Epsilon-Near-Zero and Plasmonic Dirac Point by using 2D materials

Marios Mattheakis

Co-authors:
Prof. Efthimios Kaxiras
Prof. Costas Valagiannopoulous

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Graphene as Plasmonic Platform

Graphene is an efficient plasmonic platform:

- More confined plasmons (even more localized EM energy).
- Ultra sub-wavelength plasmons.
- Tunability of plasmon frequency via doping.
- High & low energy plasmons are supported.
- Longer propagation length.

Plasmonic Thickness $\xi$

\[ \delta = \xi / 2 \quad \text{(decay length)} \]

\[ \xi = \frac{1}{2} \left( k_{sp}^2 - k_0^2 \varepsilon_d \right)^{-1/2} \]
Periodic structure of 2D metals

2D metallic layers (e.g. graphene) are extended in (y,z) plane and arranged periodically along x.

- The interlayer distance is called structural period d.
- Anisotropic uniaxial dielectric as host media $\varepsilon_z = \varepsilon_y \neq \varepsilon_x$.
- The 2D layers are characterized by surface conductivity $\sigma_s$.
- Plasmon and Bloch wavenumbers $k_z$ and $k_x$.

- Study the normal Transverse Magnetic (TM) modes.
- Looking for the dispersion relation: $k_z(k_x)$.
- Due to periodicity the allowable $k_z(k_x)$ should be arranged in bands.
Maxwell Equations (MEs)

Assumptions:
- Monochromatic harmonic in time EM waves.
- Transverse Magnetic (TM) Polarization.

Maxwell Equations read:

**Transversal Field**

\[-i \frac{\partial}{\partial z} \Psi = \mathcal{M} \cdot \Psi \Leftrightarrow \]

\[-i \frac{\partial}{\partial z} \begin{pmatrix} E_x \\ H_y \end{pmatrix} = k_0 \eta_0 \begin{pmatrix} 0 & 1 + \frac{1}{k_0^2} \frac{\partial}{\partial x} \frac{1}{\varepsilon_z} \frac{\partial}{\partial x} \\ \frac{\varepsilon_z}{\eta_0} & 0 \end{pmatrix} \begin{pmatrix} E_x \\ H_y \end{pmatrix}.\]

\[k_0 = \frac{\omega}{c} \quad \& \quad \eta_0 = \sqrt{\frac{\mu_0}{\varepsilon_0}}\]

are wavenumber and impedance in vacuum.

**Longitudinal Field**

\[E_z = \frac{i \eta_0}{k_0 \varepsilon_z} \frac{\partial H_y}{\partial x}.\]

**EigenValue Problem:**

- Assuming EM waves propagate along z: \[\Psi(x, z) = \Psi(x) e^{ik_z z}.\]
- Obtain an Eigenvalue problem: \[k_z \Psi = \mathcal{M} \Psi.\]

The eigenvalue \(k_z\) is the plasmon wavenumber.
Dispersion Relation

Periodicity: The eigenmodes are Bloch waves and arranged in bands.

\[ H_y^+(x) = H_y^-(x - d) e^{ik_x d} \]

\[ H_y^+(0) - H_y^-(0) = \sigma_s E_z(0) \]

\[ \partial_x H_y^+(0) = \partial_x H_y^-(0) \]

Graphene carries a surface current: \( J = \sigma E_z \)

\[ F(k_x, k_z) = \cos(k_x d) - \left[ \cosh(\kappa d) - \frac{\xi \kappa}{2} \sinh(\kappa d) \right] = 0 \]

- Assume very dense grid: \( \kappa d \ll 1 \)
- Around Brillouin center: \( k_x \sim 0 \)

- \( d > \xi \): Weak Plasmon Coupling \( \rightarrow \) Elliptic Band
- \( d = \xi \): Critical Plasmon Coupling \( \rightarrow \) Two Linear Bands
- \( d < \xi \): Strong Plasmon Coupling \( \rightarrow \) Hyperbolic Band

\[ k_x^2 \approx \frac{\varepsilon_x d}{\varepsilon_z(\xi - d)} k_x^2 \]
Dispersion Relation Bands

Make the choice $\xi=d$ and replace in Dispersion Relation.

- We have Saddle Point at $\left( k_x, k_z \right) = \left( 0, k_0 \sqrt{\varepsilon_x} \right)$
- Two Bands coexist

**Saddle Point + Linear Dispersion = Plasmonic Dirac Point**

- Spatial harmonics travel with the same phase velocity.
- Non-Dispersive EM wave propagation
Effective Medium Approach

Effective Medium (Metamaterial approach)

\[
\frac{k_z^2}{\varepsilon_{\text{eff}}^x} + \frac{k_x^2}{\varepsilon_{\text{eff}}^z} = k_0^2
\]

Approximate Dispersion Relation

\[
\frac{k_z^2}{\varepsilon_x} + \frac{d}{(d - \xi)\varepsilon_z} k_x^2 = k_0^2.
\]

Effective Relative Permittivities

\[
\varepsilon_{\text{eff}}^x = \varepsilon_x, \quad \varepsilon_{\text{eff}}^z = \varepsilon_z + i \frac{\eta_0 \sigma_s}{k_0 d} = \varepsilon_z \frac{d - \xi}{d}.
\]

Plasmonic Dirac Point → Epsilon-Near-Zero

\[
d = \xi \Rightarrow \varepsilon_{\text{eff}}^z = 0
\]
PDP Sensitivity

PDP is very sensitive to structural defects.

\[
\frac{\Delta k_z}{k_0 \sqrt{\varepsilon_x}} = -\frac{6}{(k_0 d)^2 \varepsilon_z} \frac{\Delta \xi}{d}.
\]

\[
\frac{\Delta \xi}{d} \sim \pm 0.05\%
\]

2D materials build planar bulk dielectrics.

- The extremely high sensitivity makes regular dielectrics impractical
- 2D media (e.g. MoS\(_2\) & hBN) build bulk dielectrics with essentially perfect planarity (atomic scale controllability).
Numerical EM Wave Simulations

- 40 graphene monolayers embedded in MoS$_2$ background ($\varepsilon_x=3.5$, $\varepsilon_z=13$).
- Drude model for graphene conductivity.
- $\lambda_0=12$ μm (THz regime).
- 2d magnetic dipole source.

Weak plasmon coupling ($\xi<d$)

PDP ($\xi=d$)

Strong plasmon coupling ($\xi>d$)

Simulations performed with COMSOL
Combinations of $\mu_c$ and $\lambda$ leading to PDP & ENZ ($\xi$ is plotted in nm).

A structure with arbitrary $d$ can be fabricated and then with suitable choice of $\mu_c$ and $\lambda$ we achieve ENZ.

The propagation distance $L/d$ of a plasmonic mode for all $\lambda$, $d$ and $\mu_c$ combinations leading to ENZ.

$$\frac{L}{d} = \sqrt{\frac{2}{\varepsilon_\infty}} \sqrt{\frac{\text{Im}[\sigma_s]}{\text{Re}[\sigma_s]}} \frac{1}{k_0 d}$$
Effective permittivity for $\lambda$ & $\mu_c$ combinations and fixed period $d=20\text{nm}$

- Dashed lines indicate the ENZ regime.
- Low losses in the ENZ region.
- Very negative $\varepsilon$ achieved but accompanied with high losses.
Conclusion

- Any periodic structure of 2D plasmonic materials (e.g. Graphene) exhibits **Plasmonic Dirac Point** in \((k_x, k_z)\) space.

- **Plasmonic Dirac Point** leads to **Epsilon-Near-Zero** media.
  - Systematic method for designing ENZ meta-materials.

- **Extreme sensitivity** of PDP on structural imperfection.
  - Dielectrics built by 2D materials (e.g. MoS\(_2\), hBN) have essentially **perfect planarity** (atomic scale control).

- **Graphene** multilayer in bulk MoS\(_2\) or hBN host:
  - **Dynamically tunable** dispersion by doping and frequency
  - **ENZ regime** shows relative **low losses**.
  - **Extremely negative** (up to \(\varepsilon_z = -100\)) relative permittivity.
Collaborators

- Prof. Efthimios Kaxiras, Harvard University.
- Prof. Giorgos Tsironis, University of Crete.
- Prof. Costas Valagiannopoulos, Nazarbayev University.
- Dr. Sharmila Shirodkar, Harvard University.

Thank you...

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