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

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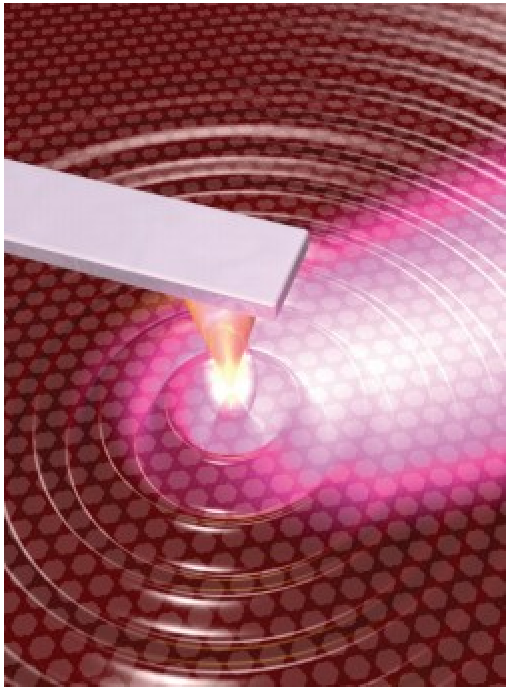
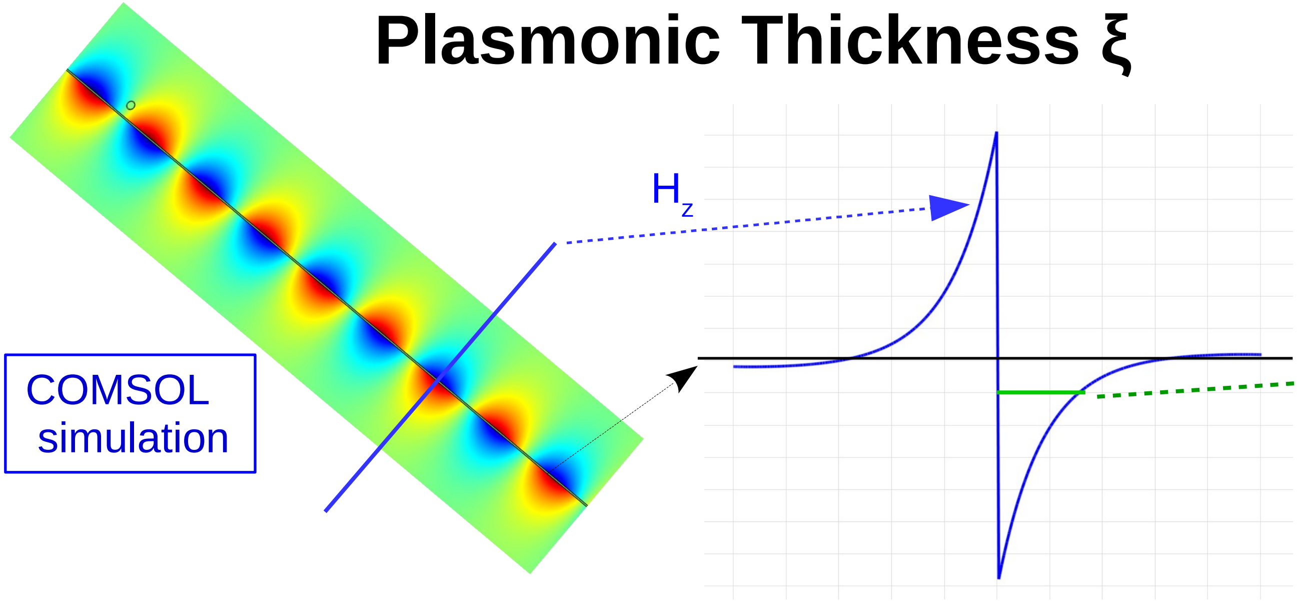
Graphene as Plasmonic Platform

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 ξ

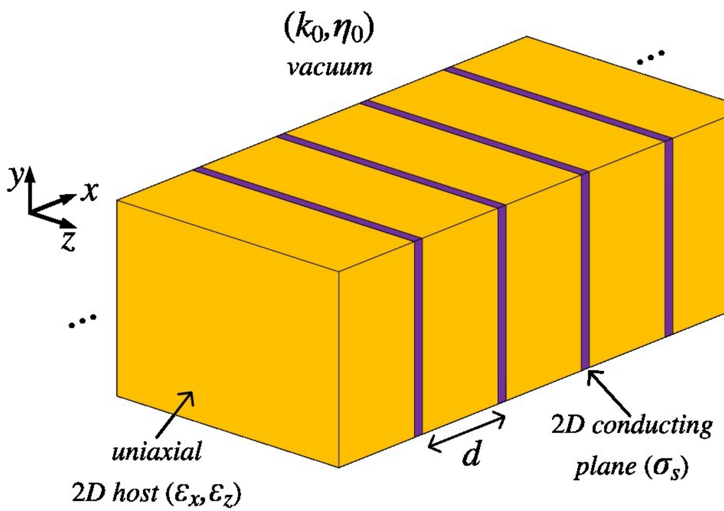


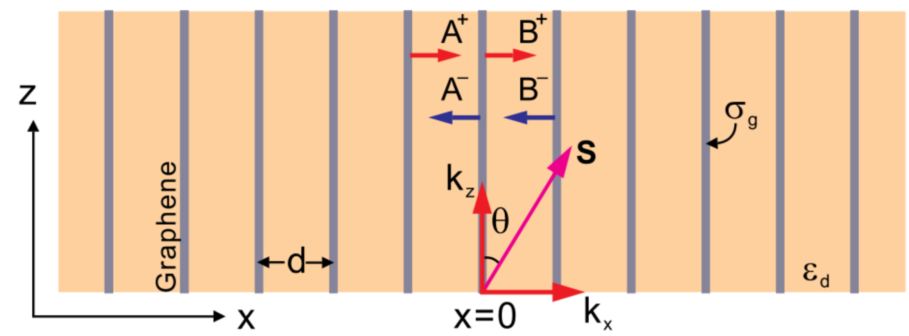
$$\delta = \xi/2 \quad \text{(decay length)}$$

$$\xi = \frac{1}{2}\left(k_{sp}^2 - k_0^2 \varepsilon_d\right)^{-1/2}$$

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 σ_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

$$-\mathrm{i}\frac{\partial}{\partial z}\mathbf{\Psi} = \mathcal{M}\cdot\mathbf{\Psi} \Leftrightarrow$$

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

Longitudinal Field

$$E_z = \frac{\mathrm{i}\eta_0}{k_0\varepsilon_z}\frac{\partial H_y}{\partial x}$$

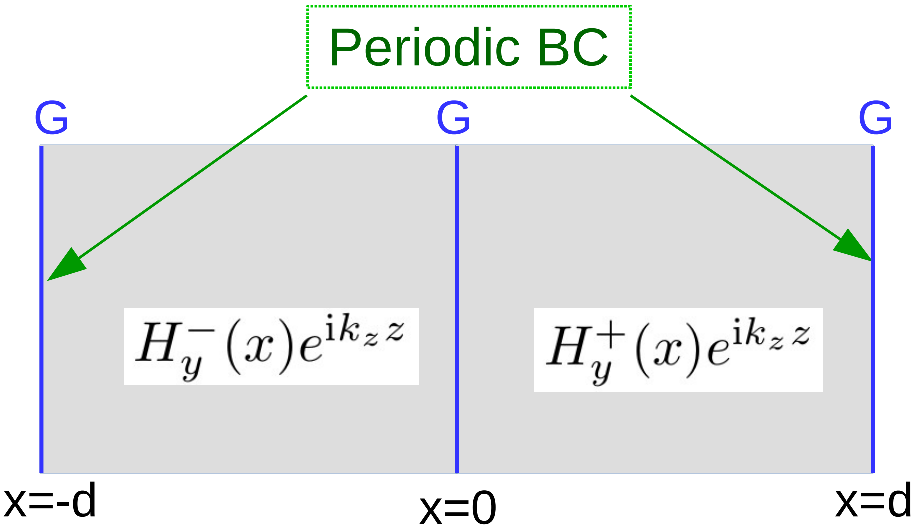
$k_0 = \omega/c$ & $\eta_0 = \sqrt{\mu_0/\varepsilon_0}$ are wavenumber and impedance in vacuum.

EigenValue Problem:

- Assuming EM waves propagate along z: $\mathbf{\Psi}(x,z) = \mathbf{\Psi}(x)e^{\mathrm{i}k_z z}$,
- Obtain an Eigenvalue problem: $k_z\mathbf{\Psi} = \mathcal{M}\mathbf{\Psi}$

The eigenvalue k_z is the plasmon wavenumber.

Dispersion Relation



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

$$H_y^+(x) = H_y^-(x-d)e^{ik_x d}$$

Graphene carries a surface current: $J=\sigma E_z$

$$H_y^+(0) - H_y^-(0) = \sigma_s E_z(0)$$

$$\partial_x H_y^+(0) = \partial_x H_y^-(0)$$

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

$$\kappa = \sqrt{\frac{\varepsilon_z}{\varepsilon_x}(k_z^2 - k_0^2\varepsilon_x)}.$$

$$\xi = -\frac{i\sigma_g\eta_0}{k_0\varepsilon_z}$$

- Assume very dense grid: $\kappa d << 1$
- Around Brilloun center: $k_x \sim 0$.

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

- d>ξ: Weak Plasmon Coupling → Elliptic Band
- d=ξ: Critical Plasmon Coupling → Two Linear Bands
- d<ξ: Strong Plasmon Coupling → Hyperbolic Band

$$k_z^2 \simeq \frac{\varepsilon_x d}{\varepsilon_z(\xi - d)}k_x^2$$

Dispersion Relation Bands

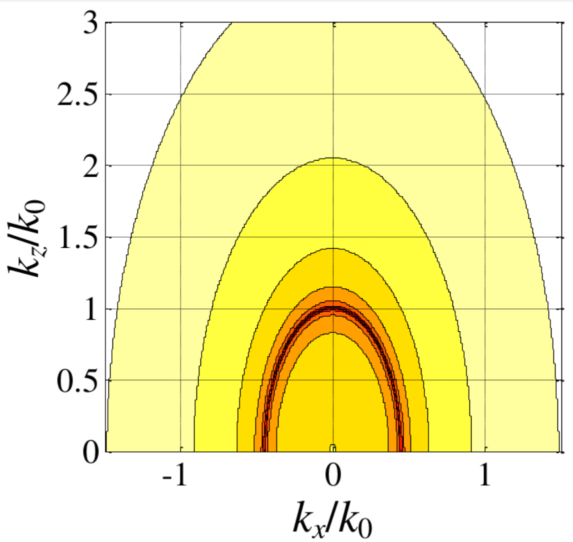
Make the choice **ξ=d** and replace in Dispersion Relation.

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

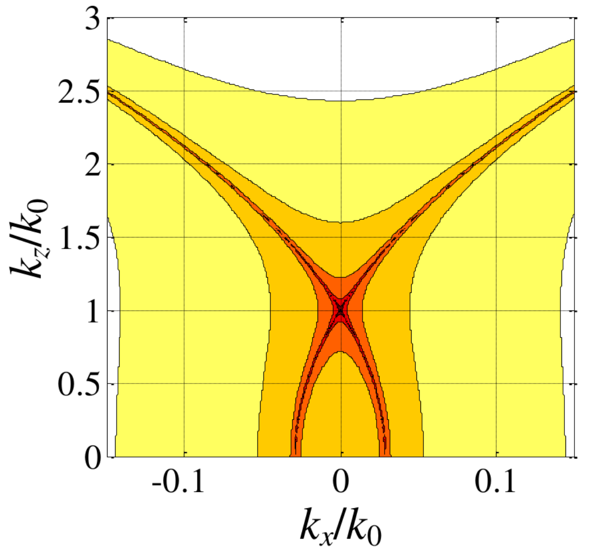
Saddle Point + Linear Dispersion = **P**lasmonic **D**irac **P**oint

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

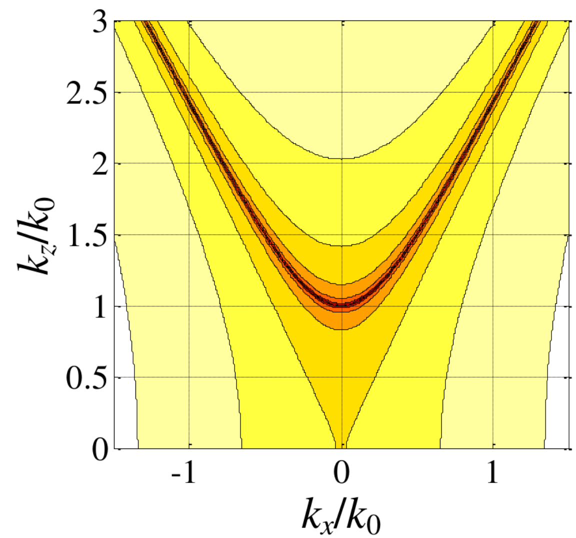
Elliptical Dispersion (ξ<d)



Linear Dispersion (ξ=d)



Elliptical Dispersion (ξ<d)



Effective Medium Approach

Effective Medium (Metamaterial approach)

$$\frac{k_z^2}{\varepsilon_x^{\text{eff}}} + \frac{k_x^2}{\varepsilon_z^{\text{eff}}} = k_0^2$$

Approximate Dispersion Relation

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

Effective Relative Permittivities

$$\varepsilon_x^{\text{eff}} = \varepsilon_x \quad , \quad \varepsilon_z^{\text{eff}} = \varepsilon_z + \mathrm{i}\frac{\eta_0 \sigma_s}{k_0 d} = \varepsilon_z \frac{d-\xi}{d}.$$

Plasmonic **D**irac **P**oint → **E**psilon-**N**ear-**Z**ero

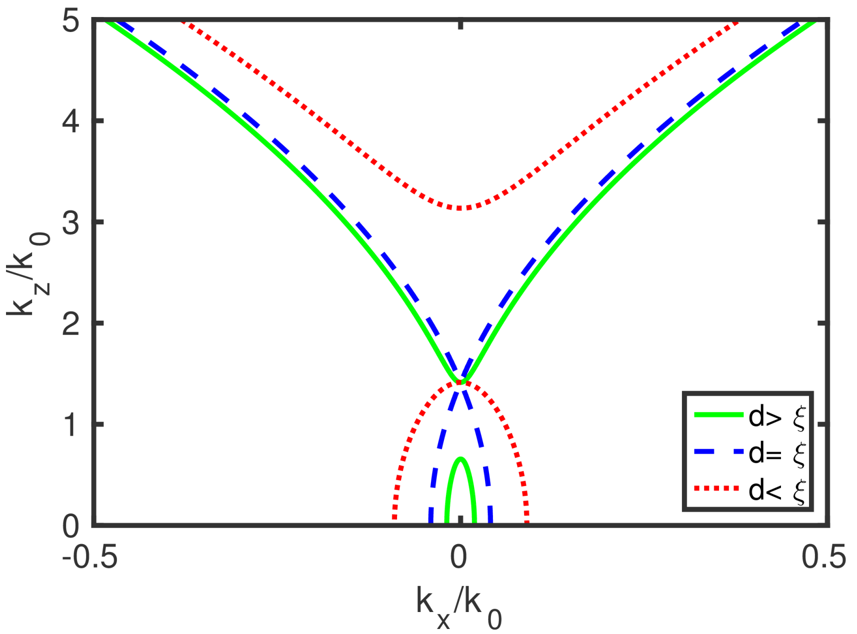
$$d = \xi \Rightarrow \varepsilon_z^{\text{eff}} = 0$$

PDP Sensitivity

PDP is very sensitive to structural defects.

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

$$\frac{\Delta\xi}{d} \sim \pm 0.05\%$$



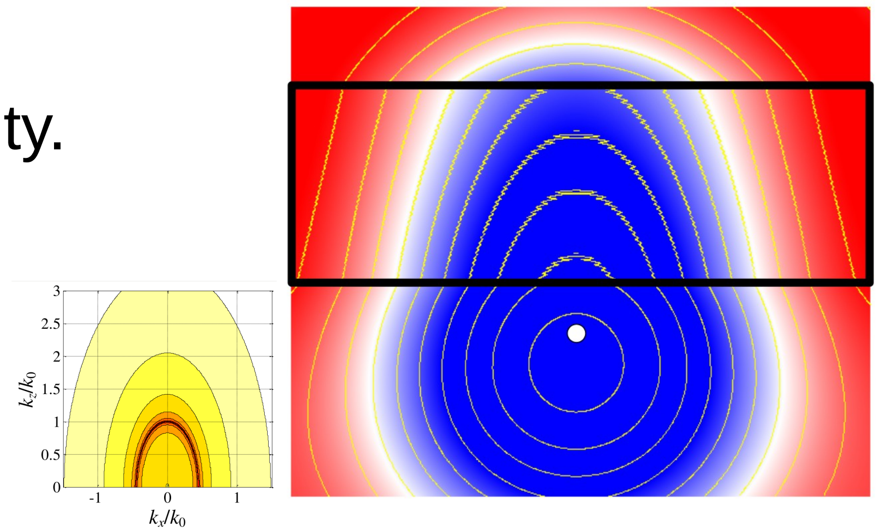
2D materials build planar bulk dielectrics.

- ✗ 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).

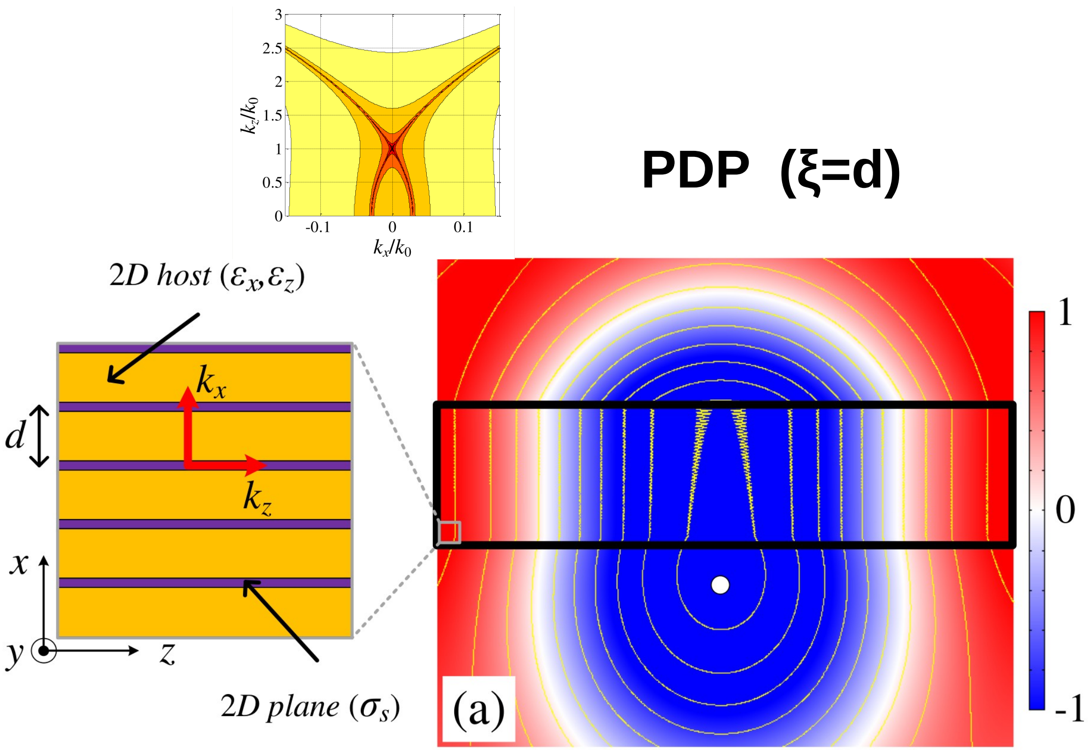
Numerical EM Wave Simulations

- 40 graphene monolayers embedded in MoS_2 background (ε_x=3.5, ε_z=13).
- Drude model for graphene conductivity.
- λ_0=12 μm (THz regime).
- 2d magnetic dipole source.

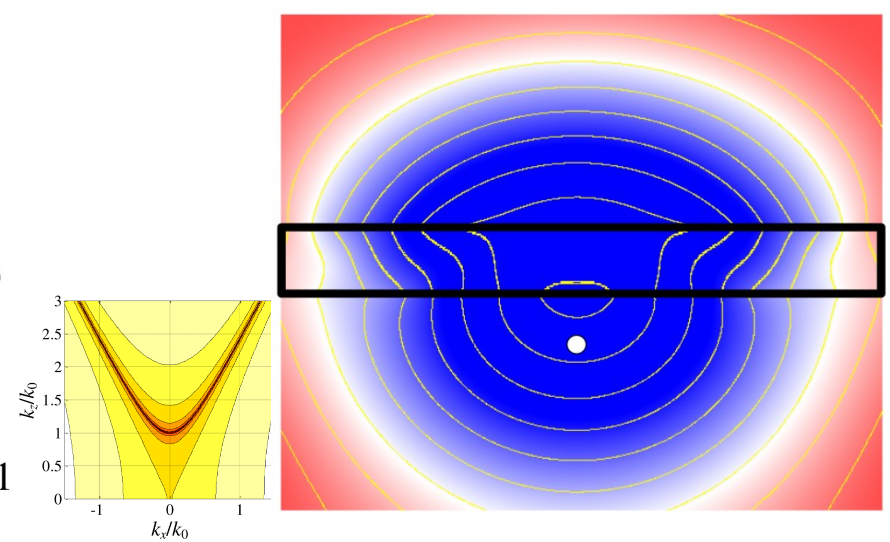
Weak plasmon coupling (ξ<d)



PDP (ξ=d)



Strong plasmon coupling (ξ>d)

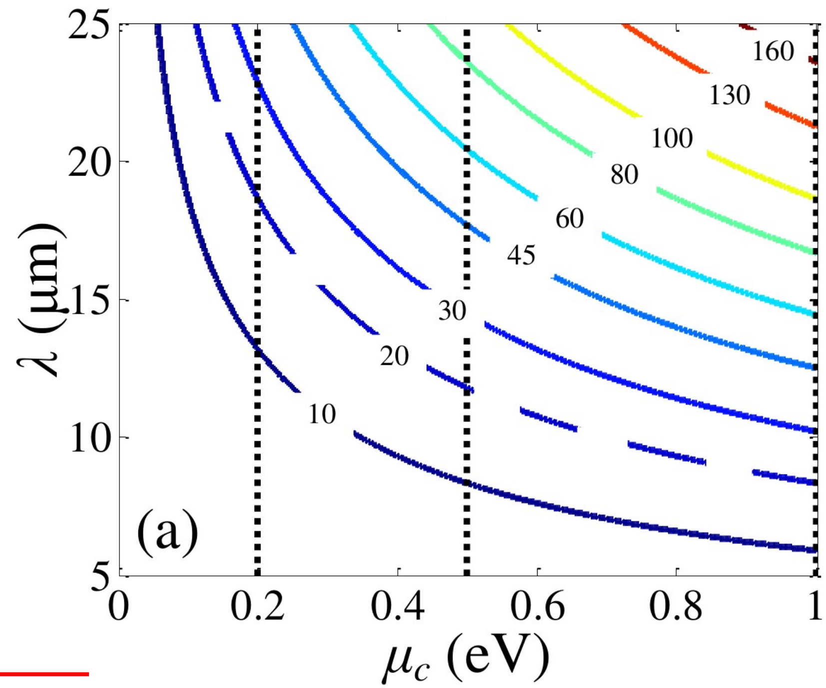


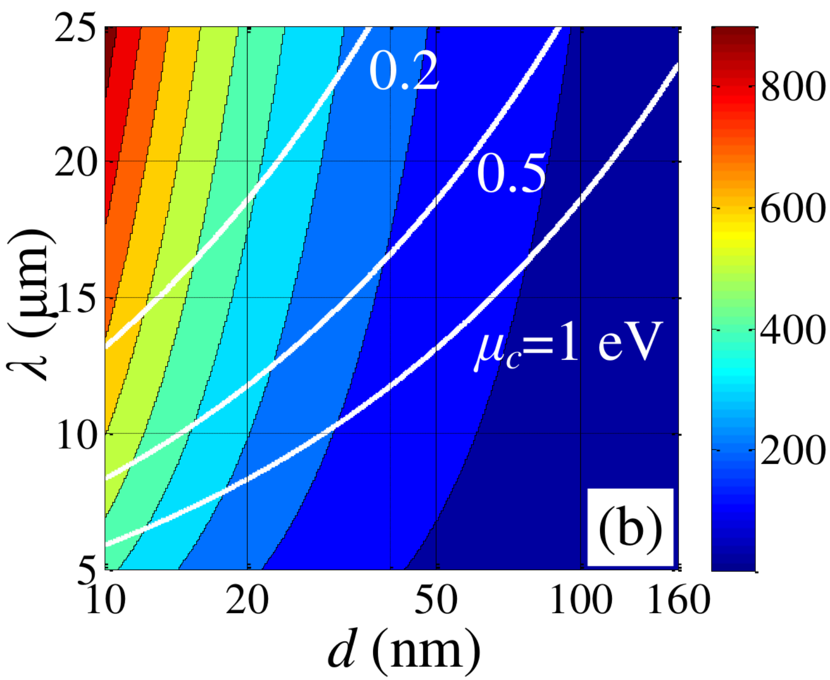
Simulations performed with COMSOL

General Investigation (maps)

Combinations of μ_c and λ leading to PDP & ENZ (ξ is plotted in nm).

A structure with arbitrary d can be fabricated and then with suitable choice of μ_c and λ we achieve ENZ.



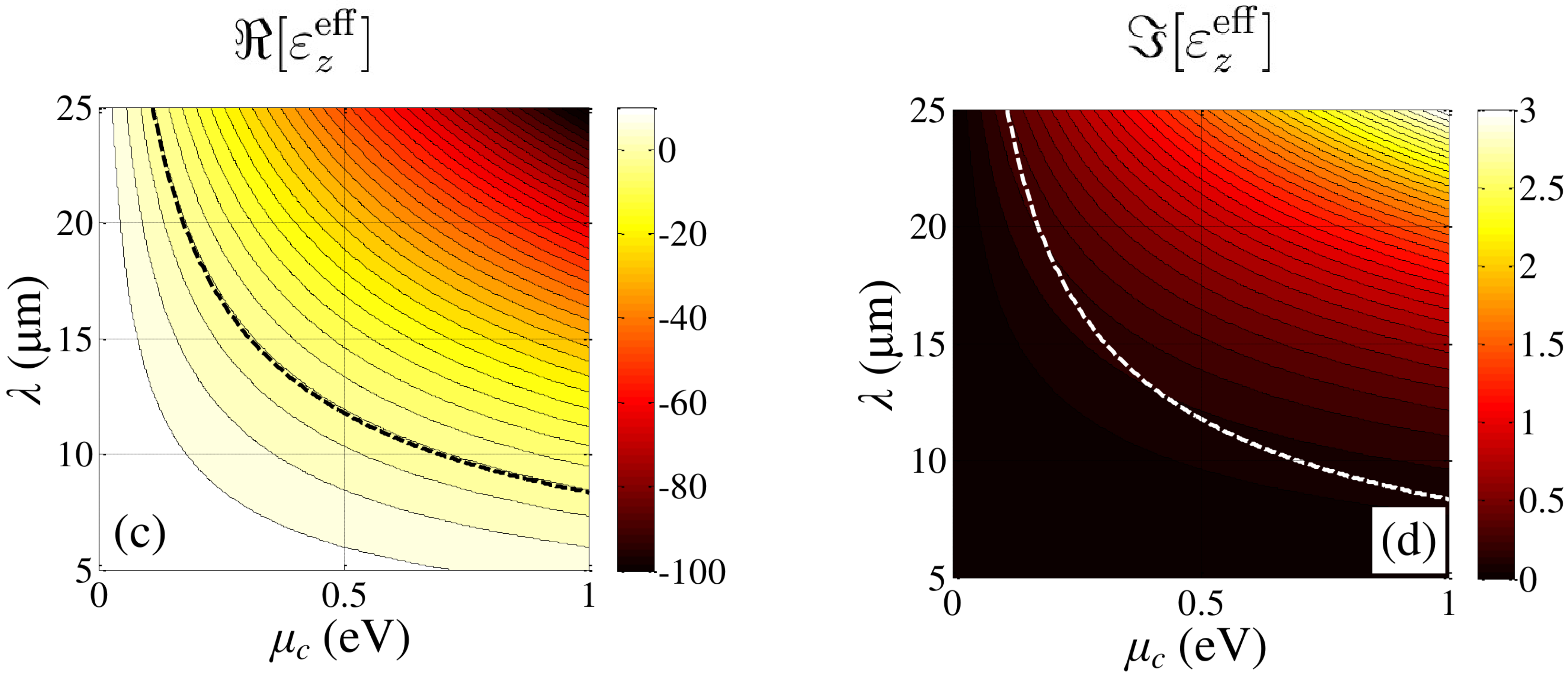


The propagation distance L/d of a plasmonic mode for all λ, d and μ_c combinations leading to ENZ.

$$\frac{L}{d} = \sqrt{\frac{2}{\varepsilon_z}} \sqrt{\frac{\mathrm{Im}[\sigma_s]}{\mathrm{Re}[\sigma_s]} \frac{1}{k_0 d}}$$

Effective Permittivity (maps)

Effective permittivity for λ & μ_c combinations and fixed period d=20nm



- Dashed lines indicate the ENZ regime.
- Low losses in the ENZ region.
- Very negative ε achieved but accompanied with high losses.

Conclusion

- Any periodic structure of 2D plasmonic materials (e.g. Graphene) exhibits **P**lasmonic **D**irac **P**oint in (k_x,k_z) space.

- **P**lasmonic **D**irac **P**oint leads to **E**psilon-**N**ear-**Z**ero 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 ε_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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