions – Between elements

$$n \times (\mathbf{E}_2 - \mathbf{E}_1) = 0$$

$$n \times (\mathbf{H}_2 - \mathbf{H}_1) = \mathbf{J}_s = \bar{\sigma}_s^{(1)} \mathbf{E} \rightarrow \sigma_c \mathbf{E}_{\text{tan}} = \sigma_c \left[ n \times (\mathbf{E} \times n) \right]$$

Galerkin procedure – Applied to the 3D vector wave-equation

$$\iiint_V \left\{ (\nabla \times \mathbf{E}_a) \cdot [\mu_r^{-1} (\nabla \times \mathbf{E})] - k_0^2 \mathbf{E}_a \cdot [\mathbf{\bar{e}}_r \mathbf{\bar{E}}] \right\} dV = i\omega\mu_0 \iint_S \mathbf{E}_a \cdot [\bar{\sigma}_s^{(1)} \mathbf{E}] dS$$

- LHS term: Bulk media
- RHS term: Sheet media; simplification

Mode Envelope (2D) → Sparse-array system → Numerical solution
Nonlinear Propagation – Perturbation Method

Nonlinear Perturbation:
\[
\nabla \times \tilde{H} = \left( -i\omega \varepsilon_0 \varepsilon_{r} + \sigma_{s}^{(1)}(r) \right) \tilde{E} - i\omega \left( \tilde{P}_{NL} + i\omega^{-1}\tilde{J}_{NL} \right)
\]

Narrowband 3rd order NL effects
Kerr/TPA, FWM

\[
P_{j,NL} = \frac{3\varepsilon_0}{4} \sum_{klm} \chi_{jklm}^{(3)} E_k E_l^* E_m
\]

\[
J_{s,j,NL} = \frac{3}{4} \sum_{klm} \sigma_{s,jklm}^{(3)} E_k E_l^* E_m
\]

Slowly Varying Envelope:
\[
\tilde{E}(r, \omega) = \tilde{A}(z, \omega - \omega_0)e(x,y,\omega_0)\exp(+i\beta_0z) / \sqrt{N}
\]

Propagation Equation:
\[
\frac{\partial A}{\partial z} = \frac{i\omega_0 e^{i(\omega_0 t - \beta_0 z)}}{2\sqrt{4N}} \int \int e^* \left( \tilde{P}_{NL} + i \frac{\omega}{\omega_0} \tilde{J}_{NL} \right) dS + LA
\]

 Single-mode waveguide:
\[
\frac{\partial A}{\partial z} = -\frac{1}{2L_{prop}} A + i\gamma_{NL} |A|^2 A + L_{disp} A
\]

NL parameter:
\[
\gamma_{NL} = \gamma_{b} + \gamma_{s} \quad \text{(bulk + sheet nonlinearity)} \rightarrow \text{Per mode!}
\]

\[
\gamma_{b} = \frac{\omega_0 \varepsilon_0}{(2N)^2} \int \int \chi_3 \left( \frac{1}{2} |e|^4 + \frac{1}{4} |e\cdot e|^2 \right) dS
\]

\[
\gamma_{s} = i \frac{1}{(2N)^2} \int \sigma_3 \left( \frac{1}{2} |e_t|^4 + \frac{1}{4} |e_t\cdot e_t|^2 \right) dl
\]
Linear Regime Applications of Graphene Waveguides

Absorption & Phase Modulation
Voltage-control of optical waveguide absorption & phase

**Capacitor model:** $\Delta V_{\text{bias}} \rightarrow \Delta \mu_c \rightarrow \Delta \text{Re}\{\sigma_c\} \& \Delta \text{Im}\{\sigma_c\}$ for graphene sheet(s)

**Waveguide:** Graphene-Alumina-Graphene (GAG) stack on SOI waveguide
- Si-wire design by [Liu et al., Nano Lett., 2012], at 1550 nm (0.8 eV)
- This work → Optimized design using a Si-rib design

**Modulation** → From **interband** surface conductivity term
- Absorption Modulation: High Re$\{\sigma_c\}$ for $\mu_c(V_{\text{bias}}) < 0.4$ eV
- Phase Modulation: Local peaking of Im$\{\sigma_c\}$ at $\mu_c(V_{\text{bias}}) \sim 0.4$ eV

![Diagram](image)

Modulation $\sim 0.4$ dB/um

$\pi$-length $\sim 45$ um
Propagation in Nonlinear Graphene Waveguides

Nonlinear Parameter Calculation
Third-order NL effects in waveguides

Applications: Wavelength conversion, switching, soliton propagation ...

Overruling quantity: Nonlinear phase $\Phi_{NL} = \gamma_{NL} \times L_{\text{eff}} \times P$
- $\gamma_{NL}$: NL parameter $\rightarrow$ Waveguide: Structure & material nonlinearity
- $L_{\text{eff}}$: Effective waveguide length $\rightarrow$ Limited by waveguide losses ($L_{\text{prop}}$)
- $P$: Threshold power for NL effect manifestation $\rightarrow$ Typically for $\Phi_{NL} \sim \pi$

Figure-of-Merit (FoM) in units [1/Watt]:

FoM = $\gamma_{NL} L_{\text{prop}}$

Optical Waveguides
- Silicon wire
- Silicon slot
- Metal stripe
- Metal slot
+ Nanoribbon (@THz)

Maximize interaction with graphene sheet

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<tr>
<th>Silicon wire</th>
<th>Metal stripe</th>
<th>Nanoribbon</th>
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Graphene
- Silicon (3.48)
- Oxide (1.45)
- PMMA (1.49)
- Silver (0.145+11.4i)
Silicon wire @ 1550 nm

**Waveguide** – Materials & fixed parameters

- Silicon \((n_0=3.48, n_2=2.5\times10^{-18} \text{ m}^2/\text{W})\) wire, 340 nm thickness
- PMMA \((n_0=1.49)\) cladding, 20 nm gap between graphene and Si
- Graphene \((\mu_c=0.5 \text{ eV}, \sigma_3=-i7.2\times10^{-23} [\text{S/(m/V)}^2])\), inf. width

- Graphene losses and nonlinearity have the same trend
- Polarization dependence \(\Rightarrow \gamma_{gr}\) is larger for TM modes (due to longitudinal \(E_z\))
  - \(\gamma_{gr} << \gamma_{Si}\): Mode profile interacts weakly with graphene
  - Increased losses, compared to Si-wire without graphene (1 dB/cm)
  - **Overall**: FoM is lower than regular Si-wires...
Waveguide – Materials & fixed parameters

- Two 400 nm-wide Air-clad Si-wires, Graphene (inf. width) on top
- Supports a strongly-confined TE-polarized mode inside the slot

\[ \gamma_{gr} \text{ (and losses) increase as dimensions decrease but...} \]

**Overall:** FoM still remains low... Other waveguide designs?
Plasmonic optical waveguides + Graphene

**Stripe**
- Patterned Ag stripe, 20 nm thick
- TM y-antisymmetric mode
- Oxide substrate / Air cladding

- $\gamma_{\text{sheet}}$ improves for smaller widths
- Metal loss dominates over graphene losses
- **Overall**: $\text{FoM} \sim 0.003/W$

**Slot**
- Two (semi-inf.) stripes, 20 nm thick
- Oxide substrate / Air cladding
- TE x-polarized mode

- $\gamma_{\text{sheet}}$ is greatly increased
- Losses from metal and graphene are comparable
- **Overall**: $\text{FoM} > 0.1/W$
Graphene Nanoribbon (GNR) @ Terahertz

**GNR waveguide**
- Finite graphene stripe: width 1 um, $f=10$ THz ($\lambda=30$ um, $E=0.04$ eV)
  - Linear regime: **Plasmonic waveguiding** → “Edge” modes
  - Graphene: Like a zero-thickness metal stripe → **Extreme confinement**
- $\sigma_3$ in THz is much higher than optical; increases for lower $\mu_c$
- $\gamma_{NL}$ is **exceedingly** high
- Tolerable losses: $L_{prop} \sim 10\lambda$

**Overall:** FoM $\sim 10^4$/W (!)
- Ample tuning via $\mu_c$ (e.g. electric gating)
- Promising potential, but experiments are required!
Conclusions & Outlook

Graphene-comprising Waveguides
Conclusions & Outlook

Graphene-comprising Waveguides
- Sheet/2D material → Rigorous framework for numerical modeling
- Waveguide design → Maximize graphene/field interaction
- Voltage controlled conductivity → Zero-bandgap semiconductor

Linear Optical Regime / Experimentally confirmed
- Graphene → Perturbation to index-contrast (or plasmonic) waveguiding
  ✓ Phase modulation → $L_n \sim 45$ μm is theoretically possible
  ✓ Absorption modulation → 0.16 dB/μm with 5 V (measured); up to 0.4 dB/μm

Nonlinear Regime / Uncharted territory
- Ambiguity for $\sigma_3$ (in-plane nonlinearity) magnitude → More experiments!
  ✓ Best NL performance @ 1550 nm → Plasmonic “slot” waveguide
  ✓ Nanoribbon waveguides @ THz → Potential for gigantic NL performance

Future work
- Match theoretic modeling with experimental measurements
- Deeper study of carrier dynamics in graphene
- More complex graphene configurations: multiple sheets & orientations
Alexandros Pitilakis acknowledges the support of the:

“IKY Fellowships of Excellence for Postgraduate Studies in Greece – Siemens Programme”.
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http://photonics.ee.auth.gr
Maxwellian Derivation & Sheet/2D Representation

Maxwell’s curl equations $\rightarrow$ Linear and nonlinear contributions

\[
\begin{align*}
\nabla \times \tilde{E} &= +i\omega\mu_0 \mu_r \tilde{H} \\
\nabla \times \tilde{H} &= -i\omega(\varepsilon_0 \tilde{E} + \tilde{P}) + \tilde{J}
\end{align*}
\]

\[
\tilde{J} = \tilde{J}_{\text{lin}} + \tilde{J}_{\text{NL}},
\tilde{P} = \tilde{P}_{\text{lin}} + \tilde{P}_{\text{NL}},
\]

\[
\begin{align*}
\tilde{J}_{\text{NL}} &\ll \tilde{J}_{\text{lin}} = \sigma^{(1)} \tilde{E} \\
\tilde{P}_{\text{NL}} &\ll \tilde{P}_{\text{lin}} = \varepsilon_0 \chi^{(1)} \tilde{E}
\end{align*}
\]

Bulk current density, expanded similarly to polarization

\[
\tilde{J}_b = \sigma^{(1)} |\tilde{E}| + \sigma^{(2)} |\tilde{E}\tilde{E}| + \sigma^{(3)} |\tilde{E}\tilde{E}\tilde{E}| + \ldots
\]

Surface current density on graphene (sheet/2D):

\[
\tilde{J}_s = \sigma^{(1)}_s |\tilde{E}| + \sigma^{(2)}_s |\tilde{E}\tilde{E}| + \sigma^{(3)}_s |\tilde{E}\tilde{E}\tilde{E}| + \ldots
\]

Total current density (units: [A/m²])

- Using the “surface” Dirac function $\delta_s$

\[
\tilde{J} = \tilde{J}_b + \tilde{J}_s \delta_s(\mathbf{r})
\]

Surface conductivity $\sigma^{(1)}_s$ (units: [Siemens])

\[
\tilde{J}_s = \sigma^{(1)}_s \tilde{E} \rightarrow \sigma_c \tilde{E}_\parallel = \sigma_c \left[ \mathbf{n} \times (\tilde{E} \times \mathbf{n}) \right]
\]

Set of surface-conductivity tensors, $\sigma^{(n)}_s$: rank $(n+1)$, units [S(m/V)^{n-1}]
Equivalent Bulk/3D representation – Nonlinear index $n_{2,eq}$

**Derived from theoretical models**
- Solid-curves: Positive $\text{Re}\{n_{2,eq}\}$.
- Dashed-curves: Negative $\text{Re}\{n_{2,eq}\}$.
- Sign transitions near $|\text{Re}\{n_{0,eq}\}| = |\text{Im}\{n_{0,eq}\}|$

**Value range of $\sim 10^{-15}$ m²/W**
For comparison,
- Si $\sim 10^{-18}$ m²/W,
- Chalcogenides $\sim 10^{-17}$ m²/W,
- polymers (DDMEBT) $\sim 10^{-17}$ m²/W.

**Attention…**
The high $n_{2,eq}$ value does not directly translate into a high $\gamma_{NL}$ value!
Waveguide engineering is required to maximize interaction with graphene sheet.

$$n_{2,eq} = \frac{3}{4} \times \frac{i\sigma_3}{1 + i\sigma_c} \frac{(\omega\varepsilon_0 d_{gr})}{Z_0}$$
Silica microfiber on MgF$_2$ (1.37) substrate – $L_{\text{prop}}$ & $\gamma_{\text{NL}}$ calculation

**Configurations:**
(a)+(d) : $x$-mode interacts more strongly with graphene
(b)+(e) : $x$- and $y$-modes are approximately degenerate w.r.t graphene
(c)+(f) : Fictitious “microtube” configuration $\rightarrow$ THz?

[Wu et al., PTL, 2014]: FWM experiment hints at higher $\sigma_3$ (via $\gamma_{\text{sheet}}$)
Silicon wire @ 1550 nm – Mode Profiles

**Waveguide:** SOI-wire / PMMA cladding / graphene / Air @ 1550 nm
- Si-wire is 400 nm-wide and 340 nm-thick / graphene @ $\mu_c \sim 0.5$ eV
- Supports TE and TM modes

- $E$-field intensity tangential to graphene: $I_{\text{tan}} = |E_{\text{tan}}|^2 = |E_x|^2 + |E_z|^2$
Plasmonic optical waveguides

Rounded corners
✓ Avoid plasmonic field “singularity”
✓ Closer to real fabricated structures
✓ Faster & reliable mode convergence

Material choices
✓ Material-symmetry → Mode symmetry
✓ Graphene → At higher-index material side

Metal stripe →

Metal slot →