Anomalous scattering of light by slit structures in metallic slabs

Hai Zhang

Department of Mathematics, HKUST

Workshop on Qualitative and Quantitative Approaches to Inverse Scattering Problems
Sep 25, 2018

Joint work with Junshan Lin, Auburn University, USA
Extraordinary Optical Transmission Through a Small Hole Array


Size of each hole: 150 nm, metal thickness: 300 nm, skin depth: 30nm

Classical Bethe theory for diffraction by a small hole
Applications: Near-field optical imaging, biosensing, novel optical devices....
Possible Enhancement Mechanisms

- Surface plasmonic resonances in noble metals

- Non-plasmonic resonances (e.g., resonances induced by the geometry of the structure)

- Non-resonant enhancement,....
Motivations

- There has been a long debate on the interpretation of enhancement effects. For instance, surface plasmonic resonances strengthen or inhibit the enhancement? interplay between different enhancement mechanisms?

- Other questions: How large is the field enhancement and at what frequencies?

- **Quantitative analysis** of the field enhancement would be desirable!
Focus on a Prototype Structure: Narrow Slits

Field enhancement for slit structures in perfect conducting (PEC) metals:

- Single slit and an array of slits.

Related work:

- Gao, Li, Yuan (2017): field enhancement for a subwavelength cavity.
- High transmission for the periodic structures: G. Bouchitté, B. Schweizer, G. Kriegsmann, and many others in physics literatures.
Transmission with metal thickness = 1, gap size = 0.02.

- **Resonant effect**

- **Non-resonant effect**
Scattering Problem II

- Normalization: $\ell = 1$.
- The exterior domain: $\Omega_\epsilon = \Omega_+ \cup \Omega_- \cup S_\epsilon$.
- **TM polarization**: the incident magnetic field $H^i = (0, 0, u^i)$, where $u^i = e^{ikd \cdot x}$, $k = \omega/c$.
- The total field $u_\epsilon = u^i + u^r + u^s_\epsilon$ in $\Omega^+$, and $u_\epsilon = u^s_\epsilon$ (transmitted wave) in $\Omega^-$.
- The scattering problem:

\[
\begin{cases}
\Delta u_\epsilon + k^2 u_\epsilon = 0 \quad & \text{in } \Omega_\epsilon, \\
\frac{\partial u_\epsilon}{\partial \nu} = 0 \quad & \text{on } \partial \Omega_\epsilon, \\
\lim_{r \to \infty} \sqrt{r} \left( \frac{\partial u^s_\epsilon}{\partial r} - iku^s_\epsilon \right) = 0, \quad r = |x|.
\end{cases}
\]
Fact: The scattering problem attains a unique solution if $\text{Im } k \geq 0$.

**Definition**

The *scattering resonances* are the poles of the scattering operator when continued meromorphically to the whole complex plane.

Field enhancement at resonant frequencies: $O \left( \frac{1}{|k - k_{\text{res}}|} \right)$. 
**Integral Equation Formulation**

**Integral equation formulation:**

\[
\begin{cases}
\int_{\Gamma_\epsilon^+} g^e(x, y) \frac{\partial u_\epsilon}{\partial \nu} \, ds_y + \int_{\Gamma_\epsilon^+} g^i(x, y) \frac{\partial u_\epsilon}{\partial \nu} \, ds_y = -(u^i + u^r), & \text{on } \Gamma_\epsilon^+,

\int_{\Gamma_\epsilon^-} g^e(x, y) \frac{\partial u_\epsilon}{\partial \nu} \, ds_y + \int_{\Gamma_\epsilon^-} g^i(x, y) \frac{\partial u_\epsilon}{\partial \nu} \, ds_y = 0, & \text{on } \Gamma_\epsilon^-.
\end{cases}
\]

**Boundary integral equations after scaling** (\(x_1 = \epsilon X, y_1 = \epsilon Y, X, Y \in (0, 1)\)):

\[
\begin{bmatrix}
T^e + T^i \\
\tilde{T}^i \\
T^e + T^i
\end{bmatrix}
\begin{bmatrix}
\phi_1 \\
\phi_2
\end{bmatrix} =
\begin{bmatrix}
f/\epsilon \\
0
\end{bmatrix}.
\]

where \(T^e, T^i, \text{ and } \tilde{T}^i\) are the integral operators with kernels \(G^e_\epsilon, G^i_\epsilon\) and \(\tilde{G}^i_\epsilon\), \(\phi_1(X) := -\partial \nu u_\epsilon(\epsilon X, 1)\), and \(\phi_2(X) := -\partial \nu u_\epsilon(\epsilon X, 0)\).
Asymptotic Expansions for the Integral Operators

• Asymptotic expansions of the kernels:

\[ G_\varepsilon^e(X, Y) = \frac{1}{\pi} \left[ \ln \varepsilon + \ln k + \gamma_0 \right] + \frac{1}{\pi} \ln |X - Y| + O((\varepsilon|X - Y|)^2 \ln(\varepsilon|X - Y|)); \]
\[ G_\varepsilon^i(X, Y) = \frac{\cot k}{k \varepsilon} + \frac{2 \ln 2}{\pi} + \frac{1}{\pi} \left[ \ln \left( |\sin \left( \frac{\pi(X + Y)}{2} \right) | \right) + \ln \left( |\sin \left( \frac{\pi(X - Y)}{2} \right) | \right) \right] \]
\[ + O(k^2 \varepsilon^2); \]
\[ \tilde{G}^i_\varepsilon(X, Y) = \frac{1}{(k \sin k) \varepsilon} + O\left( e^{-1/\varepsilon} \right). \]

• Asymptotic expansions of the integral operators:

\[
\begin{bmatrix}
T^e + T^i & \bar{T}^i \\
\bar{T}^i & T^e + T^i
\end{bmatrix}
= \begin{bmatrix}
\beta & \tilde{\beta} \\
\tilde{\beta} & \beta
\end{bmatrix} P + K + \begin{bmatrix}
K_\infty & \tilde{K}_\infty \\
\tilde{K}_\infty & K_\infty
\end{bmatrix} =: \mathbb{P} + \mathbb{L}.
\]

• The system of integral equations becomes \((\mathbb{P} + \mathbb{L}) \varphi = f\).
Resonant Effect I: Resonance Condition

- Look for $k$ such that $(P + L)\varphi = 0$ attains non-trivial solutions.
- The operator equation reduces to
  \[(M + I)\begin{bmatrix} \langle \varphi, e_1 \rangle \\ \langle \varphi, e_2 \rangle \end{bmatrix} = 0,\]
  where $e_1 = [1, 0]^T$ and $e_2 = [0, 1]^T$, and the matrix
  \[M = \left( \beta I + \tilde{\beta} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \right) \cdot \begin{bmatrix} \langle L^{-1}e_1, e_1 \rangle & \langle L^{-1}e_1, e_2 \rangle \\ \langle L^{-1}e_1, e_2 \rangle & \langle L^{-1}e_1, e_1 \rangle \end{bmatrix} \]
- The eigenvalues of $M + I$ are given by
  \[
  \lambda_1(k, \epsilon) = 1 + (\beta(k, \epsilon) + \tilde{\beta}(k, \epsilon)) \left( \langle L^{-1}e_1, e_1 \rangle + \langle L^{-1}e_1, e_2 \rangle \right),
  \]
  \[
  \lambda_2(k, \epsilon) = 1 + (\beta(k, \epsilon) - \tilde{\beta}(k, \epsilon)) \left( \langle L^{-1}e_1, e_1 \rangle - \langle L^{-1}e_1, e_2 \rangle \right).
  \]

Resonance condition
The resonances are the roots of $\lambda_1(k, \epsilon) = 0$ or $\lambda_2(k, \epsilon) = 0$. 
Theorem

The following asymptotic expansions hold for the resonances of the scattering problem:

\[
k_{m,1} = (2m - 1)\pi + 2(2m - 1)\pi \left[ \frac{1}{\pi} \varepsilon \ln \varepsilon + \left( \frac{1}{\alpha} + \frac{1}{\pi} (2 \ln 2 + \ln((2m - 1)\pi) + \gamma_0) \right) \varepsilon \right] + O(\varepsilon^2 \ln^2 \varepsilon),
\]

\[
k_{m,2} = 2m\pi + 4m\pi \left[ \frac{1}{\pi} \varepsilon \ln \varepsilon + \left( \frac{1}{\alpha} + \frac{1}{\pi} (2 \ln 2 + \ln(2m\pi) + \gamma_0) \right) \varepsilon \right] + O(\varepsilon^2 \ln^2 \varepsilon),
\]

for \( m = 1, 2, 3, \ldots \), and \( m\varepsilon \ll 1 \). Here \( \alpha = \langle K^{-1} 1, 1 \rangle \), \( \gamma_0 = c_0 - \ln 2 - i\pi/2 \), and \( c_0 \) is the Euler constant.

Remark The imaginary part of each resonance has an order of \( O(\varepsilon) \).
The wave field inside the slit adopts the following expansion at the odd and even resonances respectively:

\[ u_\varepsilon(x) = \frac{1}{\varepsilon} \cdot \frac{2i}{k \sin(k/2)} \cdot \cos(k(x_2 - 1/2)) + O(\ln^2 \varepsilon) \]

and

\[ u_\varepsilon(x) = -\frac{1}{\varepsilon} \cdot \frac{2i}{k \cos(k/2)} \cdot \sin(k(x_2 - 1/2)) + O(\ln^2 \varepsilon). \]
Expand the wave field in the slit as the sum of wave-guide modes:

\[ u_\varepsilon(x) = a_0 \cos k x_2 + b_0 \cos k (1 - x_2) + \sum_{m \geq 1} \left[ a_m \exp \left( -k_2^{(m)} x_2 \right) + b_m \exp \left( -k_2^{(m)} (1 - x_2) \right) \right] \cos \frac{m \pi x_1}{\varepsilon}, \]

where \( k_2^{(m)} = \sqrt{(m \pi / \varepsilon)^2 - k^2}. \)

**Theorem**

No significant magnetic field enhancement is gained. However, the electric field

\[ |E_\varepsilon| \sim O(1/k) \text{ or } |E_\varepsilon| \sim O \left( 1/(k \ell) \right) \text{ if } \ell \neq 1. \]
Scattering by A Periodic Array of PEC Slits

- A periodic array of slits: $S_{\varepsilon} = \bigcup_{n=-\infty}^{\infty} \left( S_{\varepsilon}^{(0)} + nd \right)$.

- The scattering problem: $\Delta u_{\varepsilon} + k^2 u_{\varepsilon} = 0$ in $\Omega_{\varepsilon}$ and $\partial_{\nu} u_{\varepsilon} = 0$ on $\partial \Omega_{\varepsilon}$.

- Look for quasi-periodic solutions such that $u_{\varepsilon}(x_1 + d, x_2) = e^{i\kappa d} u_{\varepsilon}(x_1, x_2)$.

- Outgoing radiation condition: the scattered field
  \[ u^s_{\varepsilon}(x_1, x_2) = \sum_{n=-\infty}^{\infty} u^s_{n,\pm} e^{i\kappa_n x_1 \pm i\zeta_n x_2} \quad \text{in } \Omega^\pm, \]

  where
  \[ \kappa_n = \kappa + \frac{2\pi n}{d} \quad \text{and} \quad \zeta_n(k) = \begin{cases} \sqrt{k^2 - \kappa_n^2}, & |\kappa_n| \leq k, \\ i\sqrt{\kappa_n^2 - k^2}, & |\kappa_n| > k. \end{cases} \]
Three Configurations of Periodic Slits

- Normalization: $\ell = 1$.
- Three configurations of periodic slits:
  1. $\varepsilon \ll d \sim \lambda \sim O(1)$: diffraction regime.
  2. $\varepsilon \ll d \ll \lambda$: homogenization regime I
  3. $\varepsilon \sim d \ll \lambda \sim O(1)$: homogenization regime II
Diffraction Regime: $\varepsilon \ll d \sim \lambda$

- Reduce to the first Brillouin zone: $\kappa \in (-\pi/d, \pi/d]$.

- Exterior Green’s function in $\Omega^\pm$: $g^e(x, y) = g^d(x, y) + g^d(x', y)$, where

  $$g^d(x, y) = -\frac{i}{2d} \sum_{n=-\infty}^{\infty} \frac{1}{\zeta_n(k)} e^{i\kappa_n(x_1-y_1) + i\zeta_n(k)|x_2-y_2|},$$

  and

  $$\kappa_n = \kappa + \frac{2\pi n}{d} \quad \text{and} \quad \zeta_n(k) = \begin{cases} \sqrt{k^2 - \kappa_n^2}, & |\kappa_n| \leq k, \\ i\sqrt{\kappa_n^2 - k^2}, & |\kappa_n| > k. \end{cases}$$
Diffraction Regime: Integral Equation and Asymptotic Expansion

\begin{align*}
\int_{\Gamma^+_\varepsilon} g_{\#}^\varepsilon(x,y) \frac{\partial u_\varepsilon}{\partial y} dy + \int_{\Gamma^+_\varepsilon \cup \Gamma^-_\varepsilon} g_i^\varepsilon(x,y) \frac{\partial u_\varepsilon}{\partial y} dy &= -(u^i + u^r), \quad \text{on } \Gamma^+_\varepsilon, \\
\int_{\Gamma^-_\varepsilon} g_{\#}^\varepsilon(x,y) \frac{\partial u_\varepsilon}{\partial y} dy + \int_{\Gamma^+_\varepsilon \cup \Gamma^-_\varepsilon} g_i^\varepsilon(x,y) \frac{\partial u_\varepsilon}{\partial y} dy &= 0, \quad \text{on } \Gamma^-_\varepsilon.
\end{align*}

Boundary integral equation after scaling:

\[
\begin{bmatrix}
T_{\#}^\varepsilon + T^i \\
\tilde{T}^i
\end{bmatrix}
\begin{bmatrix}
\phi_1 \\
\phi_2
\end{bmatrix} =
\begin{bmatrix}
f/\varepsilon \\
0
\end{bmatrix}.
\]

\(T_{\#}^\varepsilon\) is the integral operator with kernel \(G_{\#}^\varepsilon\):

\[
G_{\#}^\varepsilon(X,Y) = \frac{1}{\pi} \left( \ln \varepsilon + \ln 2 + \ln \frac{\pi}{d} \right) + \frac{1}{2\pi} \sum_{n \neq 0} \frac{1}{|n|} - \frac{i}{d} \sum_{n=-\infty}^{\infty} \frac{1}{\zeta_n(k)} + \frac{1}{\pi} \ln |X - Y| + O(\varepsilon|X - Y|).
\]

Asymptotics of integral operators and the resonance condition can be obtained!
Diffraction Regime: Rayleigh Anomaly Frequencies

• Rayleigh anomaly frequencies: \( k = \kappa_n = \kappa + 2\pi n/d \) or \( \zeta_n = 0 \) for some \( n \).

Note that the scattered field

\[
u^s(x_1, x_2) = \sum_{n=-\infty}^{\infty} u^s_n e^{i\kappa_n x_1 \pm i\zeta_n x_2}, \quad \zeta_n(k) = \begin{cases} \sqrt{k^2 - \kappa_n^2}, & |\kappa_n| \leq k, \\ i\sqrt{\kappa_n^2 - k^2}, & |\kappa_n| > k. \end{cases}
\]

• Resonances away from the Rayleigh anomaly frequencies: consider the domain

\[
D_{\kappa,\delta,M} := \mathbb{C} \setminus B_{\kappa,\delta} \cap \{z \mid |z| \leq M\}, \quad \text{where } B_{\kappa,\delta} := \bigcup_{n=-\infty}^{\infty} B_\delta(\kappa + 2\pi n/d).
\]
Diffraction Regime: Resonances and Eigenvalues

**Theorem**

For each $\kappa \in (-\pi/d, \pi/d]$, if $m\pi \in D_{\kappa, \delta, M}$, there exists a resonance or an eigenvalue $k_m$ in the neighborhood of $m\pi$.

- If $m\pi > |\kappa|$, $k_m$ is a **resonance**. Otherwise, $k_m$ is an **eigenvalue**.

- The following asymptotic expansion holds for $k_m$ if $m\epsilon \ll 1$:

  $$k_m = m\pi + 2m\pi \left[ \frac{1}{\pi} \epsilon \ln \epsilon + \left( \frac{1}{\alpha} + \gamma(m\pi, \kappa, d) \right) \epsilon \right] + O(\epsilon^2 \ln^2 \epsilon),$$

  Here $\alpha = \langle K^{-1} 1, 1 \rangle$, $\gamma(k, \kappa, d) = \frac{1}{\pi} \left( 3\ln 2 + \ln \frac{\pi}{d} \right) + \left( \frac{1}{2\pi} \sum_{n \neq 0} \frac{1}{|n|} - i \frac{1}{d} \sum_{n=-\infty}^{\infty} \frac{1}{\zeta_n(k)} \right)$.

- $\text{Im} \gamma(m\pi, \kappa, d) = -\frac{1}{d} \sum_{|\kappa_n| < m\pi} \frac{1}{\zeta_n(m\pi)} < 0$ if $m\pi > |\kappa|$, and the resonance has an imaginary part of $O(\epsilon)$.

- $\text{Im} \gamma(m\pi, \kappa, d) = 0$ if $m\pi < |\kappa|$.

- The eigenvalue occurs only if $d < 1$.

- The eigenmode $u_\epsilon^s$ is a **surface bound state** (decaying exponential away from the grating surface).
Surface Bound State
In the slit $S^{(0)}_\epsilon$

The wave field adopts the following expansion at the odd and even resonances respectively:

$$u_\epsilon(x) = \frac{1}{\epsilon} \cdot i \cdot \frac{i}{\text{Im} \gamma(m\pi, \kappa, d) \cdot k \sin(k/2)} \cdot \cos(k(x_2 - 1/2)) + O(\ln^2 \epsilon)$$

and

$$u_\epsilon(x) = -\frac{1}{\epsilon} \cdot i \cdot \frac{i}{\text{Im} \gamma(m\pi, \kappa, d) \cdot k \cos(k/2)} \cdot \sin(k(x_2 - 1/2)) + O(\ln^2 \epsilon).$$
Homogenization Regime I. $\varepsilon \ll d \ll \lambda$

- No scattering resonance or eigenvalue exists if $k \ll 1$ (or $\lambda \gg 1$).

- If $\varepsilon \ll 1$ and $k = \varepsilon^\sigma$, in the reference slit,

$$u_\varepsilon(x) = \left( \frac{\alpha}{\varepsilon \cdot \lambda_1} + \frac{\alpha}{\varepsilon \cdot \lambda_2} \right) \cdot \frac{\cos(kx_2)}{k \sin k} + \left( \frac{\alpha}{\varepsilon \cdot \lambda_1} - \frac{\alpha}{\varepsilon \cdot \lambda_2} \right) \cdot \frac{\cos(k(1-x_2))}{k \sin k} + H.O.T$$

$$= \begin{cases} 
2x_2 + O(\varepsilon^{2\sigma}) + O(\varepsilon^{1-\sigma}) & \text{if } 0 < \sigma < 1, \\
1 + id \cdot \cos \theta (2x_2 - 1) \varepsilon^{\sigma-1} + O(\varepsilon^{\sigma+1}) + O(\varepsilon^{2(\sigma-1)}) & \text{if } \sigma > 1,
\end{cases}$$

- No magnetic enhancement is gained. However, the leading-order term has a slope of 2 and $O(\varepsilon^{\sigma-1})$ respectively.
Homogenization Regime I: Non-resonant Field Enhancement

If \( \varepsilon \ll 1 \) and \( k = \varepsilon^{\sigma} \), then \( E_\varepsilon = [E_{\varepsilon,1}, E_{\varepsilon,2}, 0] \) in the reference slit, where

\[
E_{\varepsilon,1} = \begin{cases} 
\frac{2i}{\sqrt{\tau_0/\mu_0}} \cdot \frac{1}{\varepsilon^{\sigma}} + H.O.T \quad & \text{if } 0 < \sigma < 1, \\
\frac{d \cos \theta}{\sqrt{\tau_0/\mu_0}} \cdot \frac{1}{\varepsilon} + H.O.T \quad & \text{if } \sigma > 1,
\end{cases}
\]

and \( E_{\varepsilon,2} \sim O(e^{-1/\varepsilon}) \).
Homogenization Regime II: $\epsilon \sim d \ll \lambda$

- $\eta := \epsilon/d$, where $0 < \eta < 1$.

- Asymptotic expansion of the scattering solution can be obtained, using the expansion for the periodic Green's function:

$$G_\epsilon^e(X, Y) = \frac{1}{\pi} \ln 2 - \frac{i\eta}{\zeta \epsilon} + \frac{1}{\pi} \ln |\sin(\pi\eta(X - Y))| + \frac{\kappa\eta}{\zeta}(X - Y) + O(\epsilon),$$

where $\kappa^2 + \zeta^2 = k^2$. 
Homogenization Regime II: “Surface Plasmon"

There exist two groups of dispersion relations satisfying $|\kappa| > k$, and their leading orders are: $\kappa = k \sqrt{1 + \eta^2 \left( \frac{\sin k}{\cos k \pm 1} \right)^2}$, $\eta = \varepsilon / d$.

- The associated eigenmodes $u_\varepsilon$ are surface bound states.
- The dispersion relations and surface bound states resemble the ones for surface plasmon polaritons in the dielectric-metal configuration.
Homogenization Regime II: Total Transmission

Scattering by an incident plane wave $u^i = e^{i(\kappa x_1 - \zeta (x_2 - 1))}$, where $\kappa = k \sin \theta$, $\zeta = k \cos \theta$, and $|\kappa| < k$.

The leading orders of the reflection and transmission coefficients are

$$R_0 = \frac{i \tan k \cdot (\eta^2 - \cos^2 \theta)}{-i \tan k \cdot (\eta^2 + \cos^2 \theta)} + 2 \eta \cos \theta,$$

$$T_0 = \frac{2 \cos \theta \cdot \eta}{-i \sin k \cdot (\eta^2 + \cos^2 \theta) + 2 \cos \theta \cdot \eta \cos k}.$$

Total transmission is achieved when $k = m\pi$ (Fabry-Perot resonance), and all frequencies for a special incident angle $\theta$ such that $\cos \theta = \eta$ (Brewster angle).
Field enhancement for PEC metals:

- **Single slit**: resonant and non-resonant enhancement effects.
- **An array of slits**: resonant and non-resonant enhancement effects, surface bound states, “surface plasmon", and total transmission.
- Asymptotics of resonances/eigenvalues are derived, and the enhanced wave modes are characterized.
Field enhancement for a single slit in a real metallic slab

1. **Multiscale problem**: size of slit aperture $\delta$, skin depth of metal $\delta_m$, thickness of slab $d$, and wavelength $\lambda$;

2. The skin depth effect **weakens** the Fabry-Perot resonance, and induces **small shifts** of the FP resonance;

3. The slit structure can excite **plasmonic surface waves** (plasmonic resonance) along the metal interface;

4. The plasmonic resonance can **interact** with the FP resonance, an vice visa.
Numerical results

\[ \varepsilon_m = -100 + 10i \]

\[ \nu \]

\[ \delta = 0.02 \]

\[ \delta = 0.05 \]

\[ \delta = 0.1 \]

\[ \delta = 0.2 \]

Figure: The transmittance \( T \) over the frequency band \([0.5, 15]\) for various slit sizes.

1. For numerical results, see “An integral equation method for numerical computation of scattering resonances in a narrow metallic slit”, J. L and H. Z, submitted;

2. For theoretical results, coming soon.
1. 3D subwavelength structures: quantitative analysis

2. Applications in sensing and control of light.

Thank you for your attention!