Metamaterials Comprising of Plasmonic Nano-spheres and Nanorods: Modeling Using Dipole Moment and Characteristic Basis Function Methods

by

Arash Rashidi

Submitted to the Department of Electrical and Computer Engineering on April 3, 2012, in partial fulfillment of the requirements for the degree of Doctorate of Philosophy in Electrical and Computer Engineering
To my mother,

to those kind professors who support talented students,

& to those scientists who devoted their life to find the truth.
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Abstract

This dissertation presents physical modeling and numerically efficient analyses of the interaction between electromagnetic waves and clusters of metamaterials comprising of core-shell nano-particles and plasmonic nanorods. Chapter 1 is the introduction for this thesis. The main idea of chapter 2 is to design an array of core-shell plasmonic nanoparticles manipulating a desired near-field focusing pattern in optical spectrum. The interactions between the array elements are formulated by using Dyadic Green’s Function analysis and by employing the closed-form formula for electric polarizability of each plasmonic particle (Dipolar Mode (DM) approach).

In chapter 3 we introduce a set of Macro Basis Functions (MBFs) for efficient representation of the currents induced on metal wires and elements comprising of junctions of wires or strips. The use of these functions leads to a relatively small and well-conditioned matrix, only a 3x3 size for a cross-shaped element. An important advantage of using these basis functions is that the fields they generate can be expressed in close forms.

In chapter 4 we introduce a numerically efficient computational technique to model the problem of scattering from plasmonic nanorod antennas. The key to achieving the numerical efficiency is to utilize MBFs to reduce the size of matrix equation. Closed form formulations are presented for computing the fields by the MBFs that enable us to generate the required matrix elements rapidly.

The goal of chapter 5 is to present a computational scheme to characterize reflection and transmission coefficients for a periodic array of plasmonic nanorods illuminated by an obliquely incident plane wave. The problem is formulated by using the Characteristic Basis Function Method (CBFM) to reduce the number of unknowns. The concept of progressively expanding rings is employed along with Parseval's theorem to evaluate the Galerkin’s integrals for the periodic structure.

In chapter 6, by taking advantage of CBFM we solve the scattering problem of finite arrays of plasmonic nanorods for two different cases. In case 1, the elements are arbitrarily tilted
(rotated around their centroids). And in case 2, the finite array includes a Fibonacci arrangement of two kinds of nanorods with different lengths and consequently different resonance frequencies.

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Chapter 1

Introduction

Metamaterials comprising of plasmonic nano-spheres and nanorods have been used in a wide range of nanophotonics applications [1-5]. Collimation and near-field concentration of the radiation of nanoscale light sources (i.e., molecules and quantum dots) can be achieved by designing array of plasmonic nanoantennas that surround the optical source [6-8]. Storing light can be effectively demonstrated by formation of long-lasting resonances via external coupling in plasmonic nanorods [9]. Nanoantennas can also be deposited on layered substrates to enable solar cells and energy harvesting applications [10-11]. Biosensing technology is another application that can be improved by using a porous plasmonic nanorod layer supporting special optical response and guided modes [12].
1.1. Metamaterials Comprising of Core-Shell Nano-Particles

Next chapter, chapter 2, devotes to design an array of core-shell plasmonic nanoparticles manipulating a desired near-field focusing pattern in optical spectrum. Tightly localizing light and subwavelength near field focusing are well understood topics in recent theoretical and experimental optics [13,14]. The major physical obstacle for confining the light in very small spots is the diffraction limit, in which there is a considerable attenuation in evanescent waves for the finer spatial details (smaller than a wavelength) [15]. Super-resolution aperture scanning microscope was successful but expensive in fabricating a small aperture in a thin diaphragm to obtain information about the small details features [16]. Theoretically, it can be shown that in a medium of negative index property, evanescent waves can be enhanced in amplitude by perfect lens realization and its unique transmission process [17]. One L-C loaded left-handed transmission line medium sandwiched between two commensurate unloaded printed grids experimentally demonstrated the super lens phenomenon [15,18], but the low inductor quality factor is the primary cause of the loss degrading the performance considerably. Some efforts were done recently to theoretically design a near field focusing plates by back-propagation of the desired near field and then solving an integral equation to find the passive surface impedance [19,20]. One corrugated near field plate theoretically prompted a sub-wavelength focal pattern with a null-to-null beamwidth of $\lambda/10$ [21]. Another approach has been based on synthesizing the focused pattern by displaced slot elements which enable spatially shifted beams in the near field [22]. The desired weighted magnetic current for each slot is realized by finding the slot dimensions in optimized iteratively full wave simulations. However, the focus in all of these approaches has been in microwave spectrum where the metal acts like a high-conductivity structure.
The main question is to how manipulate the waves in THz spectrum and provide sub-wavelength near-field focusing in optical region. Notice that, in this frequency spectrum, the metals have dispersion properties with negative permittivity parameters. And one would need to take this property into the account for a novel optical concentrator design. Recently, there have been some efforts to shape the light beams in nanometer scale providing far-field directive emission, with the use of optical Yagi-Uda plasmonic nanoantennas (functioning based on the resonant plasmonic core-shell particles) [23].

In chapter 2, we will use the same strategy, but for shaping the light in the near-field region establishing a narrow-beamwidth pattern in the focal plane. Our formulation has this capability that we can obtain any two dimensional subwavelength focusing function as the preferred near-field pattern. Such array of plasmonic particles can be exploited as an array of optical nanoantennas manipulating the waves in the near-field region. The geometry of each concentric core-shell spherical particle, the inner and outer radii, can be tailored for the application of interest. Instead of using time-consuming and convoluted iteratively full wave simulation to design the inner and outer radii of each element, here we introduce an analytical work based on the Dipolar Mode (DM) analysis and finding the intersection of the amplitude and phase contours for the polarizability in a plane created by two independent variables, the radii ratio \(a/b\) and the normalized shell radius \(b/\lambda\) of the nanoparticles. The other point in chapter 2 is that we will find the dipole mode polarization for each element in an Inverse Scattering Problem (ISP), in which one attempts to infer the properties of the scatterer from the scattered field measured outside the scatterer [24]. In general, an ISP can be a non-linear problem and in our case nonlinearity between the polarizabilities of the elements and the sample points of the desired near field pattern can be observed. This is due to the excitation of both \(x\)- and \(y\)-directed
polarizations in a plasmonic particle. The array of plasmonic nanoparticles shapes the beam of the dipole source excitation located at the center. The dipole moments with general polarizations are induced on each element so that we have an array of dipoles where by tailoring the geometry of each element the required optical near field concentration is established.

Choosing plasmonic particles as the array elements in our work is due to the fact that plasmonic materials have extreme interactions with the electromagnetic waves in optical regime. Designing and fabricating nano-antennas by using plasmonic particles have had a great development in recent years [25-27]. The frequency response of the amplitude of the polarizability of a plasmonic particle can possess a very high peak even though the size of the particle is very small in comparison with the wavelength [23]. The amplitude and phase of the polarizability have significant variations around the resonant frequency. Hence, for the concentric core-shell nano plasmonic particle in which the core has a positive permittivity and the plasmonic shell has a negative permittivity, by changing \((a/b)\) and \((b/\lambda)\) wide-range amplitude and phase of the polarizability can be obtained. This property of the concentric core-shell nano plasmonic particle is of great advantage when one uses it as an element in the array configuration.

1.2. Metamaterials Comprising of Junctions of Wires

In chapter 3, we introduce a set of Macro Basis Functions for efficient representation of the currents induced on elements comprising of junctions of wires. The use of half-triangular MBFs near the junction of a metallic cross-shaped element, established in this chapter, is very useful to study a more complicated case in which the plasmonic nanorod scatterer is considered (the
subject of chapter 4), where similarly half-triangular MBFs can model the non-zero currents efficiently at the two ends.

Tripoles and Cross-shaped elements, comprising of junctions of wires or strips, are frequently used as building blocks for artificial dielectrics such as metamaterials, Electromagnetic Bandgaps (EBGs), and Frequency Selective Surfaces (FSS), and an efficient numerical analysis of these structures is often desired [28,29]. The Characteristic Basis Function Method (CBFM) [30-32] has been found to be a time- and memory-efficient technique for analyzing either the isolated or array-type problems. Solving the problem of scattering by an isolated element using a relatively small number of MBFs to represent the induced current, regardless of the angle of incidence is an essential step in the application of CBFM. The use of the MBFs helps to substantially reduce the size of the associated matrix in the Method of Moments (MoM) formulation, as compared to the conventional formulation based on sub-domain basis functions. In chapter 3, it will be shown that only a 3×3 matrix is adequate for the representation of the induced current on the cross-shaped element, regardless of the angle of incidence of the incident plane wave. Another attribute of these basis functions is that the fields radiated by them can be expressed in closed forms. Furthermore, the three MBFs are chosen such that Kirchhoff Current Law (KCL) is automatically satisfied at the junction of the cross, and the use of these MBFs obviates the needs to handle fictitious singularities of the electric field generated by the triangular (sinusoidal) BFs at the junction. The proposed formulation leads to a well-conditioned 3×3 matrix, whose generation does not require the need to deal with the singularities of any Green’s function. We show that the results generated by using the present approach agree very well with those given by FEKO, which utilizes thin-wire modeling in the context of conventional MoM even near the resonance where
the current changes rapidly with frequency. The computational memory and time are reduced significantly.

1.3. Characterizing the Optical Performance of Plasmonic Nanorod Antennas

The goal of chapter 4 is introducing an efficient, fast and accurate technique to characterize the optical performance of plasmonic nanorod antennas comprising of Drude materials that have negative permittivity values and are dispersive as well. Conventional EM simulation techniques are often inaccurate or highly time-consuming and memory-intensive to run and, hence, a robust computational method that can efficiently model such structures is highly desired. The challenge is to accurately model the surface plasmon mode along the rod of thin cross-section, which requires a fine meshing to generate accurate solutions, and this, in turn, renders them computationally intensive. A number of publications [33-38] have addressed the problem of scattering by thin dielectric rods, but they have limited their attention to those with positive epsilon. Typically, such problems are formulated by using Surface or Volume Integral Equations (SIEs or VIEs) [35-38]; however, the large aspect ratio of the rod (length/cross section), requires a relatively large number of unknowns when the problem is solved by the Method of Moment (MoM) with small pulse Basis Functions (BFs). Another important issue in the application of the SIE to the problem of a thin rod is that the resulting matrix equation is ill-conditioned [37]. Difficulties also arise when we use alternative numerical techniques such as Finite Difference Time Domain (FDTD) or the Finite Element Method (FEM), since both of them require the use of a fine mesh when analyzing thin rods [39-40]. We note that similar challenges also exist when we attempt to characterize Carbon Nanotubes (CNTs), for which the ratio of the length to cross-section is considerably larger, by orders of magnitude [41], and it, too, presents a considerable
challenge when we attempt to model it accurately and efficiently. While the objective of chapter 4 is to develop accurate and efficient numerical techniques for solving the problem of scattering by plasmonic nanorod antennas, the methodology developed is useful for CNT-based devices as well. The key to saving computational time as well as memory is to employ a physics-based approach that utilizes MBFs, and closed form expressions for the fields radiated by these BFs, in the context of MoM, to generate a relatively small matrix equation which characterizes the problem at hand accurately as well as efficiently.

The MBFs are chosen to be piecewise sinusoidal functions and we show how we can generalize the closed form expressions presented in [42], and how we utilize a combination of the full and half piecewise sinusoidals to model plasmonic nanorod antennas that require both the longitudinal and transverse MBFs. We are able to realize considerable savings in both time and memory, by orders of magnitude, by taking advantage of the fact that we can derive closed-form expressions for all of the macro basis functions needed to characterize the plasmonic nanorods. In addition, in contrast to the conventional MoM formulation based on the use of Green’s functions, the proposed method requires no singularity extraction.

1.4. Scattering Analysis of Arrays of Plasmonic Nanorod Antennas

Chapter 5 is about the optical performance of doubly periodic array of plasmonic nanorod antennas illuminated by an obliquely incident planewave. Arrays of plasmonic antennas demonstrate interesting physical attributes and find a wide range of applications in photonics. Arrays of hetero-structure gold nanorods loaded with poly(3-hexylthiophene) (P3HT), an electronically active semiconductor [43], can concentrate the light in the nanoscale gap between
the two antenna arms [44]. One-dimensional arrays of plasmonic nanoparticles have been reported to operate as optical waveguides supporting different guided modes with different polarization properties [45]. Array of rectangular gold nanorod antennas surrounded by an insulating SiO$_2$ region and deposited on a semiconductor interface can act like a Schottky diode to generate hot electron-hole pairs, resulting in a photocurrent [46]. It has been demonstrated in [47] that nano-optical Yagi-Uda antennas, comprising of plasmonic nanorods can both enhance and direct the interaction of a single quantum emitter with electromagnetic fields. Another interesting example that is worth mentioning is the immobilization of bacteria at designated positions in space to study their metabolism without damaging them by utilizing an array of plasmonic nanoantennas that produces strong gradients of light intensity for the trapping mechanism [48].

Scattering analyses of arrays of plasmonic nanorods comprising of dispersive and negative-permittivity materials carried out by using conventional EM-simulation packages are often either inaccurate or highly time- and memory-consuming. In the context of MoM, grating-type problems are most commonly formulated by using the Periodic Green’s Function (PGF) [49]. However, the PGF is usually expressed in the form of an infinite series, whose evaluation may suffer from the problem of slow convergence [50,51]. To mitigate this problem, various acceleration techniques such as Poisson’s summation and Kummer’s decompositions [52], Shanks’ transformations [53], $\rho$-algorithm [54], Ewald’s and Veysoglu’s transformations [55,56], etc., have been applied to accelerate the convergence of the relevant series arising in the PGF formulation.

Thus, we face two main challenges when attempting to solve the problem of the array of plasmonic nanorods: first, how to model the elements (especially thin elements with small
features) in the unit-cell by using as few unknowns as possible; and, second, how to address the issue of slow convergence for the PGF. To address the first challenge, macro BF (MBF) method [57-59], which uses high-level BFs, is employed to model the induced current with few unknowns. For the scattering problem involving thin plasmonic nanorods, employing the MBF technique results in a small-size and well-conditioned matrix equation. We take advantage of this by first solving a single-element problem efficiently utilizing the MBF approach as illustrated in the organizational flowchart, shown in Fig. 1-1. The number of unknowns can be further reduced employing Characteristic BFs (CBFs) that are higher-level MBFs [30]. The CBFs are calculated via a Singular Value Decomposition (SVD) procedure applied to the previously obtained MBFs for the isolated element by using different incident fields with different wave vectors and polarizations. This step, depicted as step-2 in Fig.1-1, serves to remove the redundancy of the MBFs. Next, to address the problem of slow convergence encountered when using a PGF-based formulation, we follow a different procedure that simulates relatively small-size truncated arrays and derive a small-size matrix equation by using Galerkin’s testing on the central element. Furthermore, we take advantage of the fact that the shape of the macro-CBF, comprising of a linear combination of the CBFs, remains essentially unchanged and its level only fluctuates as the size of the truncated array is increased. This fact can obviate the need to compute the electric field due to relatively large number of elements in the large truncated array. To find the shape of the macro-CBF we solve a relatively small size matrix equation associated with a small truncated array. This step, which is step-3 in the flowchart shown in Fig. 1-1, can be carried out computationally efficiently. Next, to determine the level of the macro-CBF, we take advantage of the rapid convergence of the Galerkin integral when performed in the spectral domain by using the Parseval theorem. We show that the convergence of the weight coefficient of composite-
CBF, i.e., the solution of the finite array problem, is fast and does not have the oscillatory behavior as do the results when the problem is solved in the spatial domain. Following this step, which is step-4 in Fig. 1-1, we go on to obtain closed form formulas for the reflection and transmission coefficients by finding the contribution of the visible Floquet mode component of the scattered field in the spectral domain, which is step-5 in Fig. 1-1.

To summarize, the principal contributions of chapter 5 are three: first, we minimize the number of unknowns in the array problem by using CBFs, which results in a small-size and well-conditioned matrix equations; second, we obviate the need for time-consuming evaluation of PGFs by finding the shape of the final current, which we obtain by solving a relatively small truncated array and also find the weight coefficient of the final current by taking advantage of the fast convergence of the Galerkin’s integral in the spectral domain; and, third, we find closed-form formulas for reflection and transmission coefficients for an obliquely incident plane-wave. We validate our method by using the FDTD technique which requires considerably more runtime (typically more than two orders of magnitude). Finally, we mention that the formulation developed in chapter 5 is a general recipe for solving the problem of scattering by periodic structures, e.g., metamaterials, and by arrays of Carbon Nano-Tubes (CNTs) with large aspect-ratios [41].
1.5. Finite Clusters of Plasmonic Nanorods

In chapter 6, we formulate and investigate the optical performance of finite arrays of plasmonic nanorod antennas in randomly tilted disordered and Fibonacci configurations. Although a wide range of applications of two dimensional finite arrays of plasmonic nanorods has been demonstrated recently [10,48], an efficient formulation that quantifies the optical performance of such arrays has not yet been investigated. There is significant interest to be able of characterizing the physics of finite arrays of nanoantennas which are not necessarily periodic, due to the novel phenomena that one can achieve such
as multi-band or wideband results [60,61]. In chapter 6, we apply a powerful model based on CBFM to accurately characterize the optical performance of such arrays, considerably fast and efficient. The effect of small random rotation around the centroid of the nanorods, an uncontrollable disorder, is studied. The formulation is also employed to investigate the electromagnetic response of the Fibonacci plasmonic quasi-lattice comprising of two different nanorods with two different lengths.
Chapter 2

Array of Plasmonic Particles Enabling Optical Near-Field Concentration

The main idea of this chapter is to design an array of core-shell plasmonic nanoparticles manipulating a desired near-field focusing pattern in optical spectrum. The interactions between the array elements are formulated by using Dyadic Green’s Function (DGF) analysis and by employing the closed-form formula for electric polarizability of each plasmonic particle (Dipolar Mode (DM) approach). The point matching technique is applied to optimize the plasmonic array field performance as close as to the desired near-field pattern. The final equation for finding the polarizability of each element will be a system of non-linear equations that can be solved successfully by Levenberg-Marquardt technique. Controlling the inner and outer radii of each element using magnitude and phase contours of polarizability demonstrates a near-field subwavelength concentration. The accuracy of our theoretical model is successfully compared with a full-wave numerical analysis using CST commercial software. Interesting physical features for the optical near-field engineering are illustrated.
2.1. Formulation: Step-by-Step Design Process

Fig. 2-1(a) depicts the configuration for an array of dielectric-plasmonic particles located at $z=0$ plane. The array has $N = M^2 - 1$ concentric elements, where $M$ is the number of elements along the row and column in the geometry (shown in Fig. 2-1(a)). The excitation is located at the center and is oriented along the $y$, which its performance must be shaped in the focal plane by using array elements. The unit-cell sizes along the $x$ and $y$ directions are considered to be $d_x$ and $d_y$, respectively. Here, for the sake of simplicity a square unit-cell with $d_x = d_y = d$ is assumed. The configuration of each element is depicted in Fig. 2-1(b). Each element is a concentric core-shell spherical particle with the inner and outer radius of $a$ and $b$, respectively. The core is a dielectric material with positive permittivity $\varepsilon_1$ and the shell is made of a plasmonic material with negative and dispersive permittivity $\varepsilon_2$. The objective is to find the pair $(a,b)$ for each element to engineer a desired pattern for $y$-component of the electric field, $E_{y,des}$, at focal plane, $z=L$. This goal will be realized through an outlined step-by-step design process describing below. It is evident that any other component of the electric or magnetic field can also be tailored with the proper array of plasmonic particles. Notice that our problem can in fact be considered as an Inverse Scattering Problem (ISP) in which the scattered field by the elements (or scatterers) is given in one plane (focal plane), and the geometry of the scatterers must be determined. During the design process, this ISP is turned out to be a non-linear problem due to the coupled induced polarizations for the plasmonic nanoparticles.

The first step in the design approach is to obtain the dipolar mode equations, which is to find the $x$- and $y$-polarized electric dipole moments induced on each plasmonic element. Since the array elements have subwavelength sizes, from Mie theory, one can approximate the n’th plasmonic particle with the electric dipole moment $p_n$ and the polarizability $\alpha_n$ [7,62]. The dipole mode approximation is valid as long as the size of particles is small and further they are not in the near-touching zone where higher order
modes can be generated [63,64]. The design in this chapter will be in the region that the electric dipole mode is sufficient to represent the physics [65,66] (the diameter of the particles (2b) is less than 0.1λ and their surface to surface spacing is larger than 0.05b). Obviously, utilizing multipole expansion one can provide more accurate results when the distances between the particles are very small and in touching-zone. This requires an extensive modeling and optimization. Here, a dipole mode approximation is used.

For the n’th plasmonic element, one can then assume $p_n = \alpha_n E_n$, where $E_n$ is the total electric field radiated by all other elements and the source. The vector dipolar mode equation can be expanded in two scalar equations as below

$$p^n_x = \alpha_p \left( \sum_{m=1, m \neq n}^{N} (G_{xx, z=0}^{nn} p^n_x + G_{xy, z=0}^{nn} p^n_y) + G_{xy, z=0}^{n0} P_{source} \right),$$

(2.1a)
\[ p_y^n = \alpha_n \left( \sum_{m=1, m \neq n}^{N} (G_{yy,z=0}^{nm} P_y^m + G_{yy,z=0}^{nm} P_y^m) + G_{yy,z=0}^{n0} P_{source} \right) \]  

(2.1b)

In equation (2.1), \( p_x^n \) and \( p_y^n \) are x- and y-polarized electric dipole moments at the location of n’th plasmonic element. For the dipole source at the center of the array, the electric dipole moment is \( p_{source} = \hat{y}p_{source} \). The Green’s function \( G_{wz,z=0}^{nm} \), where \( w_s \in \{xx, xy, yx, yy\} \), is the electric field component in \( w \)-direction at the location of n’th element radiated by the unit electric dipole moment along \( s \)-direction at the location of m’th element. In other word, \( G_{wz,z=0}^{nm} \) is the \( ws \)-component of the electric Dyadic Green’s Function (DGF), \( \mathbf{G}(r, r') \), where \( r \) is the location of n’th observation element and \( r' \) is the location of m’th source element. A closed form formula for the DGF is given as [67]:

\[
\mathbf{G}(r, r') = \frac{1}{4\pi\epsilon_0 R^3} \left\{ \left[ (k_0 R)^2 - jk_0 R - 1 \right] \mathbf{I} - \left[ (k_0 R)^2 - j3k_0 R - 3 \right] \mathbf{RR} \right\},
\]

(2.2)

where \( \mathbf{I} \) is the identity dyad, \( \mathbf{R} = r - r' \), \( R = |\mathbf{R}| \) and \( k_0 = \omega\sqrt{\epsilon_0\mu_0} \) is the free space wave number.

It must be mentioned that, for the array depicted in Fig. 2-1(a), there are no induced dipoles along the \( z \)-direction for the plasmonic particles. The reason is explicable by using the closed form formula of DGF given in (2.2). As is observed, DGF includes two dyads: \( \mathbf{I} \) and \( \mathbf{RR} \). Therefore for the excitation which is along \( \hat{y} \), the radiated electric field at the source plane, \( z=0 \), has two components: one is parallel to \( \mathbf{I}\hat{y} = \hat{y} \), and the other is parallel to \( \mathbf{R}(\mathbf{R}\hat{y}) \) or \( \mathbf{R} \) vector. Since we have a planar array at \( z=0 \), \( \mathbf{R} \) is in \( x-y \) plane and does not include any \( z \)-component, that is why there is no \( z \)-polarized induced dipole. It is obvious that if there is an array of plasmonic particles over a curved surface, let us say a paraboloid or a sphere, then \( \mathbf{R} \) can have all the components, and as a result all the \( x \)-, \( y \)-, and \( z \)-polarized induced dipoles may exist.
Equations (2.1a) and (2.1b) introduce 2N dipolar mode equations and one can recast a compact matrix form for them as follows

\[
\begin{bmatrix}
[G_{xx,z=0}] & [G_{xy,z=0}] \\
[G_{yx,z=0}] & [G_{yy,z=0}]
\end{bmatrix}
\begin{bmatrix}
[p_x] \\
[p_y]
\end{bmatrix}
= \begin{bmatrix}
-\Psi_{x,z=0} \\
-\Psi_{y,z=0}
\end{bmatrix},
\]  

(2.3)

\( [G_{ws,z=0}] \) is a \( N \times N \) matrix, where its diagonal terms are related to the particles polarizabilities and its off-diagonal terms are obtained from the Green’s functions \( G_{ws,z=0}^{nn} \). The \( N \times 1 \) matrix \([p_s]\), \( s \in \{x, y\} \), is defined with \( m \)'th element equals to \( p_s^m \). The source dipole effect is appeared in the right-hand side, in \( N \times 1 \) matrix \( [\Psi_{ws,z=0}] \), \( w \in \{x, y\} \), which its \( n \)'th element is \( G_{ws,z=0}^{nn} \). From (2.1) and (2.3) one can readily obtain the below expressions for the diagonal terms of the \( [G_{ws,z=0}] \) matrix:

\[
G_{xx,z=0}^{nn} = G_{yy,z=0}^{nn} = -\alpha_n^{-1},
\]  

(2.4)

\[
G_{xy,z=0}^{nn} = G_{yx,z=0}^{nn} = 0.
\]  

(2.5)

Polarizabilities, \( \alpha_n \)'s and the matrix \([p_s]\) are the unknowns terms in equation (2.3), which are solved as below.

The second step in our design approach involves collocation (point matching method) to relate the required x- and y- polarized dipoles, which satisfies (2.3), to the desired electric field pattern in the focal plane. As it was discussed earlier, the plasmonic particles array is designed to provide the required two-dimensional narrow beamwidth near-field pattern for a component of the electromagnetic fields, let us say \( E_y \), at the focal plane \( z=L \). Assuming one needs to achieve desired field pattern \( f(x, y) \) as below:
\[ E_y(x, y, L) = f(x, y). \] (2.6)

One needs N point-matching equations to obtain the required polarizabilities. These required collocation equations are achieved by applying point-matching on equation (2.6) at N points. These points are chosen to be the locations of plasmonic particles in the array. The obtained equation will be as below:

\[
f_n = \sum_{m=1}^{N} \left( G_{yx,z=L}^{nm} P_x^m + G_{yy,z=L}^{nm} P_y^m \right) + G_{yy,z=L}^{n0} P_{source}.
\] (2.7)

Here \( f_n \) is the value of the desired focusing function at the location of \( n \)'th plasmonic element. In \( G_{ws,z=L}^{n,m} \), the source point is at the location of the \( m \)'th plasmonic element at \( z=0 \), and the observation point is at the focal plane, \( z=L \), which its projection on \( z=0 \) is the location of the \( n \)'th element. The compact form associated with the equation (2.7) is turned out to be:

\[
\begin{bmatrix}
G_{yx,z=L}^{n}\left[ G_{yy,z=L}^{-1} \right] [p_x] \\
G_{yy,z=L}^{-1} [p_y]
\end{bmatrix} = [f] - [\Psi_{y,x=L}].
\] (2.8)

[\( f \)] is constructed by \( f_n \) and the \( n \)'th element of \( [\Psi_{y,x=L}] \) includes the radiation of the central dipole which is equal to \( G_{yy,z=L}^{n0} P_{source} \).

The third part of this design procedure is to set up an equation only in terms of the polarizabilities, \( \alpha_n \)'s. This equation can be achieved by eliminating the electric dipole moment matrices [\( p_x \)] and [\( p_y \)] from dipolar mode equation (2.3), and point matching equation (2.8), obtaining the below matrix equation:

\[
\begin{bmatrix}
G_{yx,z=L}^{n}\left[ G_{yy,z=L}^{-1} \right] \begin{bmatrix}
G_{xx,z=0}^{-1} & G_{xy,z=0}^{-1} \\
G_{yx,z=0}^{-1} & G_{yy,z=0}^{-1}
\end{bmatrix}^{-1} \begin{bmatrix}
-\Psi_{x,z=0} \\\n-\Psi_{y,z=0}
\end{bmatrix} = [f] - [\Psi_{y,x=L}].
\] (2.9)
The recent equation is an Inverse Scattering Equation, ISE, because it relates the properties of the scattered field at \( z=L \), ([\(\mathbf{f}\)]-\(\mathbf{\Psi}_{y,z=L}\)), to the scatterers, \( \alpha_n \)'s. In this ISE, the only unknowns are the diagonal components of \( [G_{xx,z=0}] \) and \( [G_{yy,z=0}] \), which are \(-\alpha_n^{-1}\). It is of value to consider that the ISE given in (2.9), is a system of nonlinear equations in terms of \( \alpha_n^{-1} \). The inverse of the middle matrix creates the nonlinear effect. To solve this nonlinear matrix equation, there are several nonlinear solver techniques to be used [68-70]. Levenberg-Marquardt technique [70] has been found to be more appropriate for our study, and will be applied here to successfully solve the nonlinear ISE given in (2.9). A discussion about this powerful approach for solving the nonlinear set of equations is presented in Appendix I.

The final step, forth step, is to design the geometry of each concentric spherical particle which is finding the inner and outer radii \( a \) and \( b \) of each plasmonic particle, satisfying the obtained required polarizability. As discussed earlier, by full analytical Mie scattering analysis [71], the concentric core-shell particle depicted in Fig. 2-1(b) can be modeled by an induced electric dipole moment with the polarizability \( \alpha \). The higher-order terms are ignored considering the subwavelength sizes of the particles. As a result the polarizability which is the dipolar coupling between the electric field and the concentric core-shell particle is given as [23]

\[
\alpha = -\frac{j6\pi\varepsilon_0}{k_0^3} \frac{U}{U - j\mathcal{V}},
\]

where \( \mathcal{V} \) time convention is assumed throughout this chapter and \( U \) is given by

\[
U = \begin{bmatrix}
    j_1(k_1a) & j_1(k_2a) & y_1(k_2a) & 0 \\
    j_1(k_1a)/\varepsilon_1 & j_1(k_2a)/\varepsilon_2 & y_1(k_2a)/\varepsilon_2 & 0 \\
    0 & j_1(k_2b) & y_1(k_2b) & j_1(k_0b) \\
    0 & j_1(k_2b)/\varepsilon_2 & y_1(k_2b)/\varepsilon_2 & j_1(k_0b)/\varepsilon_0
\end{bmatrix}
\quad (2.11)
\]
$j_1(x)$ and $y_1(x)$ are spherical Bessel functions of the first and second kind respectively and of the first order. Moreover $\tilde{z}(x) = d(xz(x))/dx$, where $z$ can be any of $j_1$ and $y_1$. Also $k_1$ and $k_2$ are the wave numbers of dielectric core and plasmonic shell respectively. $V$ is similar to $U$, but in the forth column in the determinant, $\tilde{j}_1$ and $j_1$ should be replaced by $\tilde{y}_1$ and $y_1$, correspondingly.

As mentioned before, the core is considered to be a dielectric material, and the shell a plasmonic material with Drude dispersive model as below [29]:

$$\varepsilon_2 = \varepsilon_0 \left( 1 - \frac{\omega_p^2}{\omega(\omega - j\omega_D)} \right).$$

(2.12)

where $\omega_p$ and $\omega_D$ are the plasma and damping frequencies of the plasmonic material. Noble materials like Silver in optical regime can be used as the plasmonic shell for array elements. The numerical values for $\omega_p$ and $\omega_D$ can be achieved by fitting the experimental data of the noble metals’ permittivity to the Drude model [72]. For example at $\lambda = 620 \text{ nm}$, $\dot{\lambda} = 2\pi / k_o$, for $\omega_p = 9.121 \times 10^{15}$ and $\omega_D = 3.378 \times 10^{13}$ the permittivity of the shell will be $\varepsilon_2 = \varepsilon_0 (-8 - j0.1)$.

After obtaining the magnitude and phase of polarizability ($|\alpha|$ and $\angle \alpha$) from equation (2.9), one can determine the inner and outer radii of the plasmonic particles, or equivalently the radii ratio $a/b$ and normalized outer radius $b/\lambda$ (by plotting $|\alpha|$ and $\angle \alpha$ using equation (2.10) in a plane constructed by the two independent variables $a/b$ and $b/\lambda$ and finding the intersection of these two contours). The above methodology offers a successful design procedure to create the required plasmonic array nanoparticles for a desired near-field manipulation, as will be highlighted for a typical example in the next section.
2.2. Plasmonic Particles Concentrators

In this section, the design procedure for an array of plasmonic particles engineering the near field patterns in a specified focal plane is demonstrated. One needs to solve the nonlinear ISE equation given by (2.9) to achieve the required parameters. In all the cases studied in this section, the unit-cell size of $d = 0.1\lambda$ is considered, and the focal length $L = 0.15\lambda$ is assumed. Also, the desired pattern at $z=L$ is a two dimensional Sinc function with the null to null beamwidth of $\lambda/5$ given as below

$$f(x, y) = \frac{\sin(qx) \sin(qy)}{qx \ qy}.$$  
(2.13)

Here $q = 5k_0$ is considered to obtain a $\lambda/5$ beamwidth. The resolution enhancement is defined as $R_e = q / k_0$ (=5) [19]. The goal is to match the required near-field profile with the nulls of the Sinc function and its peak value at the main beam. The permittivity of the core and shell for the elements are $\varepsilon_1 = \varepsilon_0 (2.2 - j0.001)$ and $\varepsilon_2 = \varepsilon_0 (-8 - j0.1)$ at the operational optical wavelength $\lambda = 620 \text{ nm}$ (orange light in visible spectrum), respectively.

For the sake of simplicity and to demonstrate the physical meanings conveniently, we start with a $5 \times 5$ array of plasmonic particles. The objective is to determine the induced dipoles and the array elements configurations consequently. To achieve this, we should follow the equations derived in section 2.1. Namely, for obtaining the desired pattern (equation (2.13)), one must first obtain the required $p_x$, $p_y$, $\alpha$, and then the geometry configurations $a$ and $b$ for each element, as they are summarized in Tables 2-I - 2-IV. As obtained from Tables 2.I(a) and 2.II(a), the dominant polarization is $p_y$ (since the source is polarized along the $y$). Another observation is the phase alternation of $p_y$ between around $0^\circ$ and $180^\circ$ controlling the weighting functions.
for the field profile of each plasmonic particle, featuring the focusing phenomenon. To better understand this feature, in Fig. 2-2(a) we plot the field pattern for the $y$-polarized dipoles of the middle row in table 2-I when they have the same electric dipole moment. In Fig. 2-2(b) the performance of the dipoles with the proper weighting factors associated with the middle row in table 2-I is illustrated. Combination of these patterns will narrow the beam along the $x$-axis as is shown in Fig. 2-2(c). In this figure we also show the performance of a single dipole for the sake of comparison and to highlight the success of our focusing approach.

TABLE 2-I: Magnitude and phase of the induced dipoles along the $y$ for the array of $5\times5$ nanoparticles. (a) $|p_y|$ (b) $\angle p_y$

<table>
<thead>
<tr>
<th></th>
<th>0.23</th>
<th>0.39</th>
<th>0.42</th>
<th>0.39</th>
<th>0.23</th>
</tr>
</thead>
<tbody>
<tr>
<td>$</td>
<td>p_y</td>
<td>$</td>
<td>0.80</td>
<td>1.20</td>
<td>1.00</td>
</tr>
<tr>
<td>$\angle p_y$</td>
<td>0.23</td>
<td>0.39</td>
<td>0.42</td>
<td>0.39</td>
<td>0.23</td>
</tr>
</tbody>
</table>

TABLE 2-II: Magnitude and phase of the induced dipoles along the $x$ for the array of $5\times5$ nanoparticles. (a) $|p_x|$ (b) $\angle p_x$

<table>
<thead>
<tr>
<th></th>
<th>0.06</th>
<th>0.09</th>
<th>0.11</th>
<th>0.11</th>
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<td>p_x</td>
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<td>$\angle p_x$</td>
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<td>0.16</td>
<td>0.09</td>
<td>0.11</td>
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TABLE 2-III: Magnitude and phase of the polarizability of each of the core-shell nanoparticles for the 5×5 array.

(a) |α|/α₀ (b) ∠α (in Deg.)

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TABLE 2-IV: Geometry of each nanoparticle for the 5×5 array (a) b/λ (b) a/b

|          | 0.044    | 0.049    | 0.043    | 0.049    | 0.044    |
|          | 0.045    | 0.048    | 0.049    | 0.048    | 0.045    |
|          | 0.045    | 0.040    | 0.040    | 0.045    | 0.045    |
|          | 0.045    | 0.048    | 0.049    | 0.048    | 0.045    |
|          | 0.044    | 0.049    | 0.043    | 0.049    | 0.044    |

|          | 0.615    | 0.555    | 0.665    | 0.555    | 0.615    |
|          | 0.605    | 0.575    | 0.600    | 0.575    | 0.605    |
|          | 0.605    | 0.650    | 0.605    | 0.650    | 0.605    |
|          | 0.605    | 0.575    | 0.600    | 0.575    | 0.605    |
|          | 0.615    | 0.555    | 0.665    | 0.555    | 0.615    |
Fig. 2-2: Focusing phenomenon for the real part of $E_y$ in the focal plane ($z = 0.15\lambda$) (a) Normalized shifted beams for the identical $y$-polarized infinitesimal dipoles located at $r_{a2} = -0.2\lambda \hat{x}$ (green with circle marker), $r_{a1} = -0.1\lambda \hat{x}$ (purple with diamond marker), $r_0 = 0$ (black with solid line), $r_{a4} = 0.1\lambda \hat{x}$ (blue with pentagram line), and $r_{a3} = 0.2\lambda \hat{x}$ (red with square marker), (b) The shifted patterns multiplied by their weighting factors, $w_{a2} = 0.42 \angle 6^\circ$, $w_{a1} = 1\angle 179.7^\circ$, and $w_0 = 1\angle 0^\circ$, and (c) Subwavelength beam which is the superposition of the five weighted dipoles patterns (blue with solid line) and the pattern of a single dipole (red with circle marker).

The main challenge is next to create the dielectric-plasmonic core-shell nanoparticles array realizing the required induced dipoles. The advantage of considering core-shells is the fact that one has more flexibility in the design space. For instance in Fig. 2-3, we demonstrate $|\alpha|$ and $\angle \alpha$ in terms of $b/\lambda$ and $a/b$ which will be the design rule for achieving the required plasmonic particles. The magnitude of the polarizability $|\alpha|$ is normalized by a normalization factor $\alpha_0 = 4\pi\varepsilon_0/k_0^3$ for simplicity. A typical contour plot is shown in Fig. 2-4 that demonstrates how for example one can obtain the required core and shell radii, $(b/\lambda, a/b) = (0.043, 0.63)$, to achieve the required polarizability, $\alpha/\alpha_0 = 0.05\angle -3^\circ$. The obtained $\alpha$’s ensure the required $p_x$ and $p_y$ manipulating the near field pattern in the focal plane. It must be mentioned that not always one can achieve the exact required $\alpha$. Therefore one has to make an approximation in obtaining the required core-shell particle providing the best
closest $\alpha$ in our design space. In this case, the phase of polarizability can be changed slightly to make the two contours have an intersection point in expense of suffering from some approximation. The accuracy of this procedure is highlighted well later in this section through the demonstrated results. Note that, the outer radius of each element should be less than the half of unit-cell size i.e. $b < d/2$. In our case $d/(2\lambda) = 0.050$ and in Table 2-IV(a), the constraint $b/\lambda < 0.050$ is satisfied for all the plasmonic particles.

Fig. 2-3: (a) Normalized amplitude of the polarizability, $|\alpha|/\alpha_0$ in terms of a/b and b/\lambda. (b) The phase performance, $-\angle\alpha$.

Fig. 2-4: Design-rule curve for the geometry realization of the core-shell plasmonic particles, using polarizability magnitude and phase contours.
Let us now investigate the results for the design of a $5\times5$ plasmonic particles array design. Fig. 2-5(a) shows the required Sinc function pattern in the focal plane and obviously our goal is to ensure the plasmonic particles can manipulate the near field in the focal plane as close as possible to the Sinc function. The merit function is the nulls of the Sinc (2 at each side) and its peak at the main beam (since we have 5 spheres). Using more number of points can provide a better matching to the desired field profile (as will be investigated next). For the sake of comparison, the field pattern of a single dipole in the focal plane is also calculated in Fig. 2-5(b). The field performances for the array of induced dipoles and their approximated values (modeled by plasmonic nanoparticles) are plotted in Figs. 2-5(c) and 2-5(d), respectively. The approximated result refers to the case in which the phase of polarizability can be changed slightly to make the two polarizability phase and magnitude contours have an intersection point. As observed, our designed plasmonic particles can successfully engineer the near field in the required focal plane and enable the narrow-beam performance. To demonstrate better the field performance of the array, the two-dimensional plots along the x and y axes are also demonstrated in Figs. 2-6(a) and 2-6(b), respectively. As observed from these figures, we are able to narrow the beam in both x and y directions with the use of our designed core-shell dielectric plasmonic particles. The results derived for the exact induced dipole array successfully follow the nulls of the desired Sinc function. The approximated core-shell dielectric-plasmonic particles performance is slightly deviated from the exact model result; however, still a narrow beam characteristic is successfully developed.
Fig. 2-5. The magnitude of normalized $E_y$ at the focal plane $z = 0.15\lambda$ for (a) Desired Sinc function (b) A single infinitesimal dipole. (c) Exact polarizabilities $5\times5$ array performance found by Levenberg-Marquardt technique, and (d) The approximated polarizabilities $5\times5$ array model.
Fig. 2-6. The magnitude of normalized $E_y$ at the focal plane $z = 0.15\lambda$ for the $5 \times 5$ array obtained by using the exact polarizabilities (blue with squarer marker), by using approximated polarizabilities (green with circle marker), for a single dipole along $y$ at the origin (red with diamond marker), and for a desired sinc pattern (purple solid line). (a) Along $x$-axis (b) Along $y$-axis.

To validate the accuracy of the proposed theoretical model, we apply a full-wave analysis based on CST commercial software to characterize the performance of the array of $5 \times 5$ dielectric-plasmonic core-shells. The results are shown in Fig. 2-7 along the $x$ and $y$ directions. A good comparison is illustrated. The slight difference is due to the fact that in our modeling we approximate each nanoparticle with a dipole located at its center, while in CST the whole spherical particle is modeled. Considering the near-field calculation, this slight difference is very much reasonable. A relatively good comparison is achieved, realizing beam focusing in the focal plane. Notice that in CST analysis the size of the dipole excitation is considered around $0.05\lambda$ (in the order of outer radius of the nano-particles).
Fig. 2-7. The magnitude of normalized $E_y$ at the focal plane $z = 0.15\lambda$ for the $5 \times 5$ array obtained based on our theoretical model (green with circle marker) and using full wave CST simulation (brown solid line). (a) Along $x$-axis (b) Along $y$-axis. A relatively good comparison is illustrated.

Increasing the number of array elements allows achieving a better near field performance in regard of narrowing the beam. Figs. 2-8(a) and 2-8(b) obtain the three-dimensional plots for the exact and approximated $11 \times 11$ polarizabilities designs, respectively. The successful beam narrowing is demonstrated. The two-dimensional plots are shown in Fig. 2-9. It is obtained that the $11 \times 11$ array design has a better characteristic than that of the $5 \times 5$ case (Fig. 2-6). One can see the null-to-null beamwidth for the $11 \times 11$ array along the $x$ direction is about $0.36\lambda$ and along the $y$ direction is about $0.2\lambda$. The desired null-to-null beamwidth for both the $x$ and $y$ directions is $0.2\lambda$. We need to mention that from all the obtained near-fields in the focal plane, one can observe narrowing the beam along the $y$ axis is more successful than along the $x$-axis. This is because of having narrower beam for the dipole excitation itself along the $y$-direction. Thus, there is more challenge to manipulate and focus the beam along the $x$-direction. One
solution to this will be if one uses more number of dielectric-plasmonic elements along the \( x \) direction, so that the beam can be narrowed to our interest in this direction.

Fig. 2-8. The magnitude of normalized \( E_y \) in the focal plane \( z = 0.15\lambda \) for the \( 11\times11 \) array of plasmonic core-shell particles. (a) Exact polarizabilities array performance, and (b) Approximated polarizabilities model.

Fig. 2-9. The magnitude of normalized \( E_y \) at the focal plane \( z = 0.15\lambda \) for the \( 11\times11 \) array obtained by using the exact polarizabilities (blue with square marker), by using approximated polarizabilities (green with circle marker), for a single dipole along \( y \) at the origin (red with diamond marker), and for a desired Sinc pattern (purple solid line) (a) Along \( x \)-axis (b) Along \( y \)-axis. The \( 11\times11 \) array can narrow the beam more successfully than the \( 5\times5 \) case (obtained in Fig. 2-6).
The concept and formulations developed in this chapter allow successful optical near field engineering with the use of array of plasmonic particles that can be uniform or non-uniform depending on the application of interest. Although a simple planar (rectangular) array is utilized here, where the elements are placed along a rectangular grid [73], our formulation can be applied to other general arrays configurations enabling state-of-the-art optical applications. Other particles configurations such as multi-shells of different materials (increasing the design flexibility), and arrangements in unique patterns, can demonstrate desired physics.
Chapter 3

Macro Basis Functions for Solution of Scattering from Elements Comprising of Junctions of Wires

In this chapter we introduce a set of macro basis functions for efficient representation of the currents induced on elements comprising of junctions of wires. The use of these functions leads to a relatively small and well-conditioned matrix, only a $3 \times 3$ size for a cross-shaped element, for instance. Furthermore, an important advantage of using these basis functions is that the fields they generate can be expressed in close forms, circumventing the need to use the Green’s function and to handle the singularity problem associated with these functions. We show that by taking advantage of these two features we can solve the scattering problem, in an accurate and numerically efficient manner. The results are presented and compared well with those generated by a commercially available EM simulation software package. Our proposed method is accurate and fast. The computational time is reduced by orders of magnitude.
3.1. Problem Definition and MBFs Formulation

Fig. 3-1 depicts a cross-shaped antenna element, with two equal arms of length \( L \) and radius \( a \), illuminated by an obliquely incident plane wave  \( \mathbf{E}^{\text{inc}} = E_0 e^{i k \mathbf{r}} \). For the sake of simplicity we assume the cross is PEC, however, our method is general and can be applied to dielectric and frequency dispersive materials based scatterer as well. Three Macro Basis Functions (MBFs) namely, \( S_a \), \( S_b \) and \( S_c \), shown in Fig. 3-2, are chosen to represent the induced current. We refer \( S_a \) and \( S_b \) as common MBFs along x- and y-axis, respectively, and \( S_c \) as the differential MBF. The mathematical expression for the common MBF is \( S_a(x) = \sin[k(L/2-|x|)] \), along the x, where \( k = 2\pi/\lambda \), and \( S_b(y) \) has the corresponding expression with y replacing x. The differential MBF takes the form \( S_c(r) = S_{c1}(x) - S_{c2}(y) \) (see Fig. 3-2(c)), where \( S_{c1} \) (\( S_{c2} \)) is the same as \( S_a \) (\( S_b \)) and its domain is \( 0<x<L/2 \) \( (0<y<L/2) \).

![Fig. 3-1: A cross-shaped antenna in x-y plane illuminated by an obliquely incident plane wave.](image)
It is interesting that the differential MBF automatically satisfies KCL. Hence, for a general oblique incidence the induced current, $I(r)$ can be expressed as a superposition of the introduced MBFs, as follows

$$I(r) = I_a S_a(r) + I_b S_b(r) + I_c S_c(r),$$  \hspace{1cm} (3.1)

where $I_a$, $I_b$ and $I_c$ are three unknowns to be determined.

For the full triangular sinusoidal MBF along $z$, depicted in Fig. 3-3, including the two right- and left-half MBFs, we can find in [42] a closed form representation for the electric field radiated from the full triangular MBF with the length of $2H$. We next extend the above point for the two half triangular MBFs. Using the cylindrical coordinate system $(\rho, \varphi, z)$ we can write:
\[ G_{zz}^{MBF,Right} = -\frac{j\eta}{4\pi} \left[ f - z \sin(kH) \frac{e^{-jkR_0}}{kR_0^3} \right], \tag{3.2} \]

\[ G_{\rho\rho}^{MBF,Right} = \frac{j\eta}{4\pi\rho} \left\{ zf + \sin(kH) \rho^2 \left( \frac{e^{-jkR_0}}{kR_0^3} - H \frac{e^{-jkR_1}}{R_1} \right) \right\}, \tag{3.3} \]

where \( G_{ss}^{MBF,Right}, s \in \{z, \rho\}, \) is the s-component electric field radiated by the right MBF shown in Fig. 3-2, \( R_i = \sqrt{\rho^2 + (z-H)^2} \), \( R_0 = \sqrt{\rho^2 + z^2} \), and \( f \) is given by as

\[ f = \frac{e^{-jkR_1}}{R_1} - \frac{e^{-jkR_0}}{R_0} \left( \cos(kH) + j \frac{z}{R_0^2} \sin(kH) \right). \tag{3.4} \]

The fields radiated by the left MBF shown in Fig. 3-2, is the same as those for the right one, with H replaced by –H. Equations ((3.2)-(3.4)) can now be employed to find the electric fields radiated by the MBFs, \( S_a, S_b \) and \( S_c \), for the cross problem.

To solve the scattering problem at hand, we need to impose the Boundary Condition (BC) on the surface of the cross, say at \( z=a \), where we enforce \( E^{scat} = E^{inc} \). For the u-MBF shown in Fig. 3-1, \( u \in \{a,b,c\} \), one can write the BC as

\[ \sum_{w=a,b,c} I_w E^{aw} = -E^{inc}_u, \tag{3.5} \]

where \( E^{aw} \) is the component of electric field along the axis of the wire included in the domain of \( u \)-MBF radiated by the \( w \)-MBF.

Fig. 3-4 shows the magnitude of \( |E^{aw}| \) on the x-branch of the cross, \( u=a \), due to \( a \)-, \( c1 \)-, \( c2 \)-, and \( c \)-MBFs. We use an identical scale for all the plots in Fig. 3-4, to facilitate comparison of the magnitude of the electric fields radiated by MBFs. The cross is assumed to be \( \lambda/2 \) in length and its radius is \( a=\lambda/100 \) at the frequency of 1 GHz. It is interesting to note that although the electric fields due to the half \( c1 \)- and \( c2 \)-MBFs have the fictitious singularities near the origin
(see Figs. 3-4(b) and 3-4(c)), they are eliminated when we construct the field radiated by the differential MBF shown in Fig. 3-4(d), and this is the second advantage of using the differential MBF. We also note that, owing to procedure of the symmetry, the electric field due to the \( b \)-MBF on the domain of \( a \)-MBF is zero, i.e., \( E_{ab} = 0 \).

\[
\begin{align*}
\text{(a)} & \\
\text{(b)} & \\
\text{(c)} & \\
\text{(d)} & 
\end{align*}
\]

Fig. 3-4: Magnitude of the radiated electric field on the domain of \( a \)-MBF due to (a) \( a \)-MBF, (b) \( c_l \)-MBF, (c) \( c_2 \)-MBF (d), \( c \)-MBF.

Applying the Galerkin’s testing on (3.5), we can derive the 3x3 matrix equation which is

\[
\begin{bmatrix}
Z_{aa} & 0 & Z_{aa}/2 \\
0 & Z_{aa} & -Z_{aa}/2 \\
Z_{aa}/2 & -Z_{aa}/2 & 2Z_{cc} \\
\end{bmatrix}
\begin{bmatrix}
I_a \\
I_b \\
I_c \\
\end{bmatrix}
=
\begin{bmatrix}
V_a \\
V_b \\
V_c \\
\end{bmatrix},
\]

(3.6)

where

\[
V_a = -\int_{-L/2}^{L/2} S_a(x) E_{inc,x}^a (x, y = 0, z = a) dx,
\]

(3.7)
As can be seen from (3.12) and (3.13), the current is located on the axis of each branch and the observation point is placed on the surface of the wire. Hence, the minimum distance between the source and the observation point is equal to the radius $a$ and, hence, there are no singularities associated with the integrands in (3.12) and (3.13). For $L=\lambda/2$ and $a=\lambda/100$, we obtain $Z_{aa}=-73 - j39$ and $Z_{ce}=-20-j4.5$ ($f=1$ GHz). Also, we find that the $Z$-matrix is very well-conditioned, and its condition number is only 16.

3.2. Simulation and Numerical Results

Let us assume that the cross antenna is illuminated by an obliquely incident plane wave $E^{inc} = E_0 e^{-jkr}$, with $E_0 = (\hat{x} + 2\hat{y} + 3\hat{z})/\sqrt{14}$ and $(\theta=36.7^\circ \text{ and } \phi=63.4^\circ \text{ in spherical coordinates})$ and $k = (3\hat{x} - 3\hat{y} + \hat{z})/\sqrt{19}$ ( $\theta=76.7^\circ \text{ and } \phi=-45^\circ$). In all the results, it is assumed that the center frequency is $f_0=1$ GHz ($\lambda_0=30$ cm), $L=\lambda_0/2$, and $a=\lambda_0/100$. Fig. 3-5 shows the magnitude of currents along x- and y- branches of the cross antenna which can be obtained by solving the 3×3 matrix equation given in (3.6). We observe the current magnitude as well as the current jump are very sensitive functions of frequency in the neighborhood of resonance (Note: The legend in Fig. 3-5 is $\Delta f/f_0=(f-f_0)/f_0$) According to Fig. 3-5, the resonant frequency for which the magnitude of the current is maximum is $f_{res}=1.05 f_0$, 5% above the central frequency. To gain a better insight
about how the induced current varies rapidly around the resonant frequency, we define the following variables

\[
I_{\text{com-}x} = |I(x = 0^-)|, \quad I_{\text{com-}y} = |I(y = 0^-)|, \quad I_{\text{jump-}x} = |I(x = 0^+) - |I(x = 0^-)||, \quad I_{\text{jump-}y} = |I(y = 0^+) - |I(y = 0^-)||
\]

(3.14) (3.15) (3.16) (3.17)

Fig. 3-5: Magnitude of the induced current on the cross antenna by using the introduced 3x3 matrix, for a frequency range around the central frequency. (a) Along the x-arm, (b) Along the y-arm.

We can see from Fig. 3-5 that the resonant frequency is 5% above \( f_0 \), for which \( I_{\text{com-}x} \) and \( I_{\text{com-}y} \) are maximum. We also observe from Fig. 3-6 that the current jump approaches a minimum near the resonance, and that the current magnitude is quite sensitive near the resonant frequency.
Next we compare our results with those obtained from the commercial software FEKO. The FEKO results for the magnitude of currents around the resonant frequency are shown in Fig. 3-7, and we note that the resonant frequency at which the current reaches a maximum is $1.03 f_0$, whereas we predicted this frequency to be $1.05 f_0$. Next in Fig. 3-8 we compare the result of 3×3 MBF technique with those of FEKO, and find out that the comparison is good. It is worthwhile to point out that the slight difference between FEKO and MBF technique can be attributed to the effective length of the wire used in FEKO.

The MBF technique is numerically very efficient, not only because it uses very small number of MBFs, but also because the availability of the closed-form expression for the fields generated by the MBFs enables us to generate the matrix equation very efficiently. The running time for all the frequencies used to generate the plots in Fig. 3-5, is just 1 second on a 2.2 GHz Intel Core(TM)2 Duo CPU machine, whereas it takes 5 minutes on the same machine for FEKO results in Fig. 3-7. This is a reduction of about 300 times.
Fig. 3-7: Comparison of the resonant results for MBF technique and FEKO. (a) $|I(x)|$, (b) $|I(y)|$, (c) Phase of $I(x)$, (d) Phase of $I(y)$.
Chapter 4

Scattering Analysis of Plasmonic Nanorod Antennas

In this chapter we introduce a versatile and numerically efficient computational technique to model the problem of scattering from plasmonic nanorod antennas. The key to achieving the numerical efficiency is to utilize Macro Basis Functions (MBFs) that taking into account the physics of the problem to reduce the size of matrix equation we need to solve. Closed form formulations are presented for computing the fields by the transverse and longitudinal MBFs that enable us to generate the required matrix elements rapidly, while ensuring that the matrix is well-conditioned. We show that the transverse and longitudinal components of polarization current and all of the components of the scattered fields can be computed very accurately by employing only a few MBFs, i.e., by solving a relatively small-size matrix equation. The accuracy of our modeling technique has been successfully demonstrated by comparing the simulation results with those derived by using the Finite Difference Time Domain (FDTD) technique, which is considerably more time-consuming than the present approach. Interesting physical phenomena
such as surface plasmon modes for polarization currents and resonance behaviors of plasmonic nanorods are illustrated.

### 4.1. Problem Formulation

Fig. 4-1 depicts a plasmonic nanorod antenna of radius $a$ and length $L$ located along the $z$-axis and illuminated by an obliquely incident plane wave as $\mathbf{E}^{\text{inc}} = E_0 e^{-jkr}$, where $\mathbf{k}$ is the incident wave vector and $\mathbf{r}$ is the observation vector. The permittivity of the nanorod is characterized by a frequency-dependent Drude model given by [75]

$$
\varepsilon_r = \varepsilon_{\infty} - \frac{f_p^2}{f(f - jf_d)},
$$

(4.1)

where $f_p$ is the plasma frequency, and $f_d$ is the damping frequency representing the loss. We see from Fig. 4-2 that for silver with $\varepsilon_{\infty} = 5$, $f_p = 2175$ THz, and $f_d = 4.35$ THz, the real part of the permittivity has a negative value at optical frequency of interest.
Fig. 4-2: Drude permittivity behavior of silver with $\varepsilon_{\infty} = 5, f_p = 2175$ THz, and $f_d = 43.5$ THz.

The plasmonic antenna resonates when its length is approximately half-wave in terms of the effective wavelength $\lambda_{\text{eff}}$. This is because in contrast to microwave frequencies where the incident plane wave is totally scattered by the rod, in optics the wave penetrates into the metal and gives rise to oscillations of the free-electron gas. Therefore, the plasmonic nanorod no longer responds to the free-space wavelength but to a shorter effective wavelength instead. The computation of effective wavelength can be carried out by solving the characteristic transcendental equation including the cylindrical Hankel and Bessel function or by using approximate algebraic formulas. The physical concepts of effective wavelength for an optical nanorod and the corresponded transcendental and algebraic characteristic equations were first presented in [76]. The $\lambda_{\text{eff}}$ for the silver nanorod of length $L = 300 \text{ nm}$ and radius $a = 10 \text{ nm}$ is plotted over an optical frequency range in Fig. 4-3. It should be mentioned that for plasmonic configurations the shape and the aspect ratio of structure play critical roles in dictating the resonant frequency, as has been fully investigated in [77]. Extending classic concepts of radio-frequency antenna theory to the
visible regime for the proper design and matching of plasmonic nanoantennas has been exploited in [78] and [79].

Fig. 4-3: Effective length normalized by effective wavelength over an optical frequency range for a silver plasmonic nanorod with length $L=300$ nm and radius $a=10$ nm. The effective length is equal to $L+2a$.

To solve the scattering performance we employ volume equivalent theorem [80] to replace the rod with a volume polarization current $\mathbf{J}$ radiating the scattered field $\mathbf{E}^{\text{scat}}$: 

$$j\omega\varepsilon_0(\varepsilon_r-1)(\mathbf{E}^{\text{inc}} + \mathbf{E}^{\text{scat}}) = \mathbf{J}.$$ 

(4.2)

We note that in contrast to the case of the PEC rod which only requires longitudinal currents the volume polarization current can have both the longitudinal ($z$-component) as well as transverse ($x$- and $y$-components). Since the nanorod is electrically thin, $ka<<1$, we can assume that the total polarization current vector $\mathbf{I}$ is uniformly distributed across the cross-section, i.e. $\mathbf{J} = \mathbf{I}/(\pi a^2)$. 

For the sake of simplicity, we assume that the rod has a circular cross-section, although we can
also accommodate arbitrary shapes, if desired, since in general we can write $\mathbf{J} = \mathbf{I} / A$, where $A$ is the area of the cross-section.

To model the scattering performance of the thin nanorod, we assume that the polarization current $\mathbf{I}$ exists along the axis of the rod, $(\rho = 0$ in cylindrical coordinates $(\rho, \phi, z)$) instead of working with the volume current $\mathbf{J}$. Our next step is to express $\mathbf{I}$ in terms of $N$ Macro Basis Functions (MBFs) as illustrated in Fig. 4-4. The $w$-component of $\mathbf{I}$, $I_w (w \in \{x,y,z\})$, is written as:

$$I_w(z) = \sum_{n=1}^{N} I_w^n t_n(z),$$

(4.3)

where $I_w^n$ is the unknown coefficient of the $n$'th MBF for the $w$-component of current, yet to be determined.

![Fig. 4-4: Representation of polarization current by $N$ triangular sinusoidal MBFs. The first and last MBFs are half-triangular and the rest are full-triangular sinusoidal MBFs.](image1)

The length $L$ of rod is split into $N-1$ equal segments of length $H$. Segment $#n$ extends from $z = z_n$ to $z_{n+1}$, where $z_n = -L/2 + (n-1)H$. Except for the first and last MBFs that are half triangular, other MBFs have two nulls at $z_{n-1}$ and $z_{n+1}$ and a cusp at $z_n$. For this case, one can express the $n$'th MBF as follows:

$$t_n(z) = \sin[\beta(H - |z - z_n|)] \quad z_{n-1} < z < z_{n+1},$$

(4.4)
In (4.4), the wave number associated with the current distribution is $\beta$, which is not necessarily equal to the free space wave number $k$. For a plasmonic nanorod $\beta=(2\pi/\lambda_{\text{eff}} - 4a)$ and is greater than the free space $k$ [76]. Equation (4.4) is also valid for the first and last MBFs, if we define $z_0 = z_1$ and $z_{N+1} = z_N$. The reason for using half triangles at the two endpoints of the rod is that, unlike a PEC rod for which the current is zero at the two ends, the current does not vanish at the endpoints for non-metallic wires [38].

In (4.2), the $s$-component of scattered field, $E_{s\text{scatt}}$, where $s \in \{x,y,z\}$, can be expressed by a weighted summation of the $s$-component electric field radiated by each $w$-component of the $n$'th MBF, $G_{sw,n}^{MBF}$, i.e., we can write:

$$E_{s\text{scatt}} = \sum_{w=x,y,z} \sum_{n=1}^{N} I_w^n G_{sw,n}^{MBF},$$

(4.5)

Our goal is to obtain the $G_{sw,n}^{MBF}$ in a computationally efficient manner, in order to reduce the total calculation time. With this in mind, we devote the next section to the problem of evaluating electric fields radiated by the MBFs in closed-forms.

### 4.2. Closed Form Expression for the Radiation of MBFs

Let us consider a full triangular-sinusoidal MBF including left and right half MBFs as shown in Fig. 4-5. As mentioned earlier, the current is assumed to exist only at the axis of the rod along the $z$-direction. The width of the half MBF is $H$. The $w$-component of the current is assumed to have a triangular-sinusoidal variation given by $I_w = \sin[\beta(H - |z'|)]$, where $-H < z' < H$. For the $w$-component of current associated with the right MBF, the corresponding auxiliary magnetic vector potential $A$ has only $w$-component obtained from [80]:

63
\[ A_w = \int_0^H \sin(\beta(H - z')) g \, dz', \]  
(4.6)

where \( g = \mu \exp(-jkR)/(4\pi R) \) is the scalar Green’s function and \( R=\sqrt{(z-z')^2 + \rho^2} \). It is worth mentioning that in (4.66), the wave number of current \( (\beta) \) can be different from that for scalar Green’s function \( (k) \). In the rest of formulation we assume that \( \beta \geq k \) which is the case for plasmonic nanorod.

![Diagram](image)

**Fig. 4-5:** Full-triangular sinusoidal MBF including right (orange) and left (green) MBFs. The current flows along the axis and can have all three components.

We expand \( \sin(\beta(H - z')) \) as a combination of two exponentials, namely \( \exp(\pm j\beta(H - z')) \), and introduce a change the variable, from \( z' \rightarrow -z' \) for the negative exponent, to get

\[ A_w = \frac{\mu_0}{8\pi j} \left[ \text{Int}(z, \rho; H) + \text{Int}(-z, \rho; -H) \right], \]

(4.7)

where

\[ \text{Int}(z, \rho; H) = \int_0^H \frac{\exp[-jk(R + \zeta(z'-H))]}{R} \, dz', \]

(4.8)

where \( \zeta = \beta/k \geq 1 \). To derive an efficient and robust computational model, one needs to pay special attention to the problem of deriving the expressions for electric field radiated by each MBF, which contains second order partial derivatives of auxiliary potential \( A_w \) in (4.7). If we implement such partial derivative operations in (4.8), in which the integrand is a function of observation point \((\rho, z)\), the resultant expressions contain integrals whose integrands comprise of
exp(-jkR)/R^2 and exp(-jkr)/R^3, and this in turn results in complexity of the expressions for the radiated electric field. Since we must evaluate the above integrals numerically, we can lose accuracy and lose the speed advantage of closed-form formulations. To obtain the integral in closed form, one needs to work with a formulation in which the integrand is independent of the observation point. Toward this end, we use a change of variables of \( u = k(R - \zeta(z - z')) \) to reduce (4.8) to the form:

\[
\text{Int}(z, \rho; H) = \exp[-j\beta(z - H)] \int_{k(R_0 - \zeta)}^{k(R_1 - \zeta)} \frac{\exp(-ju)}{\sqrt{u^2 + (\zeta^2 - 1)(k\rho)^2}} \, du, \tag{4.9}
\]

where \( R_1 = \sqrt{\rho^2 + (z - H)^2} \) and \( R_0 = \sqrt{\rho^2 + z^2} \), as depicted in Fig. 4-5. We can observe that if \( \zeta = 1 \), the integrand in (4.9), is not a function of the observation point. Hence, we have shown that working with the MBFs that are associated with the free space wave number can highly improve the speed and accuracy of the numerical algorithm, because with this choice of the MBFs the derivation of the electric field no longer depends on the numerical evaluation of the integrals, including those involving the first and second derivatives of the scalar Green’s function. Although this approach still requires us to numerically compute the integral containing the scalar green’s function, this can be done by employing Gaussian Quadrature Rule (GQR) [81]. Admittedly, if we employ the MBFs with effective wave numbers that are different from that of the free space wave number, we would be able to use fewer MBFs to represent the currents. However, as pointed out earlier, this would require us to calculate the integrals of derivatives of scalar Green’s function numerically, and will therefore result in loss in overall speed and accuracy. This leads us to conclude that it is more advantageous for us to use MBFs associated with free-space rather than the effective wavelength. This is especially true because, as we show later, only the \( x \)-component (y-component) of the electric field radiated by the \( x \)-
component (y-component) of the MBF, i.e., the \( xx \)-term (yy-term), requires the evaluation of an integral containing the scalar Green’s function, while all the other terms can be expressed in closed forms. In addition, we have found that only 5 MBFs for each current component are sufficient for deriving accurate and fast-convergent results. Therefore in the rest of this chapter we assume \( \zeta = 1 \). It must be also said that in the context of MoM, the BF can have any arbitrary shape \([49,82]\), for instance triangular, pulse and sinusoidal, and the weighting coefficients of each BF are found by solving a matrix equation. Finally, we point out the well-known fact (see for instance \([49]\)), that accurate solution for the current distribution can be found regardless of the choice of the BFs, though the total number of these functions will vary in general.

To find the electric field radiated by each MBF, we need to find the electric field \( \mathbf{E} \) from the vector potential \( \mathbf{A} \), by using:

\[
\mathbf{E} = \frac{\nabla \times \nabla \times \mathbf{A}}{j \omega \mu_0 \varepsilon_0}.
\]  

(4.10)

For an \( x \)-polarized MBF, the \( x \)-component of the electric field is given by

\[
E_x = \frac{-1}{j \omega \mu_0 \varepsilon_0} \left( \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) A_x.
\]  

(4.11)

The derivative of \( \text{Int} \) function can be carried out with respect to \( y \) and \( z \) to obtain:

\[
\frac{\partial \text{Int}(z, \rho; H)}{\partial y} = \frac{e^{-jkR}}{R_1(R_1 + H - z)} - \frac{e^{-jk(R_0-H)}}{R_0(R_0 - z)}
\] \hspace{1cm} \text{and} \hspace{1cm}

\[
\frac{\partial \text{Int}(z, \rho; H)}{\partial z} = -jk \text{Int}(z, \rho; H) - \frac{e^{-jkR}}{R_1} + \frac{e^{-jk(R_0-H)}}{R_0}.
\]  

(4.12) \hspace{1cm} \text{and} \hspace{1cm} (4.13)

Then, from (4.12) and (4.13), we can arrive at:

\[
\frac{\partial}{\partial y} \left[ \text{Int}(z, \rho; H) + \text{Int}(-z, \rho; -H) \right] = \frac{2y}{\rho^2} \left[ e^{-jkR} - e^{-jkR} \left( \cos(kH) + j \frac{z}{R_0} \sin(kH) \right) \right],
\]  

(4.14)
\[ \frac{\partial}{\partial z} \left[ \text{Int}(z, \rho; H) + \text{Int}(-z, \rho; -H) \right] = -jk \left[ \text{Int}(z, \rho; H) - \text{Int}(-z, \rho; -H) \right] + j2 \sin(kH) \frac{e^{-jkR_0}}{R_0}. \]  

(4.15)

Taking the derivative with respect to \( y \) and \( z \) from (4.14) and (4.15) yields:

\[ \frac{\partial^2}{\partial y^2} \left[ \text{Int}(z, \rho; H) + \text{Int}(-z, \rho; -H) \right] = \]
\[ \frac{2(x^2 - y^2)}{\rho^4} \left[ e^{-jkR_1} - e^{-jkR_0} \left( \cos(kH) + j \frac{z}{R_0} \sin(kH) \right) \right] \]
\[ - j \frac{2k y^2}{\rho^2} \left[ e^{-jkR_1} - \frac{e^{-jkR_0}}{R_0} \left( \cos(kH) + j \frac{z}{R_0} \sin(kH) \right) \right] \]
\[ - z \sin(kH) \frac{e^{-jkR_0}}{k R_0^3} \],

(4.16)

\[ \frac{\partial^2}{\partial z^2} \left[ \text{Int}(z, \rho; H) + \text{Int}(-z, \rho; -H) \right] = \]
\[ -k^2 \left[ \text{Int}(z, \rho; H) + \text{Int}(-z, \rho; -H) \right] \]
\[ + j2k \left[ e^{-jkR_1} - \frac{e^{-jkR_0}}{R_0} \left( \cos(kH) + j \frac{z}{R_0} \sin(kH) \right) \right] \]
\[ - z \sin(kH) \frac{e^{-jkR_0}}{k R_0^3} \],

(4.17)

Next we add (4.16) and (4.17), and substitute them in (4.11), to get the \( x \)-component of the electric field radiated by the \( x \)-component of the right-half triangular sinusoidal, \( G_{xx}^{MBF, \text{Right}} \), which reads:
We represent the $s$-component of the electric field due to the $w$-component of the right MBF with $G_{sw}^{MBF, Right}$. Because of reciprocity, $G_{sw}^{MBF, Right} = G_{ws}^{MBF, Right}$. $G_{yx}^{MBF, Right}$ and $G_{zx}^{MBF, Right}$ can be obtained in similar manner and they are:

\[
G_{yx}^{MBF, Right} = \frac{\eta y}{4\pi k \rho^2} \left[ \frac{2}{\rho^2} \left( e^{-jkR_i} - e^{-jkR_0} \right) \left( \cos(kH) + j \frac{z}{R_0} \sin(kH) \right) \right] 
+ jk \left[ \frac{e^{-jkR_i}}{R_1} - \frac{e^{-jkR_0}}{R_0} \left( \cos(kH) + j \frac{z}{R_0} \sin(kH) \right) - z \sin(kH) \frac{e^{-jkR_0}}{kR_0^3} \right],
\]

\[
G_{zx}^{MBF, Right} = \frac{j\eta x}{4\pi \rho^2} \left[ \frac{z}{\rho^2} \left( e^{-jkR_i} - e^{-jkR_0} \right) \left( \cos(kH) + j \frac{z}{R_0} \sin(kH) \right) \right] 
+ \sin(kH) \rho^2 \frac{e^{-jkR_0}}{kR_0^3} - H \frac{e^{-jkR_0}}{R_1^3} \right].
\]

Next, we obtain, $G_{yy}^{MBF, Right}$, and $G_{zy}^{MBF, Right}$, from (4.18) and (4.20), respectively, with replacing $x$ with $y$. The only term that still remains to be derived is $G_{zz}^{MBF, Right}$. Using (4.10), the $z$-component of the electric field can be written:

\[
E_z = \frac{-1}{j\omega \mu_0 \epsilon_0} \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) A_z,
\]

(4.21)
with $A_z$ given by (4.7). The double derivative of $\text{Int}$ function with respect to $y$ is given in (4.16).

To compute $\frac{\partial^2 A_z}{\partial x^2}$, we replace $y$ by $x$ in (4.16), and add the two double derivatives in (4.21), to get:

$$G_{zz}^{\text{MBF,Right}} = -\frac{j \eta}{4\pi} \left[ e^{-jkr_L} - \frac{e^{-jkr}}{R_0} \left( \cos(kH) + j \frac{z}{R_0} \sin(kH) \right) \right. \\
- \left. z \sin(kH) \frac{e^{-jkr_{R_H}}}{kR_{0_H}} \right].$$

(4.22)

It can be shown that the radiation of the left MBF, depicted in Fig. 4-5, is equal to that of the right when $H$ is replaced by $-H$, i.e.,

$$G_{sw}^{\text{MBF,Left}}(z, \rho; H) = G_{sw}^{\text{MBF,Right}}(z, \rho; -H).$$

(4.23)

The radiation of full triangular-sinusoidal MBF, can then be determined by adding the corresponding left and right MBFs, namely:

$$G_{sw}^{\text{MBF,Full}}(z, \rho; H) = G_{sw}^{\text{MBF,Right}}(z, \rho; H) + G_{sw}^{\text{MBF,Left}}(z, \rho; H).$$

(4.24)

An attractive feature of the formulas derived above for the electric field radiated by the MBFs is that only the $xx$- and $yy$-components of the $G_{sw}^{\text{MBF}}$ require numerical evaluation of $\text{Int}$ function, while the rest of the $sw$-components can be obtained analytically in closed forms. The numerical integration to evaluate $\text{Int}$ function in (4.8), can also be carried out very rapidly by using an 8-point Gaussian Quadrature Rule (GQR) [81].

Traditionally, the fields due to the MBFs are obtained by the convolution of currents with Dyadic Green’s Function (DGF). This requires an integration of the type:

$$G_{sw}^{\text{MBF,Right}} = \int_{0}^{H} \mathbf{\hat{s}}G(r, r') \cdot \mathbf{\hat{w}} \sin(k(H - z')) dz'.$$

(4.25)
where \( \mathbf{G}(\mathbf{r}, \mathbf{r}') \) is the electric DGF given by [6]

\[
\mathbf{G}(\mathbf{r}, \mathbf{r}') = -\frac{j\eta e^{-jk_o R}}{4\pi R^3} \left\{ \left[ (k_o R)^2 - jk_o R - 1 \right] \mathbf{I} - \left[ (k_o R)^2 - j3k_o R - 3 \right] \mathbf{RR} \right\}.
\] (4.26)

In (4.26), \( \mathbf{I} \) is the identity dyad, \( \mathbf{r} \) and \( \mathbf{r}' \) are the locations of observation and source points, respectively, and \( \mathbf{R} = \mathbf{r} - \mathbf{r}' \), \( R = |\mathbf{R}| \). A comparison between the formulas derived herein for the radiation of MBFs and the 20-point equally-spaced integration of the convolution of DGF and MBF, given in (4.25), is presented in Fig. 4-6. The observation line in Fig. 4-6 is at \( \rho = \lambda/3 \), \( \phi = 33^\circ \), and \( 0 \leq z \leq 10H \). The width of the half triangular-sinusoidal is assumed to be \( H = \lambda/5 \). (\( \lambda = 1000 \text{ nm} \)). We notice excellent agreement between the two approaches for both the magnitude and phase, validating the accuracy of our method. The average computational time for our method on an Intel Core(TM)2 Duo at 2.2 GHz CPU frequency with 4.00 GB RAM is about 16 ms, which is about 100 times faster than the traditional MoM method employing DGF. This time advantage becomes really significant when we consider the problem of scattering by plasmonic nanorods, which is discussed in Section 4.4.
Fig. 4-6: Comparisons between the closed-form electric fields radiated by MBFs (solid line) and those obtained by using numerical integration of the convolution of the MBF and corresponded DGF by using 20-point equally-spaced integration (triangular brown marker). The observation line is at $\rho = \lambda / 3$, $\phi = 33^\circ$, and $0 \leq z \leq 10H$. The width of the half triangular-sinusoidal is $H = \lambda / 5$. (a) $|G_{xx}^{MBF, Right}|$, (b) $\angle G_{xx}^{MBF, Right}$, (c) $|G_{yx}^{MBF, Right}|$, (d) $\angle G_{yx}^{MBF, Right}$, (e) $|G_{zx}^{MBF, Right}|$, (f) $\angle G_{zx}^{MBF, Right}$, (g) $|G_{zz}^{MBF, Right}|$, (h) $\angle G_{zz}^{MBF, Right}$. 
4.3. Derivation of Matrix Equation

Having found closed form expressions for the fields radiated by different MBFs used to represent the polarization current, we proceed in this section to generate a matrix equation for the nanorod scattering problem. We start with (4.2), which relates the polarization current $I = \pi a^2 J$ with the scattered field, $E^{\text{scat}}$. Then, according to (4.5), the scattered field can be expanded as a linear combination of electric fields radiated by MBFs, $G_{sw,n}^{\text{MBF}}$. Taking advantage of the closed form formulas in the previous section, $G_{sw,n}^{\text{MBF}}$ can be obtained in terms of the fields radiated by the MBFs replacing $z$ by $z - z_n$ (see Fig. 4-4), as follows:

$$
G_{sw,n}^{\text{MBF}} = \begin{cases} 
G_{sw,\text{Right}}^{\text{MBF}} & n = 1 \\
G_{sw,\text{Left}}^{\text{MBF}} & n = N \\
G_{sw,\text{Full}}^{\text{MBF}} & \text{Otherwise}
\end{cases} \quad (4.27)
$$

To find $I^n_w$’s, comprising of a set of $3N$ unknowns, we test (4.2) on the surface of the nanorod, at $\rho = a$, by using the Galerkin’s testing [49,82] procedure. For each of the vector components ($x$, $y$, $z$), both sides of (4.2) are multiplied by $t_m(z)$ (given in (4.4)) and then an integral is taken from $z_{m-1}$ to $z_{m+1}$. This results in a $3N \times 3N$ matrix equation as below:

$$
\begin{bmatrix}
[z_{xx}] - [z_{res}] & [z_{xy}] & [z_{xz}] \\
[z_{yx}] & [z_{yy}] - [z_{res}] & [z_{yz}] \\
[z_{zx}] & [z_{zy}] & [z_{zz}] - [z_{res}]
\end{bmatrix}
\begin{bmatrix}
[I_x] \\
[I_y] \\
[I_z]
\end{bmatrix} = 
\begin{bmatrix}
[V_x] \\
[V_y] \\
[V_z]
\end{bmatrix},
$$

where $[z_{sw}]$ and $[V]$ are $N \times N$ and $N \times 1$ matrices, respectively, and:

$$
[z_{sw}]_{mn} = \int_{z_{m-1}}^{z_{m+1}} t_m(z) G_{sw,n}^{\text{MBF}} dz, \quad (4.29)
$$
\[
[V_s]_m = \int_{z_{m-1}}^{z_{m+1}} E^\text{inc}_r(z) t_m(z) dz,
\]

(4.30)

The \( N \times N \) matrix \([z]\_\text{res}\) is generated by taking the inner product of the right hand side of (4.2), \( J \), with the testing function \( t_m(z) \). We can show that \([z]\_\text{res}\) can be expressed as:

\[
[z]\_\text{res} = -\frac{j \eta}{\pi \alpha^2 k (\varepsilon_r - 1)} \begin{bmatrix}
  s_{ff}/2 & s_{h'k'} & 0 & \ldots & 0 \\
  s_{h'k'} & s_{ff} & s_{h'k'} & \ddots & \vdots \\
  0 & s_{h'k'} & s_{ff} & \ddots & 0 \\
  \vdots & \ddots & \ddots & \ddots & s_{h'k'} \\
  0 & \ldots & 0 & s_{h'k'} & s_{ff}/2
\end{bmatrix},
\]

(4.31)

where \( \eta \) is the intrinsic impedance of the free space and

\[
s_{ff} = \int_{z_m}^{z_{m+1}} t_m^2(z) dz = H \left( 1 - \frac{\sin(2kH)}{2kH} \right),
\]

(4.32)

\[
s_{h'k'} = \int_{z_m}^{z_{m+1}} t_m(z) t_{m+1}(z) dz = \frac{H}{2} \left( \frac{\sin(kH)}{kH} - \cos(kH) \right).
\]

(4.33)

In (4.32) and (4.33), \( t_m(z) \) is a full- and a half-MBF, respectively, as it may be seen by referring to the limits of the integrals. It should be pointed out that the Galerkin’s testing for the transverse components of the electric field, i.e., \( E_x \) and \( E_y \), must be carried out with the care, by ensuring that the \( E_x \)-component is matched at \( \phi = 90^\circ \), while \( E_y \) at \( \phi = 0^\circ \), as shown in Fig. 4-7.

Note that, since we have used the thin-wire assumption that the polarization current is located at the axis of the rod, and we apply the boundary condition on the surface of the rod, we do not encounter any singularity issues. It is also interesting to observe that the size of matrix equation in (4.28) is only \( 3N \times 3N \), where \( N \) is the number of MBFs for each of the \( x \)-, \( y \)-, and \( z \)-components of the polarization current; Hence the proposed method is numerically very efficient, because the matrix elements can also be generated relatively quickly by taking
advantage of the closed form representations of the fields radiated by MBFs, except for the \( xx \)-
and \( yy \)- terms which can be evaluated relatively quickly by using an 8-point GQR.

![Diagram](image)

Fig. 4-7: Suitable points on the surface of the plasmonic nanorod for matching the transverse components of the
electric field, \( E_x \) and \( E_y \).

### 4.4. Plasmonic Nanorod Simulation and Results

We now proceed to analyze a plasmonic nanorod antenna which is made of silver Drude
medium with \( \varepsilon_{re}=5 \), \( f_p =2175 \) THz, and \( f_d=4.35 \) THz (see (4.1)). We assume that its length is
\( L=300 \) nm, and that it has radius of \( a=10 \) nm. The frequency response, which shows the surface-
plasma resonance of the nanorod is plotted in Fig. 4-8, when it is illuminated at broadside by a
vertically polarized plane wave. The \( z \)-component of the scattered electric field is computed at
\( \rho =500 \) nm over an optical range of frequency. The scattered field is \( \varphi \)-symmetric for the
normally incident wave. It is found that numerical convergence is achieved with only 5 MBFs.
The resonant frequency obtained by using the MBF formulation, at which the magnitude of
scattered electric field is maximum, is found to be \( f_{res}=187 \) THz (1.6 \( \mu \)m), which is almost the
same as predicted by the FDTD analysis. The effective length of the nanorod at the resonant
frequency is \( L_{eff} =0.461 \lambda_{eff} \) (see Fig. 4-3), which is not exactly equal to half of the effective
wavelength because of the finite radius of the nanorod, which is $a=0.015 \lambda_{eff}$. The permittivity of the silver at the resonance frequency is $\varepsilon_r = -130 - j3.15$. For the normally incident excitation, only the $z$-component of current is non-zero and, hence, the size of required matrix equation is only $5 \times 5$. The condition number of the matrix $[z_{xx}] - [z_{res}]$ is only 41 at $f=200$ THz. The computational time to derive the scattering characteristics over the entire frequency band by using the MBF method is ~5 seconds for 500 frequency samples, while the corresponding time is on the order of 4 hours when we use the FDTD method, and the MBF simulation is performed on an Intel Core(TM)2 Duo at 2.2 GHz CPU frequency with 4.00 GB RAM. Because of the generation of surface plasmon mode on the curve boundary of the nanorod, it is necessary to use a fine mesh in the FDTD to obtain accurate results. We see that a significant reduction of the computational time is achieved, by more than 3 orders of magnitude relative to the FDTD, when we use the MBF approach described in this chapter.

![Fig. 4-8: Frequency response of the plasmonic nanorod illuminated by a normal incident vertically polarized plane wave. The scattered field is computed by using 5 MBFs (solid blue line) and FDTD (circular red marker).](image)

We now turn to a second example, for which the angle of incidence is now oblique, and the incident field is given by $\mathbf{E} = E_0 e^{-jkr}$, where $E_0 = (x + 2y + 3z)/\sqrt{14} \quad (\theta = 36.7^\circ, \phi = 63.4^\circ)$ in
spherical coordinates) and \( \mathbf{k} = (3\hat{x} - 3\hat{y} + \hat{z})/\sqrt{19} \) \( (\theta = 76.7^\circ, \phi = -45^\circ) \), as shown in Fig. 4-9. We assume that the operating wavelength is 1.5 \( \mu \text{m} \) \( (f=200 \text{ THz}) \) which is close to the plasmonic resonance. In contrast to the previous example, one needs to consider the transverse components of the polarization current, in addition to the longitudinal one, for the oblique incidence case. Five MBFs are found to be sufficient, for each of the \( x \)-, \( y \)-, and \( z \)-components of the polarization current, to achieve convergence, hence, the size of the matrix equation is \( 15 \times 15 \). The magnitudes and phases of the polarization currents \( (I_x, I_y, \text{ and } I_z) \) are depicted in Figs. 4-10 to 4-12. It can be observed that the magnitude of the transverse current is on the order of one-thousandth of the longitudinal one. However, in general, the transverse components of the current can be more significant, but still less than longitudinal component, once we are away from the resonance, as may be seen from Figs. 4-13 to 4-15 for the operation at 600 nm wavelength \( (f=500 \text{ THz}) \), where the magnitude of transverse current is on the order of one-tenth of the longitudinal one. Note that the length of the rod is \( L=300 \text{ nm}=\lambda/5 \) at 1.5 \( \mu \text{m} \) excitation, which in terms of the effective wavelength is about \( 2.2\lambda_{\text{eff}} \) (see Fig. 4-3).

Fig. 4-9: Plasmonic nanoantenna illuminated by an obliquely plane wave with polarization of \( \mathbf{E}_0 = (\hat{x} + 2\hat{y} + 3\hat{z})/\sqrt{14} \) (small red vectors) and wave vector of \( \mathbf{k} = (3\hat{x} - 3\hat{y} + \hat{z})/\sqrt{19} \) (big green vectors).
Fig. 4-10: $x$-component of the polarization current of plasmonic nanorod for the configuration depicted in Fig. 4-9 at $f=200$ THz ($\lambda=1.5$ µm). (a) Magnitude, (b) Phase.

Fig. 4-11: $y$-component of the polarization current of plasmonic nanorod for the configuration depicted in Fig. 4-9 at $f=200$ THz ($\lambda=1.5$ µm). (a) Magnitude, (b) Phase.

Fig. 4-12: $z$-component of the polarization current of plasmonic nanorod for the configuration depicted in Fig. 4-9 at $f=200$ THz ($\lambda=1.5$ µm). (a) Magnitude, (b) Phase.
Fig. 4-13: $x$-component of the polarization current of plasmonic nanorod for the configuration depicted in Fig. 4-9 at $f=500$ THz ($\lambda=600$ nm), away from the resonance. (a) Magnitude, (b) Phase.

Fig. 4-14: $y$-component of the polarization current of plasmonic nanorod for the configuration depicted in Fig. 4-9 at $f=500$ THz ($\lambda=600$ nm), away from the resonance. (a) Magnitude, (b) Phase.

Fig. 4-15: $z$-component of the polarization current of plasmonic nanorod for the configuration depicted in Fig. 4-9 at $f=500$ THz ($\lambda=600$ nm), away from the resonance. (a) Magnitude, (b) Phase.
The scattered near-fields along the $x$-axis for $0.05\lambda < x < 0.5\lambda$ are shown in Fig. 4-16 and are compared with the corresponding FDTD-generated data. The $y$- and $z$-components are seen to be in excellent agreement with the FDTD results, however there is some discrepancy between the $E_x$ results, especially when we close to the rod. As may be seen from the results plotted in Fig. 4-16, $E_x$ decays more rapidly as we move away from the rod relative to the other components and its radiation pattern has a null along the $x$-axis (see Fig. 4-17(a)). Consequently, a fine mesh is required for this case to accurately predict the behavior of $E_x$ very close to the rod along the $x$-axis. We also note that, $E_x$ is the field component normal to the rod, and, hence, in contrast to the tangential $E$-field components that are computed in the FDTD algorithm, directly on the surface of the object, the normal component is derived at half-a-cell away from the same. It is also important to realize that the FDTD typically utilizes a stair-casing approach to represent a curved boundary. Finally, we want to mention that the computation is the most challenging when we are operating in the proximity of the surface Plasmon resonance. We now turn to the far field radiation patterns in the $x$-$z$ plane, shown in Fig. 4-17, that are computed at $r = 10\lambda$, and note that the two results compare very well with each other. However as we have mentioned earlier the MBF approach is much faster, since it takes only 0.2 sec, the FDTD requires 4 hours to generate the same results.
Fig. 4-16: Scattered field along the x-axis for the configuration depicted in Fig. 4-9. (a) $|E_x|$, (b) $|E_y|$, (c) $|E_z|$. Great agreements between the MBF (solid blue line) and FDTD (circular red marker) are demonstrated.

Fig. 4-17: Normalized far-field in x-z plane for the configuration depicted in Fig. 4-9. (a) $|E_x|$, (b) $|E_y|$, (c) $|E_z|$. Excellent agreements between MBF (solid blue line) and FDTD (circular red marker) are observed.
Chapter 5

Analysis of Array of Plasmonic Nanorods Illuminated by an Obliquely Incident Plane Wave

The goal of this chapter is to present a computational scheme to accurately and efficiently characterize reflection and transmission coefficients for a periodic array of plasmonic nanorods illuminated by an obliquely incident plane wave. The problem is formulated by using integral equations and the Method of Moments (MoM) in conjunction with the Characteristic Basis Functions Method (CBFM) to significantly reduce the number of unknowns. The concept of progressively expanding rings is employed along with Parseval's theorem to evaluate the Galerkin’s integrals for the periodic structure under consideration. The use of this novel approach offers significant computational advantages over conventional methods using slowly-convergent periodic Green’s functions. Closed-form expressions for the reflection and transmission coefficients are derived for a plane wave illuminating the array at an arbitrary angle. The presented numerical method is general and can be applied to other periodic configurations, including metamaterials. The proposed method is validated by comparing it with
the results obtained by using the Finite Difference Time Domain (FDTD) technique. Also, we show that the proposed computational scheme achieves a speed performance that is considerably superior to that of the conventional approaches for analyzing the problem at hand.

5.1. Problem Formulation

In this section, we present the formulation of the scattering from a periodic array of plasmonic nanorods, illuminated by an obliquely incident plane wave. Let us consider a two-dimensional periodic array of plasmonic nanorods lying in the $x$-$y$ plane and illuminated by an arbitrarily incident plane wave, given by $E_{\text{inc}} = E_0 e^{-j\mathbf{k}_{\text{inc}} \cdot \mathbf{r}}$, where $\mathbf{k}_{\text{inc}}$ is the free space wave vector and $\mathbf{r}$ is the position vector, as illustrated in Fig. 5-1(a).

![Diagram](image)

Fig. 5-1: (a) Two-Dimensional array of plasmonic nanorods illuminated by an oblique incident plane wave. The periods along $x$- and $y$-axis are $\Lambda_x$ and $\Lambda_y$. (b) The plasmonic nanorod made of a Drude material as the unit-cell, (c) Real part and imaginary part of the permittivity of silver over a desired optical frequency range.

The unit-cell is assumed to be a rectangle with periodicities along $x$- and $y$-directions equal to $\Lambda_x$ and $\Lambda_y$, respectively. Fig. 5-1(b) shows the isolated element in the unit-cell which is a plasmonic
nanorod whose radius $a=7.5$ nm and length $L=150$ nm. The nanorod is composed of silver, i.e., plasmonic material, which is characterized in the optical regime by the Drude model, which has the form $\varepsilon_r = \varepsilon_{\infty} - \frac{f_p^2}{f(f - i f_d^2)}$, where $\varepsilon_{\infty} = 5$, $f_p = 2175$ THz (plasma frequency), and $f_d = 4.35$ THz (damping frequency) [75]. Fig. 5-1(c) illustrates the permittivity of silver in the optical frequency range. We use a spherical coordinate system to define the incident wave vector and polarization state, as shown in Fig. 5-2.

![Diagram of wave vectors and polarization](image)

**Fig. 5-2:** (a) Incident and reflected wave vectors, (b) Polarization of the electric field in the plane constructed by $\hat{\theta}$ and $\hat{\phi}$.

The scattered field is a summation of Floquet harmonics [49], comprising of a combination of propagating (belonging to visible range) and evanescent modes (invisible range). We assume that the dimensions of the spatial lattice, i.e., $\Lambda_x$ and $\Lambda_y$, are such that only a single Floquet mode exists in the visible region. We can characterize a periodic structure either by computing its dispersion diagram, which shows the range of frequencies within which there are no propagating...
modes, or by deriving the reflection coefficient characteristics over a range of frequencies. There are two advantages to presenting the results for the reflection coefficient, which is the focus of our work. First, one can provide the information on phase and polarization, and second, information on evanescent modes can also be made available. We will now go on to detail the various steps in our modeling procedure in the sections below.

5.1.1. Solving the Isolated Element Problem

In this section, we briefly review the technique for analyzing a plasmonic nanorod which has been presented in detail in the previous chapter. Fig. 5-3(a) shows the nanorod, which is orientated along the y-axis and illuminated by a plane wave with parallel polarization. Note that for the case of perpendicular polarization, the induced current is relatively small compared to the longitudinal current, as has been demonstrated in [57]. The basic concept of our modeling approach is based on the use of Dipole Mode (DM) method [6-8, 83]. As depicted in Fig. 5-3(b), it can be shown (see [80]) that for an electrically small dielectric sphere, with arbitrary permittivity $\varepsilon_r$, the scattering characteristics can be derived from an equivalent electric dipole moment $I_\ell = 4\pi \eta (k_0 a)^3 (\varepsilon_r - 1) E_0 / \eta k_0^2 (\varepsilon_r + 2)$, where $k_0$ and $\eta$ are free space wave number and intrinsic impedance, respectively, and $E_0$ is the incident electric field at the center of the sphere. We borrow the same concept for modeling longitudinal polarization current induced in the nanorod. In the previous chapter, we have shown that by discretizing the current using only a few piecewise sinusoidal Macro Basis Functions (MBFs), as depicted in Fig. 5-3(c), and by employing Galerkin testing on the surface of the nanorod, one can derive an accurate, fast and singularity free computational paradigm to solve the problem at hand and obtain the unknown current.
Fig. 5.3: (a) Characterization of a single nanorod illuminated by a Parallel polarization, (b) Modeling the scattering problem of plasmonic nanorod originated from Dipole Mode (DM) approach, (c) Discritization of the polarization current by piecewise sinusoidal macro basis functions, (d) Full triangular macro basis function including right and left half-MBFS.

The current induced on the axis of nanorod can be obtained by solving the matrix equation

\[
\begin{bmatrix}
Z_{\text{MBF}} & -Z_{\text{res}}
\end{bmatrix}
\begin{bmatrix}
I_{\text{MBF}}
\end{bmatrix} = \begin{bmatrix}
V_{\text{MBF}}
\end{bmatrix},
\]

where \( I_{\text{MBF}} \) is a column matrix that includes the coefficients of each MBFs, and

\[
(Z_{\text{MBF}})_{mn} = \int_{y_{m-1}}^{y_{m+1}} t_m(y) G_{n}^{\text{MBF}} \, dy,
\]

\[
(\mathbf{V}_{\text{MBF}})_{m} = \int_{y_{m-1}}^{y_{m+1}} E_{\text{inc}}(y) t_m(y) \, dy,
\]
and \( t_m(y) = \sin(k_0(H - |y - y_m|)) \) is the \( m \)th piecewise sinusoidal MBF. As depicted in Fig. 5-3(c), the first and last MBFs are one-half while the rest are full piecewise sinusoidal functions. The length of the domain of the half MBF is \( H \), and \( y_m = -L/2 + (m-1)H \) is the location of cusp of each MBF.

The electric field radiated by MBF\#\( n \) is denoted by \( G_{n}^{MBF} \) in (5.2) and is defined as:

\[
G_{n}^{MBF} = \begin{cases} 
G_{n}^{MBF,Right} (y - y_n) & n = 1 \\
G_{n}^{MBF,Left} (y - y_n) & n = N_{MBF} \\
G_{n}^{MBF,Full} (y - y_n) & \text{Otherwise}
\end{cases}
\]  

(5.4)

where \( G_{n}^{MBF,Right} \) is the electric field, radiated by the right half triangular-sinusoidal depicted in Fig. 5-3(d), which can be expressed in a closed form as:

\[
G_{n}^{MBF,Right} = \frac{-j \eta}{4\pi} \left[ e^{-j \beta_0 R_{i}} - e^{-j \beta_0 R_{0}} \right] \left( \cos(k_0 H) + j \frac{y}{R_{0}} \sin(k_0 H) \right) - y \sin(k_0 H) e^{j \beta_0 R_{0}} \left( \frac{1}{k_0 R_{i}} \right),
\]  

(5.5)

where \( R_{i} = \sqrt{x^2 + (y-H)^2 + z^2} \) and \( R_{0} = \sqrt{x^2 + y^2 + z^2} \), as shown in Fig. 5-3(d). The electric field radiated by the left half-MBF, namely \( G_{n}^{MBF,Left} \) shown in Fig. 5-3(d), can be obtained from (5.5) by replacing \( H \) with \(-H\). Also, \( G_{n}^{MBF,full} \) is the summation of the radiated electric field due to the left and right half-triangular sinusoidal MBFs. The observation point, for which the impedance matrix is constructed, is located at \((x,y,z) = (0,y,a)\), on the surface of the nanorod. And finally \( [z_{res}] \) can be obtained from:

\[
[z_{res}]_{mn} = \frac{-j \eta}{\pi \alpha} \frac{1}{k_0 (\varepsilon_r - 1)} \begin{cases} 
\delta_{ff} & m = n \neq (1 \text{ or } N_{MBF}) \\
\delta_{h^* h} & \left| m - n \right| = 1 \\
\delta_{ff}/2 & m = n = (1 \text{ or } N_{MBF}) \\
0 & \text{Otherwise}
\end{cases}
\]  

(5.6)
where $s_{ff}$ and $s_{h'h'}$ are expressed as:

$$s_{ff} = H \left(1 - \frac{\sin(2k_0H)}{2k_0H}\right), \quad (5.7)$$

$$s_{h'h'} = \frac{H}{2} \left(\frac{\sin(k_0H)}{k_0H} - \cos(k_0H)\right). \quad (5.8)$$

Solution of (5.1) enables us to obtain the unknown current on the nanorod, and we solve for this current for various incident angles and frequencies. Fig. 5-4 shows the maximum value of the induced current vs. frequency and incident angle for the nanorod illuminated by the excitation in Fig. 5-3(a). The peaks occur at $f_{res1}=260$ THz and $f_{res2}=440$ THz. The running time for 88 frequency samples and 19 incident angles is about 4 sec. on an Intel Core(TM)2 Duo at 2.2 GHz CPU frequency with 4.00 GB RAM illustrating the speed and efficiency of our model. The number of required MBFs for normal incident wave is 5 for the entire frequency range, (100:500) THz, as shown in Fig. 5-5. However, we see from Fig. 5-6 that while at lower frequencies, e.g., $f=260$ THz, the scheme converges with 5 MBFs, we need 7 to 9 MBFs at higher frequencies for $400$ THz < $f$ < $500$ THz. The convergence criterion can be defined as follows: the rms (root of the mean of the square value) of the relative difference between two successive current results is less than 2%.

![Graph showing the maximum of the magnitude of the longitudinal current versus the frequency and the azimuthal incident angle ($\varphi$) for the excitation shown in Fig. 5-3(a).](image)
Fig. 5-5: Polarization current along the plasmonic nanorod illuminated by a normally incident plane wave, $\phi=0^\circ$, (a) Magnitude at $f=260$ THz, (b) Phase at $f=260$ THz, (c) Magnitude at $f=400$ THz, (d) Phase at $f=400$ THz, (e) Magnitude at $f=440$ THz, (f) Phase at $f=440$ THz.
Fig. 5-6: Polarization current along the plasmonic nanorod illuminated by an oblique incident plane wave, $\phi = 75^\circ$, (a) Magnitude at $f=260$ THz, (b) Phase at $f=260$ THz, (c) Magnitude at $f=400$ THz, (d) Phase at $f=400$ THz, (e) Magnitude at $f=440$ THz, (f) Phase at $f=440$ THz.

### 5.1.2. Characteristic Basis Functions

Our next step is to account for the mutual interactions between the elements to obtain the polarization current accurately. Toward this end we use the Characteristic Basis Functions (CBFs) that are a set of high-level entire-domain basis functions. The advantage of using these functions is that a linear combination of just a few CBFs, for instance only two or three, can
represent the current accurately for any arbitrary angle of incidence. The motivation behind using the CBFs is to reduce the matrix size significantly, to remove the burden on the CPU in terms of memory and time, and to decrease the condition number. Mittra [30,59,84-87], has implemented CBF method (CBFM) in a variety of examples to illustrate the versatility of the approach in the context of computational physics of scattering problems.

To obtain the CBFs for a scatterer, we illuminate an object by sufficient number of plane waves \([PW_1, PW_2, \ldots, PW_{N_p}]\), as shown in Fig. 5-7, with both parallel and perpendicular polarizations. Let us assume that \(J_n(r')\) is \(x\)-, \(y\)- or \(z\)-component of the induced current vector within the object, for a specific plane wave, e.g., \(\#n, PW_n\). Next, we construct the column matrix \([J_n]\) which contains \(N_s\) samples of \(J_n(r')\) at \(N_s\) different points within the scatterer, \(r'_i, 1 \leq i \leq N_s\). Then, we construct a rectangle matrix \([J]\) whose \(n\)'th column is \([J_n]\):

\[
[J] = \begin{bmatrix} [J_1] & [J_2] & \cdots & [J_{N_p}] \end{bmatrix}
\]

(5.9)

Fig. 5-7: An arbitrary object illuminated by \(N_p\) incident plane waves with different polarizations to obtain CBFs.
The CBFs can be obtained by Singular Value Decomposition (SVD) factorization \([88]\) of \([J]\), as follows

\[
[J] = [J_U][S][W],
\]

(5.10)

where \([J_U]\) and \([W]\) are square unitary matrices, whose inverses are equal to their conjugate transposes, and \([S]\) is a \(N_s\times N_p\) quasi-diagonal matrix \([88]\) with real and positive diagonal elements that are called singular values and are arranged in a descending sequence, e.g., \(S_{11} > S_{22} > S_{33}\), and so on. The CBFs are indeed the columns of \([J_U]\). As \([J_U]\) possesses \(N_s\) columns, not all the columns are significant, and the significance of column\(\# n\), CBF\(\# n\), is determined by \(n\)th singular value, \(S_{nn}\). In practice, when the index of a singular value is above a threshold, the normalized singular value, \(S_{nn}/S_{11}\), drops significantly.

For our case study, an array of plasmonic nanorods, the CBFs can be obtained from the induced current solutions when we illuminate the nanorod by the obliquely incident plane waves with the polarization illustrated in Fig. 5-3(a), for \(-90^\circ < \varphi < 90^\circ\). If we choose an angular step equal to 10°, i.e., \(\varphi = [-90^\circ, -80^\circ, \ldots, 90^\circ]\), containing 19 different incident plane waves \((N_p=19)\) and if we solve (5.1) to obtain the current for each incident angle, then the induced current matrix can be constructed similarly to (5.9). By applying SVD on the induced current matrix, the CBFs for the nanorod can be obtained. Fig. 5-8 illustrates the magnitude, phase and the corresponding singular values of the CBFs for the plasmonic nanorod at \(f=260\) THz (first resonance), \(f=400\) THz, and \(f=440\) THz (second resonance). We use 101 equally spaced sampling points \(-L/2 \leq y \leq L/2\), \(N_s=101\), on the axis of the nanorod to construct the current matrix in (5.9). The criterion to keep the CBFs is based on the threshold for the normalized singular value to be above \(-30\) dB, i.e., \(10\times\log(S_{nn}/S_{11})> -30\). It can be observed that at \(f=260\) THz, two CBFs are
needed, whereas at higher frequencies, $f=400$ and $440$ THz, three CBFs are needed. The first CBF, CBF#1, at $f=260$ and $400$ THz, has one peak, while it possesses two peaks at $f=440$ THz. We also observe that the higher-order CBFs have more variations in both magnitude and phase compared to the lower order CBFs.

Fig. 5-8: Magnitude and phase of CBFs and singular values for plasmonic nanorod at (a) $f=260$ THz, (b) $f=400$ THz, and (c) $f=440$ THz.

5.1.3. The Shape of Macro-CBF: Ring Concept

We proceed to solve the problem of periodic array illuminated by a plane wave by utilizing the previously generated CBFs. Instead of using the periodic Green’s function (PGF) approach, which is often plagued by slow convergence [50-56], we develop an alternate strategy based, which is considerably more efficient, as is demonstrated below. We consider two different excitations, namely normal $(\psi, \theta, \phi) = (90^\circ, 0, 90^\circ)$ and oblique $(\psi, \theta, \phi) = (143^\circ, 25^\circ, 110^\circ)$.
incidence cases. The frequency is assumed to be $f=400$ THz for both cases, and the CBFs for this frequency are shown in Fig. 5-8(b). By imposing the periodicity condition [49], the $pq$-plasmonic antenna located in the $(p,q)$th cell, i.e., at $(x,y) = (p\Lambda_x, q\Lambda_y)$, where $p$ and $q$ are integers, can be represented by an induced current $I_{pq}(y) = I_e pq$, where $I(y), \quad -L/2 < y < L/2$, is the unknown induced current along the axis of the center ((0,0)th cell) element and $e_{pq}$ is the inter-element phasing factor [89] determined by the phase variation of the incident plane wave, $E^{\text{inc}} = E_0 e^{-j k_w \cdot r}$. The phase factor can be written as:

$$e_{pq} = \exp[-j (k_x^{\text{inc}} p \Lambda_x + k_y^{\text{inc}} q \Lambda_y)].$$

(5.11)

For the normal incidence case, the currents induced on the elements are in-phase, i.e., $e_{pq} = 1$. To find the unknown function $I(y)$, we need to impose the polarization current condition [57] on the center element:

$$j \omega \varepsilon_0 (\varepsilon_r - 1)(E_y^{\text{inc}} + E_y^{\text{scat}}) = I(y)/(\pi a^2), \quad -L/2 \leq y \leq L/2$$

(5.12)

where $E_y^{\text{scat}}$ is the $y$-component of the scattered electric field, generated by the infinite elements of the array. To solve (5.12), we express $I(y)$ in terms of the CBFs in the previous section, as follows:

$$I(y) = \sum_{n=1}^{N_C} I_n^{\text{CBF}} f_n(y),$$

(5.13)

where $N_C$ is the total number of CBFs, which is a relatively small number, for instance $N_C=3$ at $f=400$ THz, when we impose the -30 dB criterion on the associated singular values. The $n$th CBF is denoted by $f_n(y)$ in (5.13), and $I_n^{\text{CBF}}$ is its unknown coefficient. The scattered electric field, $E_y^{\text{scat}}$, can be expressed as an infinite summation of the fields radiated by each of the $N_C$ CBFs.
residing on each of the elements, including the center element. By taking into account of the inter-element phasing factor $e_{pq}$ introduced in (5.11), we can write $E_{y}^{\text{scat}}$ as:

$$E_{y}^{\text{scat}} = \sum_{n=1}^{N} j_{n}^{\text{CBF}} \sum_{p,q=-\infty}^{\infty} e_{pq} G_{pq}^{\text{CBF},n},$$

(5.14)

where $G_{pq}^{\text{CBF},n}$ is the $y$-component of electric field radiated by the $n$th CBF on the $(p,q)th$ element.

Since each of the CBFs is a superposition of MBFs with known coefficients, we can derive a closed-form expression for each $G_{pq}^{\text{CBF},n}$ as a linear combination of expressions for the fields radiated by the full- and half-MBFs that were presented in section 5.1.1. After replacing (5.13) and (5.14) in (5.12), we test the equation (5.12), by using $m$'th CBF, $1\leq m \leq N_{c}$, at the center element $(x,y,z) = (0,y,a)$. Such a Galerkin’s testing [82] leads to an $N_{c} \times N_{c}$ matrix equation which reads:

$$[Z_{G}^{\text{CBF}}] - [Z_{\text{res}}^{\text{CBF}}] [I^{\text{CBF}}] = -[V^{\text{CBF}}],$$

(5.15)

where

$$[Z_{G}^{\text{CBF}}]_{mn} = \int_{-L/2}^{L/2} f_{m}(y) \sum_{p,q=-\infty}^{\infty} e_{pq} G_{pq}^{\text{CBF},n} \, dy,$$

(5.16)

$$[Z_{\text{res}}^{\text{CBF}}]_{mn} = \frac{-j \eta}{\pi a^{2} k_{0}(\varepsilon_{r}-1)} \int_{-L/2}^{L/2} f_{m}(y) f_{n}(y) \, dy,$$

(5.17)

$$[V^{\text{CBF}}]_{m} = \int_{-L/2}^{L/2} E_{y}^{\text{inc}}(y) f_{m}(y) \, dy,$$

(5.18)

and $[I^{\text{CBF}}]$ is the column vector representing the $N_{c}$ unknown coefficients $I_{n}^{\text{CBF}}$. The impedance matrix in (5.16) is a doubly-infinite series, representing the contributions of infinite number of array elements. To deal with the summation included in the infinite series given by (5.16), we use the concept of progressively expanding rings, i.e., the ring concept, as illustrated in Fig. 5-9.
The first ring just includes the central element. The ring\#M (where M>1), consists of a set of nanorods whose centroids are located on the rectangular ring given by (see Fig. 5-9):

\[
\begin{cases}
|x|=(M-1)\Lambda_x, & y \leq (M-1)\Lambda_y \\
y=(M-1)\Lambda_y, & x < (M-1)\Lambda_x.
\end{cases}
\]

(5.19)

Fig. 5-9: Ring definition employed in the context of convergence of the Galerkin integrals in the spatial domain.

Our algorithm, to evaluate the infinite series in (5.16), comprises of some successive stages using the ring concept described above. At stage \#M we need to consider the truncated \((2M-1)\times(2M-1)\) array including the rings #1, #2, ..., #M to find the corresponded coefficients \([I_{\text{CBF}}^M]\). In other word, at stage \#M, we solve the matrix equation (5.15) by using (5.16)-(5.18), except that instead of using a doubly-infinite series to construct \([z_G^{\text{CBF}}]\) in (5.16), we use a truncated series in the spatial domain as follows:

\[
[z_G^{\text{CBF}}]_{\text{Spa}(M)} = \int_{-L/2}^{L/2} f_m(y) \sum_{p,q=-M}^{M} \int_{-L/2}^{L/2} G_{pq}^{\text{CBF},n} dy,
\]

(5.20)
The integral over the center element, appearing in (5.16)-(5.18) and (5.20) and ranging from $-L/2$ to $L/2$, can be evaluated efficiently and accurately by using a 20-point Gaussian Quadrature Rule (GQR) [81]. The results are performed and illustrated in Fig. 5-10 and Fig. 5-11 for normal and oblique plane-wave excitations, respectively.

![Graphs and diagrams](image-url)

Fig. 5-10: Magnitude and phase of the coefficients of the CBFs and the macro-CBF, $I_{shape}$, versus ring index in normal incidence at $f=400$ THz. (a) $|I_{1}^{CBF}|$, (b) Phase($I_{1}^{CBF}$), (c) $|I_{2}^{CBF}|$, (d) Phase($I_{2}^{CBF}$), (e) $|I_{3}^{CBF}|$, (f) Phase($I_{3}^{CBF}$), (g) $|I_{shape}|$ along the nanorod versus ring index, (h) Phase($I_{shape}$) along the nanorod versus ring index.
Fig. 5-11: Magnitude and phase of the coefficients of the CBFs and the macro-CBF, \( I_{\text{shape}} \), versus ring index in oblique incidence, \((\psi, \theta, \phi) = (143^\circ, 25^\circ, 110^\circ)\) at \( f = 400 \text{ THz} \), (a) \( |I_1^{\text{CBF}}| \), (b) \( \text{Phase}(I_1^{\text{CBF}}) \), (c) \( |I_2^{\text{CBF}}| \), (d) \( \text{Phase}(I_2^{\text{CBF}}) \), (e) \( |I_3^{\text{CBF}}| \), (f) \( \text{Phase}(I_3^{\text{CBF}}) \), (g) \( |I_{\text{shape}}| \) along the nanorod versus ring index, (h) \( \text{Phase}(I_{\text{shape}}) \) along the nanorod versus ring index. After ring #13, the coefficients will be in sync, meaning that they go up and down simultaneously, and their maxima and minima follow each others.
To facilitate the comparison between the coefficients of the CBFs plotted in Figs. 5-10 and 5-11, we normalize the magnitudes of each of the CBFs. It is worth mentioning that, the computation of $[Z_G^{\text{CBF}}]^{\text{spat}(M)}$ is time-consuming when the number of rings is large; moreover, as illustrated in Figs. 5-10 and 5-11, the convergence is slow and not monotonic. The reason for such slow convergence in the spatial domain can be explained by considering the electric field radiated by a half-MBF whose expression has been given in (5.5). The electric field due to a half-MBF is a combination of three terms, namely $\exp(-j k_0 R_1)/R_1$, $\exp(-j k_0 R_0)/R_0$, and $(y/R_0) \times \exp(-j k_0 R_0)/R_0^2$; the slow and oscillatory behaviour is due to the $\exp(-j k_0 R_{0,1})/R_{0,1}$ terms in the electric field scattered by each nanorod. We notice, however, from Figs. 5-10 and 5-11, that after a few stages (rings), the maxima and minima of the coefficients of the CBFs become essentially in sync once we go past a certain number of rings in the array. For example, for the case of normal incidence, Fig. 5-10 shows that after only 3 rings, both the magnitudes and the phases of the coefficients of the CBFs fall in sync. For the oblique incidence case, Fig. 5-11 shows that the magnitudes of the CBFs coefficients fall in sync after only 13 rings, while the phases do the same after only 10 rings. In the above algorithm, at each stage, the total polarization current on the central element, i.e., the composite-CBF (macro-CBF), can be constructed as a linear combination of the CBFs with the weighting coefficients obtained at that stage, $[I^{\text{CBF}}]^{M)}$. Because as we increase $M$, the number of rings, the elements of $[I^{\text{CBF}}]^{M)}$, goes up and down synchronously, as observed above, this results in that the shape of the composite-CBF does not change as we increase the number of rings. This observation, stabilization of the shape of the macro-CBF, is highly advantageous to handle the slow and oscillatory behavior of the series in (5.16) arising in our case study and, in general, in the scattering analysis of periodic structures.
We now define $I_{shape}$ given by:

$$I_{shape} = \sum_{n=1}^{N_r} I_n^{CBF(M)} f_n(y),$$

(5.21)

at the $M$th stage when the shape has converged. Beyond this stage, the shape of the macro-CBF, i.e., $I_{shape}$, remains essentially unchanged and only its level fluctuates as the size of the truncated array is increased, as shown in Figs. 5-10(g-h) and Figs. 5-11(g-h) for the normal incidence case and oblique incidence case, respectively. We note from Figs. 5-11(g-h) that only 5 rings are sufficient, even in the oblique incidence case, for the shape to converge. We can take advantage of this fact to find the shape of the macro-CBF by solving a relatively small-size matrix equation, 3×3 in this case, and by working with only the truncated array of 5 rings, for instance, instead of dealing with an infinite array.

In the next section, we will discuss an efficient scheme for determining the level of the macro-CBF, which will then enable us to compute the reflection and transmission coefficients for the array problem at hand.

### 5.1.4. The Level of Macro-CBF: Spectral Galerkin

In this section, we proceed to discuss a method to find the one remaining unknown, namely the level of the macro-CBF whose shape has already been determined in the previous section. The macro-CBF, $I(y)$, then can be written as

$$I(y) = CI_{shape}(y),$$

(5.22)

where $C$ is the dimensionless weight coefficient, which has yet to be determined. We have shown in Appendix A.II that $C$ can be found by testing the polarization current equation, given in
(5.12), by $I_{shape}(y)$. Following this spatial Galerkin-testing, we obtain the following expression for the level of the macro-CBF:

$$C = \frac{\left( \left[ I_{\text{CBF}} \right]_M \right)^T \left[ V_{\text{CBF}} \right]}{\left( \left[ I_{\text{CBF}} \right]_M \right)^T \left( \left[ Z_G^{\text{CBF}} \right] - \left[ Z_{\text{res}}^{\text{CBF}} \right] \right) \left[ I_{\text{CBF}} \right]_M}.$$

(5.23)

We note that, the level of macro-CBF depends on the coefficients of CBFs after $M$ rings, $\left[ I_{\text{CBF}} \right]_M$, and the impedance matrices and voltage matrix introduced in the previous section in (5.16)-(5.18). Note that the impedance matrix, $\left[ Z_G^{\text{CBF}} \right]$, appearing in the denominator of (5.23), does not correspond to a truncated array; instead, according to (5.16), it is comprised of a doubly infinite series, which converges relatively slowly and has an oscillatory behavior in the spatial domain. This prompts us to seek an efficient way to evaluate the slowly-convergent series embedded in $\left[ Z_G^{\text{CBF}} \right]$.

To address the problem of slow convergence of $\left[ Z_G^{\text{CBF}} \right]$, we switch to the spectral domain by using the Parseval's theorem. The use of Parseval's theorem is adopted by many researchers to reach a fast convergence for the integrals and series for large problems [90-95]. For a Fourier pair, $f(r) \rightarrow \tilde{f}(k)$, where $f(r)$ is a scalar function in the spatial domain whose Fourier transform (FT) is $\tilde{f}(k)$, the following property holds: when a series, including samples of $f(r)$, has a slow convergence, the corresponding series in the spectral domain, including the samples of $\tilde{f}(k)$, exhibits a fast convergence, and vice versa. We take advantage of this property of the Fourier pair to expedite the convergence of the impedance matrix $\left[ Z_G^{\text{CBF}} \right]$ defined in (5.16). The rest of this section is devoted to the computation of $\left[ Z_G^{\text{CBF}} \right]$ using a fast algorithm.
We start with the definition of the \( m \)th element of the CBF-impedance matrix given by (5.16) and rewrite it as an integral of the testing CBF\#\( m \), \( f_m(y) \), multiplied by \( E_y^{\text{scat},n} \), which is the electric field scattered by the infinite array when each element supports CBF\#\( n \). We can then write, for the \( m \)th element:

\[
[z_{G}^{\text{CBF}}]_{mm} = \int_{-L/2}^{L/2} f_m(y) E_y^{\text{scat},n} \, dy.
\]  
(5.24)

To facilitate the application of the Parseval theorem, it is beneficial to re-write the one-fold integral in (5.24) by an infinite triple integral showing the testing point, which is the top of the central element, as below:

\[
[z_{G}^{\text{CBF}}]_{mm} = \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} t_m(r) E_y^{\text{scat},n} \, dx \, dy \, dz,
\]  
(5.25)

where \( t_m(r) \) is the testing function including the CBF\#\( m \), which is defined at the top of the central element, \( z=a \):

\[
t_m(r) = \delta(x) f_m(y) \, \delta(z-a),
\]  
(5.26)

where \( \delta(x) \) is the impulse (delta) function. It is obvious that in (5.26), \( f_m(y) \) is zero for \( |y|>L/2 \). If we apply Parseval theorem to (5.25), which is discussed in Appendix A.III in (AIII.3), we obtain

\[
[z_{G}^{\text{CBF}}]_{mm} = \frac{1}{(2\pi)^3} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} e^{ik_x a} \tilde{f}_m(-k_y) \tilde{E}_y^{\text{scat},n} \, dk_x \, dk_y \, dk_z,
\]  
(5.27)

where the symbol tilde, \( \sim \), denotes the FT. We show that \( E_y^{\text{scat},n} \) can be written as a convolution of \( J_y^{\text{CBF},n} \), the current density represented by infinite array carrying CBF\#\( n \) and \( G_{yy} \), the yy-component of the free-space dyadic Green’s function [67]:

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\[ E_{y}^{\text{eval,n}} = \int \int \int_{-\infty}^{+\infty} J_{y}^{\text{CBF,n}}(r') G_{yy}(r - r') dx' dy' dz'. \]  

(5.28)

We can express \( J_{y}^{\text{CBF,n}} \) as the summation of the array elements currents, where the \( pq \)-element carries the CBF\( #n \) with the phase shift dictated by incident plane wave, as follows

\[ J_{y}^{\text{CBF,n}}(r) = \delta(z) \sum_{p,q=-\infty}^{+\infty} e_{pq} \delta(x - p\Lambda_{x}) f_{n}(y - q\Lambda_{y}). \]  

(5.29)

The corresponding \( G_{yy} \) has the following closed form [67]:

\[ G_{yy}(r) = -\frac{j k_{0} \eta}{4\pi} \left( \frac{1}{k_{0}^{2}} \frac{\partial^{2}}{\partial y^{2}} + 1 \right) e^{-jk_{0}|r|}, \]  

(5.30)

where \( r = |r| \). The FT of \( J_{y}^{\text{CBF,n}} \) can be found as a two-dimensional comb function by using the impulse-train identity in (A.III.4), as

\[ \tilde{J}_{y}^{\text{CBF,n}}(k) = \frac{4\pi^{2}}{\Lambda_{x}\Lambda_{y}} \tilde{f}_{n}(k_{y}) \sum_{p,q=-\infty}^{+\infty} \delta(k_{x} - k_{x}^{p}) \delta(k_{y} - k_{y}^{q}), \]  

(5.31)

where

\[ k_{x}^{p} = p \frac{2\pi}{\Lambda_{x}} - k_{x}^{inc}, \]  

(5.32)

\[ k_{y}^{q} = q \frac{2\pi}{\Lambda_{y}} - k_{y}^{inc}, \]  

(5.33)

and the FT of \( G_{yy} \) can be written as [67]:

\[ \tilde{G}_{yy}(k) = \frac{j \eta}{k_{0}} \frac{k_{y}^{2} - k_{y}^{2}}{k_{x}^{2} - k_{x}^{2}}. \]  

(5.34)
Hence, by using (AIII.5), the FT of $E^{scat,n}_y$ is the multiplication of $\tilde{J}^{CBF,n}_y$ and $\tilde{G}_y$ in (5.31) and (5.32). By replacing $\tilde{E}^{scat,n}_y$ in (5.27) and taking the integrals with respect to $k_x$ and $k_y$, which is performed by using the sifting property of delta functions in (5.31), we get

$$[z^{CBF}_G]_{mn} = \frac{j\eta}{2\pi k_0 c} \sum_{p,q=-\infty}^{\infty} \tilde{f}_m(-k_x^q) \tilde{f}_n(k_y^q) \left[ (k_y^q)^2 - k_0^2 \right] \text{Int}(k_{\rho} = k_{\rho}^{p,q}, r = a\hat{z}),$$

(5.35)

where $k_{\rho} = \sqrt{k_x^2 + k_y^2}$, $k_{\rho}^{p,q} = \sqrt{(k_x^p)^2 + (k_y^q)^2}$, and

$$\text{Int}(k_{\rho}, r) = \int_{-\infty}^{\infty} e^{i k_{\rho} r} \frac{dk_{\rho}}{k_{\rho}^2 - k_0^2}.$$

(5.36)

By employing a physics-based residual calculus in Appendix A.IV, we obtain the following closed form formula for $\text{Int}(k_{\rho}, r)$ in (5.36):

$$\text{Int}(k_{\rho}, r) = \pi e^{i k_{\rho} r} \times \begin{cases} -j e^{-i k_0^2 r^2/4} & k_0^2 > k_{\rho}^2, \\ \frac{1}{\sqrt{|k_0^2 - k_{\rho}^2|}} & k_{\rho}^2 > k_0^2, \\ \frac{1}{\sqrt{|k_0^2 - k_{\rho}^2|}} & k_{\rho}^2 > k_0^2. \end{cases}$$

(5.37)

where $\rho = x\hat{x} + y\hat{y}$ and $k_{\rho} = k_{x}\hat{x} + k_{y}\hat{y}$. For given integers $p$ and $q$, the resultant $k_{\rho}^{p,q} = \sqrt{(k_x^p)^2 + (k_y^q)^2}$ may be smaller or greater than $k_0$. In the next section, by using (5.37), we will express the scattered field of the array in terms of $pq$-Floquet modes. We will show that for small values of $p$ and $q$, when $|k_{\rho}^{p,q}| < k_0$, the resultant $pq$-term is a propagating (visible) Floquet mode and while for large values of $p$ and $q$, when $|k_{\rho}^{p,q}| > k_0$, the $pq$-term is an evanescent (invisible) Floquet mode. The Floquet mode corresponded to $(p,q) = (0,0)$ is always visible.
because it results in \( k_{p,0}^{0,0} = \sqrt{(k_{x}^{inc})^2 + (k_{y}^{inc})^2} \), which is always less than \( k_0 \). In this chapter, we design the unit cell dimensions, \( \Lambda_x \) and \( \Lambda_y \), such that the Floquet modes corresponding to \( (p,q) \neq (0,0) \) are invisible. This assumption requires the condition in which the Floquet modes corresponded to \( (p,q) = (1,0) \) and \( (p,q) = (0,1) \) are invisible:

\[
\begin{align*}
\left( \frac{2\pi}{\Lambda_x} - k_{x}^{inc} \right)^2 + \left( k_{y}^{inc} \right)^2 &> k_0^2 \\
\left( k_{x}^{inc} \right)^2 + \left( \frac{2\pi}{\Lambda_y} - k_{y}^{inc} \right)^2 &> k_0^2
\end{align*}
\]

(5.38)

This is because when the two above-mentioned Floquet modes are invisible, the higher order modes, such as \( (p,q) = (1,1), (2,0) \), and so on, will be invisible as well. It can be shown that the above two conditions in (5.38) can be satisfied simultaneously when the unit-cell dimensions hold the following two conditions:

\[
\begin{align*}
\Lambda_x < \lambda_0 / 2 \\
\Lambda_y < \lambda_0 / 2
\end{align*}
\]

(5.39)

For our frequency range, 100 THz < \( f < 500 \) THz, the range for free-space wavelength is 600 nm < \( \lambda_0 < 3000 \) nm; hence, both the \( \Lambda_x \) and \( \Lambda_y \) must be less than 300 nm to avoid having more than one mode in the visible region. In our numerical results, we assume \( \Lambda_x = 150 \) nm and \( \Lambda_y = 250 \) nm satisfy this criterion. By replacing the closed form for \( \text{Int}(k_{p}, r) \) in (5.37) into the spectral representation of the \( mn \)-element of the CBF impedance matrix in (5.35) and by noting that there is only one visible Floquet mode, we obtain the following

\[
[z_{G}^{\text{CBF}}]_{mn} = \lim_{N_T \to \infty} [z_{G}^{\text{CBF} \text{Spec.}(N_T)}]_{mn}
\]

(5.40)
where $N_T$ is the truncation number for the infinite series embedded in the spectral representation of $[z_G^{\text{CBF}}]_{mn}$ as follows:

$$
[z_G^{\text{CBF}}]_{mn}^{\text{Spec.}(N_T)} = \frac{\eta}{2k_0 \Lambda_x \Lambda_y} \tilde{f}_m(k_y^{\text{inc}}) \tilde{f}_n(-k_y^{\text{inc}}) \left[ (k_y^{\text{inc}})^2 - k_0^2 \right] e^{-j \sqrt{k_0^2 - (k_{p,q})^2}} \sqrt{k_0^2 - (k_{p,q})^2} 
$$

$$
+ \frac{j \eta}{2k_0 \Lambda_x \Lambda_y} \sum_{p,q=-N_y}^{N_y} \tilde{f}_m(-k_y^{\text{inc}}) \tilde{f}_n(k_y^{\text{inc}}) \left[ (k_y^{\text{inc}})^2 - k_0^2 \right] e^{-j \sqrt{k_0^2 - (k_{p,q})^2}} \sqrt{k_0^2 - (k_{p,q})^2} 
$$

(5.41)

The only issue in numerical evaluation of the series given in (5.41) is computation of the FT for the CBFs, $\tilde{f}_m(k_y)$, which can be done efficiently and quickly in an analytical closed form. In Appendix A.V, we derive an analytical closed form formula for the FT of each of the CBFs in terms of the closed form formula for the FT of half- and full-triangular sinusoidal MBFs. Fig. 5-12 depicts the FT of the CBF#1 at $f=400$ THz whose spatial variation is shown in Figs. 5-8(b).

Fig. 5-12: Magnitude and phase of the Fourier transform of the CBF#1 at 400 THz computed analytically (solid blue line), and numerically, 400-point equally spaced numerical integration, (circular red marker), (a) $|\tilde{f}_1(k_y)|$, (b) Phase($\tilde{f}_1(k_y)$).

The FT is computed in Fig. 5-12 with 400-point equally spaced integration and with much faster analytical closed form. The horizontal axis in Fig. 5-12 is $k_y$ normalized to the $y$-component.
Floquet wave number, \(2\pi/\Lambda_y\), to show that the FT of CBF decays very quickly for higher Floquet modes, which is one reason for fast convergence of the spectral representation of the CBF-impedance matrix given in (5.41). Another reason is the decaying exponential \(\exp\left(-\left|\sqrt{(k_y^p q)^2}\right|\right)\), which goes to zero for higher order Floquet modes. To compare the speed of convergence of the spatial and spectral representations of the CBF-impedance matrix, we compute the (1,1)-element of the CBF-impedance matrix by spatial and spectral techniques. In the spatial method, we find \(\mathbf{z}_{G}^{\text{CBF}}\) in (5.20), where \(M\) is the number of rings, whereas in the spectral method, we compute \(\mathbf{z}_{G}^{\text{CBF}}\) in (5.41), where \(N_T\) is the truncation number of Floquet modes in (5.41). The results are shown in Fig. 5-13 for both normal and oblique incidence cases. The horizontal axis in Fig. 5-13 is the truncation number, which is \(M\) and \(N_T\), in spatial and spectral representations, respectively. As discussed before, the convergence in spatial scheme is slow and oscillatory; however, we improved the convergence with spectral scheme, which converges fast and without oscillation. For both normal and oblique after \(N_T=20\), we obtain the correct answer for the convergent value of impedance matrix in spectral domain, which takes only 0.4 sec on a 2.2 GHz Intel Core(TM)2 Duo CPU machine. For spatial technique on the same machine, it takes 2.3 sec for 20 rings and 26 sec for 80 rings.
Fig. 5-13: Magnitude and phase of the (1,1)-element of the CBF-impedance matrix at \( f = 400 \) THz computed by two methods: spatial (square marker) and spectral (plus marker) methods, (a) \( |\mathbf{z}_{CBF}^{G}_{1,1}| \) for normal incidence, (b) Phase(\( \mathbf{z}_{CBF}^{G}_{1,1} \)) for normal incidence, (c) \( |\mathbf{z}_{CBF}^{G}_{1,1}| \) for oblique incidence, (d) Phase(\( \mathbf{z}_{CBF}^{G}_{1,1} \)) for oblique incidence. The oblique incidence is for \((\psi, \theta, \phi) = (143^\circ, 25^\circ, 110^\circ)\). The spectral method is around 25 times faster than spatial method to obtain this result.

Up to this point, we have computed the CBF-impedance matrix efficiently, and the level of macro-CBF, \( C \), can be found accurately in (5.23). To summarize, a blend of spatial-spectral scheme is used to find the macro-CBF. In other words we first find the coefficients of CBFs employing the spatial scheme by a few rings, let us say 5 rings, \( M = 5 \), to find \( \mathbf{f}_{CBF}^{M} \) to calculate the shape of macro-CBF, which is required to compute \( C \) in (5.23). Then, to find \( \mathbf{z}_{CBF}^{G} \) in the denominator of (5.23), we use the spectral scheme to compute \( \mathbf{z}_{CBF}^{G}_{\text{spec.}(N_T)} \) in (5.41) with \( N_T = 20 \), for instance. We close this section by computing the macro-CBF at the
middle of the nanorod, \( I(y = 0) = CI_{shape}(y = 0) \). The results are shown for both normal and oblique cases in Fig. 5-14. The oscillatory curve is computed fully with spatial scheme, vs. ring index, however, the solid line is the convergent value of macro-CBF at the middle of nanorod, which uses just 5 rings, and the truncation number in spectral domain is \( N_t = 20 \).

![Graphs](image-url)

Fig. 5-14: Magnitude and phase of the macro-CBF at the middle of the central nanorod at \( f = 400 \) THz computed by spatial domain, the oscillatory curve (square marker) versus ring index, and the convergent value (solid line) computed by the blended spatial-spectral method by 5 rings and the truncation number equal to \( N_t = 20 \) in the corresponded spectral series, (a) \( |I(y = 0)| \) for normal incidence, (b) Phase(\( I(y = 0) \)) for normal incidence, (c) \( |I(y = 0)| \) for oblique incidence, (d) Phase(\( I(y = 0) \)) for oblique incidence. The oblique incidence is for \( (\psi, \theta, \phi) = (143^\circ, 25^\circ, 110^\circ) \).

The oscillatory curve is computed fully with spatial scheme, vs. ring index, however, the solid line is the convergent value of macro-CBF at the middle of nanorod, which uses just 5 rings, and the truncation number in spectral domain is \( N_t = 20 \).
5.2. Reflection and Transmission Coefficients

In this section, the reflection and transmission coefficients are obtained. In the spectral domain, the FT of the scattered field, $\tilde{E}^{\text{scat}}$, by using the convolution property in (A.III.5) is:

$$\tilde{E}^{\text{scat}} = \tilde{G}(k) \hat{y} \tilde{J}_y(k),$$  \hspace{1cm} (5.42)

where $\tilde{G}(k)$ is the FT of free-space dyadic Green’s function, given by [67]:

$$\tilde{G}(k) = \frac{j \eta \mathbf{k} - k_0^2 \mathbf{I}}{k_0^2 - k^2},$$  \hspace{1cm} (5.43)

where $\mathbf{I}$ is the identity dyad, and $\tilde{J}_y(k)$ in (5.42) is the FT of the current density represented by the infinite array given by (5.31) when $\tilde{f}_s(k_y)$ is replaced by FT of the macro-CBF, $\tilde{I}(k_y)$. Therefore $\tilde{E}^{\text{scat}}$ gets the following form

$$\tilde{E}^{\text{scat}}(k) = \frac{j \eta 4 \pi^2 k \mathbf{k}}{k_0^2 \Lambda_x \Lambda_y} \frac{k y - k_0^2 \hat{y}}{k^2 - k_0^2} \tilde{I}(k_y) \sum_{p,q=-\infty}^{\infty} \delta(k_x - k_x^p) \delta(k_y - k_y^q).$$  \hspace{1cm} (5.44)

If we take the inverse FT from $\tilde{E}^{\text{scat}}$ in (5.44) by using (A.III.2) and take the integrals with respect to $k_x$ and $k_y$ we get:

$$E^{\text{scat}}(r) = \frac{j \eta}{2 \pi k_0 \Lambda_x \Lambda_y} \left( - \nabla \frac{\partial}{\partial y} - k_0^2 \hat{y} \right) \sum_{p,q=-\infty}^{\infty} \tilde{I}(k_y^q) \text{Int}(k_p = k_x^p, r),$$  \hspace{1cm} (5.45)

where $\text{Int}(k_p, r)$ is defined and evaluated in (5.36) and (5.37), respectively. Moreover, in (5.45), we use the fact that the gradient of $\text{Int}(k_p, r)$ in (5.36) can be replaced by $j \mathbf{k} \text{Int}(k_p, r)$, i.e., $\nabla = j \mathbf{k}$. After replacing $\text{Int}(k_p, r)$ given by (5.36) in $E^{\text{scat}}(r)$ given by (5.45), we conclude that the scattered field from the infinite array is the summation of Floquet modes, and from the design
criterion discussed in the previous section in (5.39), only the Floquet mode corresponded to 
\((p,q)=(0,0)\) is a true propagating mode and the rest of the modes are evanescent. The reflection 
and transmission coefficients are far-field properties of the array which relate to the Floquet 
mode corresponding to \((p,q)=(0,0)\). Therefore, in (5.45), if we take into account only the visible 
mode, we determine

\[
E^{\text{scatter}}(r) = \frac{\eta}{2k_0 \Lambda_x \Lambda_y} \left(-\nabla \frac{\partial}{\partial y} - k_0^2 \hat{y} \right) \bar{I} (-k_y^{\text{inc}}) e^{-ik_y^{\text{inc}}r} \exp\left(-\frac{\rho_{\text{scat,far}}}{k_y^{\text{inc}}}ight). \tag{5.46}
\]

Without loss of generality, we assume that the reflection side of the array is \(z>0\), the transmission 
side is \(z<0\), the incident wave is down-coming, i.e. \(k_z^{\text{inc}} < 0\). Therefore, the reflected and transmitted plane waves can be written as following closed forms:

\[
E^{\text{ref}}(r) = \frac{-\eta}{2 \Lambda_x \Lambda_y} \left( k_{\text{ref}} k_z^{\text{inc}} - k_0^2 \hat{y} \right) \bar{I} (-k_y^{\text{inc}}) e^{-ik_y^{\text{inc}}r}, \tag{5.47}
\]

\[
E^{\text{tra}}(r) = \left\{ E_0 - \frac{\eta}{2 \Lambda_x \Lambda_y} \left( k_{\text{inc}} k_z^{\text{inc}} - k_0^2 \hat{y} \right) \bar{I} (-k_y^{\text{inc}}) \right\} e^{-ik_y^{\text{inc}}r}, \tag{5.48}
\]

where the transmitted wave in \(z<0\) is the summation of the incident and scattered field and \(k_{\text{ref}}\) is \(k_p^{\text{inc}} - k_z^{\text{inc}} \hat{z}\) along the specular direction (see Fig. 5-2(a)). Furthermore, power-based reflection 
and transmission coefficients computed by using the spherical coordinates depicted in Fig. 5-2(a) 
are given by:

\[
r_{\text{coeff}} = \frac{\left| E^{\text{ref}} \right|^2}{\left| E^{\text{inc}} \right|^2} = \left( \frac{\eta}{2 \Lambda_x \Lambda_y | \langle E \rangle_0 |} \right)^2 \sin^2 \left( \theta \right) \sin^2 \left( \phi \right) \cos^2 \left( \theta \right) | \bar{I} (-k_y^{\text{inc}}) |^2, \tag{5.49}
\]

\[
t_{\text{coeff}} = \frac{\left| E^{\text{tra}} \right|^2}{\left| E^{\text{inc}} \right|^2} = 1 + r_{\text{coeff}} - \frac{\eta |E_{0,y}|}{\Lambda_x \Lambda_y \cos(\theta) | \langle E \rangle_0 |^2} \text{Re} \left\{ \bar{I} (-k_y^{\text{inc}}) \right\}, \tag{5.50}
\]
The absorption loss coefficient can then be defined as:

\[ \text{Loss} = 1 - r_{\text{coeff}} - t_{\text{coeff}}. \quad (5.51) \]

The reflection and transmission coefficients for both normal and oblique excitations are plotted in Fig. 5-15 and compared with full wave FDTD simulation. For FDTD modeling, to achieve an accurate result, fine meshing for thin cross section must be used. Considering the large aspect ratio of the rod and its dispersive material property, the simulation is time consuming and it takes about 10 hours. A coarser mesh provides a faster computation (of about 5 hours) but is obviously less accurate. As observed in Fig. 5-15(a), our CBF model provides a good comparison. For oblique excitation, we use Sin/Cos single frequency calculation [39] in FDTD with coarse meshing, and the result is shown in Fig. 5-15(b). The calculation is performed at 24 points required approximately 5 days to complete.

Fig. 5-15: Reflection and transmission coefficients (in percentage) for normal and oblique incidence cases compared with FDTD. The FDTD result is with limited accuracy due to the mesh-size. (a) Normal incidence, (b) Oblique incidence.

In comparison, the CBFM is considerably faster (by orders of magnitude), and it takes only about 30 seconds for 73 samples of frequency to generate an accurate result. We also mention that, in contrast to the FDTD, the computational time in CBFM is relatively independent of the
angle of incidence, due mainly to the fact that the CBFs include all the features of different excitations. As regards the convergence of spectral series in (5.41), the truncation number equal to \( N_T = 20 \) or 25 is sufficient regardless of the angle of incidence because of the decaying exponential for higher order Floquet modes and the decaying behavior of the FT of the CBFs for relatively large \( |k_y| \). For both normal and oblique cases, the resonance frequency occurs at \( f = 262 \) THz, which is close to the resonant of the single nanorod \( f = 260 \) THz. This is mainly because the couplings between the elements are not strong. At the resonance, the reflection coefficient for normal and oblique is 76% and 54%, respectively, whereas the corresponding transmission coefficients are 2% and 29%, respectively. Hence, the absorption loss in normal case is 22% and in oblique case is 17%. More results for other oblique incidences are depicted in Fig. 5-16, by changing \( \psi, \theta, \) and \( \phi \).
Fig. 5-16: Reflection and transmission coefficients (in percentage) for different incident angles and different polarizations, (a) For three different values of \( \theta = 25^\circ, 55^\circ, \) and \( 85^\circ \). The values of \( \phi=0 \) and \( \psi=0 \) are fixed, (b) For three different values of \( \phi=30^\circ, 90^\circ, \) and \( 120^\circ \). The values of \( \theta=60^\circ \) and \( \psi=0^\circ \) are fixed, (c) For three values of \( \psi=30^\circ, 100^\circ, \) and \( 120^\circ \). The values of \( \theta=30^\circ \) and \( \phi=60^\circ \) are fixed.
Chapter 6

Scattering Performance of Plasmonic Nanorod Antennas in Randomly Tilted Disordered and Fibonacci Configurations

In this chapter, we formulate and investigate the optical performance of finite arrays of plasmonic nanorod antennas in randomly tilted disordered and Fibonacci configurations. To efficiently model the scattering performance of a nanorod we take advantage of Characteristic Basis Function Method (CBFM) in conjunction with Macro Basis Functions. We study how random rotations of the nanorods, as a disorder, may affect their electromagnetic response. Also, the impact of quasi-periodic order on the performance of the array in the form of two-dimensional Fibonacci quasi-lattice comprising of plasmonic nanorods with two different lengths is studied.
6.1. Randomly Tilted Disordered Array of Plasmonic Nanorods

Fig. 6-1(a) demonstrates a 15×15 array of plasmonic nanorods in x-y plane. The unit cell, comprising a plasmonic nanorod, is a rectangle with the dimensions of \( \Lambda_x = 100 \) nm and \( \Lambda_y = 170 \) nm. The plasmonic nanorod possesses \( L = 150 \) nm length and \( a = 7.5 \) nm radius and is made of silver which its permittivity can be characterized with Drude model, i.e.,

\[
\varepsilon_r = \varepsilon_{\infty} - \frac{d_p^2}{\pi} \ln\left(\frac{f - i f_d}{f_d}\right), \quad \text{with } \varepsilon_{\infty} = 5, f_p = 2175 \text{ THz and } f_d = 4.35 \text{ THz} \[57].
\]

![Fig. 6-1: Finite array of plasmonic nanorods (a) periodic array, (b) disordered array.](image)

The excitation is a planwave illuminating the nanorod at broadside with vertical polarization (along y-axis). Fig. 1(b) shows the same array with a random disorder in which each of the nanorods is randomly tilted around its centroid. The tilted angle between the direction of each of the nanorods and the y-axis varies randomly between ±30°. Such a disorder can be for example due to inherent fabrication limitations, or on intention to investigate a non-periodic phenomenon.
In order to quantitatively model how the deviation from the ideal periodic arrangement may affect the optical electromagnetic response, we take advantage of the CBFM. We have already characterized the performance of a doubly infinite periodic array of plasmonic metamaterial nanorods illuminated by an obliquely incident planewave by CBFM in Chapter 5. The main advantages of utilizing CBFM for analyzing large clusters of metamaterials are namely: 1) demonstrating small sized and well-conditioned matrix equation, and 2) being faster in speed and requiring less memory, by orders of magnitude, in compared to the conventional numerical methods. To solve the array problem comprising of \( N \) nanorods demonstrated in Fig. 1, we consider one nanorod, let us say element \(#m\) whose axis, \( v\)-axis, builds the angle \( \phi_m \) with the \( y\)-axis. The equivalent polarization current on element \(#m\), flowing along \( v\)-direction, satisfies the following polarization equation

\[
 j \omega \varepsilon_0 (\varepsilon_r - 1)(E_{\text{Scat}}^v + E_{\text{inc}}^v \cos(\phi_m)) = I_m(v) / (\pi a^2),
\]

(6.1)

where \( E_{\text{Scat}}^v \) is the \( v\)-component of the electric field scattered by all the elements measured at the top of the element \(#m\), i.e., \( z = a \), and \( E_{\text{inc}}^v \) is the incident electric field. The \( I_m(v) \) in (6.1) is an unknown function yet to be determined for \( 1 \leq m \leq N \).

To solve (6.1) with CBFM, according to the recipe discussed in [97], we expand the polarization current \( I_m(v) \) in terms of CBFs, whose singular values are greater than a threshold, \(-15\) dB, for instance. Such a criterion leads to a few number of CBFs, 1, 2 or 3, in the desired optical frequency range, \( 100 \text{ THz} < f < 500 \text{ THz} \). One significant benefit of the CBFM applied on (6.1), as discussed in [97], is because each of the CBFs is a superposition of piecewise sinusoidal Macro Basis Functions (MBFs), subsequently the electric field radiated by each of the
CBFs can be obtained in closed form. If we multiply both sides of (6.1) by each of the CBFs and take the integration along each of the nanorods, Galerkin’s testing [57,97], we achieve a matrix equation. The number of unknowns is $Nc \times N$, where $Nc$ is the number of CBFs for the operational optical frequency. The integration in the Galerkin’s testing can be carried out by using Gaussian Quadrature Rule (GQR) [57]. However, to take into account the interaction between the nanorods we may use less number of points in GQR if they are electrically far, 5 points for instance, and for the self-terms and adjacent elements 20 points in GQR render the scheme convergent. Solving the resultant matrix leads to finding the polarization current and consequently the scattered field by the array is computed.

Fig. 6-2 illustrates the magnitude of the scattered electric field, $|E|$, observed at $r = 3(\mu m)\hat{z}$ (2.5$\lambda$ at 250THz) for the periodic and disordered finite arrays (15×15) for two different cases.

![Graph of scattered field magnitude vs frequency.

Fig. 6-2: Optical scattering performance for arrays of plasmonic nanorods for finite periodic, disordered and doubly infinite configurations. In case I, $\Lambda_x=100$ nm and $\Lambda_y=170$nm, and in case 2, $\Lambda_x = \Lambda_y =250$ nm.
In case I the inter-element spacing is as what mentioned before, but in case II we increase the spacing to \( \Lambda_x = \Lambda_y = 250 \) nm. The first observed thing is that the more the coupling the wider the bandwidth [98]. Case I in general has a wider bandwidth than the case II. It is also interesting to note that the resonant frequency for the array with closer elements is lower than that for the array with farther elements. The resonant frequency of the periodic array in case II is close to the frequency at which the length of the nanorod is one half of the effective wavelength, \( \lambda_{\text{eff}} / 2 \) [76].

The \( \pm 30^\circ \) disorder in the alignments of the nanorods affects slightly the performance of the case II since the couplings are less in compared to the case I (less interaction). For case I, the disorder can shift up the resonance frequency for which the \( |E| \) is maximum. For the sake of comparison we also present the results for the infinite periodic array obtained according to the closed form formula for the reflection coefficient in [97].

### 6.2. Optical Performance of the Fibonacci Quasi-Lattice of Nanorods

Next, we investigate the scattering of a plane wave by a two-dimensional Fibonacci quasi-lattice of plasmonic nanorods which is an example of Deterministic Aperiodic (DA) arrays which have recently attracted a considerable interest due to their unique capability to robustly enhance and localize electromagnetic fields at multiple frequencies within engineered optical chips for nano-plasmonic applications [99,100].

In one spatial direction, i.e., \( x \)- or \( y \)-direction, a Fibonacci array of plasmonic nanorod antennas can be generated by using binary Fibonacci sequence consisting of two seed letters \( A \) and \( B \), which \( A \) represents one plasmonic nanorod with the length \( L_A \) and \( B \) represents the other plasmonic nanorod with a different length, \( L_B \). The Fibonacci sequence of order \( n \geq 2 \), \( F_n \), can be
generated according to the recursive formula, $F_n = F_{n-1} + F_{n-2}$, where $F_1 = A$, and $F_0 = B$. For example the one dimensional Fibonacci sequence of order 6 gets the following form:

$$F_6 = \text{ABAABABAAB AAB}.$$  \hspace{1cm} (6.2)

The length of the sequence $F_6$ is 13.

We design two plasmonic nanorods $A$ and $B$, to have the resonant frequencies at $f_A = 260$ THz and $f_B = 1.05 \times f_A = 273$ THz. Such a design can be approximately carried out by taking advantage of the algebraic closed form formula for the effective wavelength of a plasmonic nanorod in [76] when the physical length of the nanorod is one half of the effective wavelength. However to increase the accuracy of the design we use CBFM to find the frequency response of the magnitude of the scattered electric field by the plasmonic nanorod illuminated at broadside by a vertically polarized planewave. The maximum of the scattered field over an optical range of frequency gives the resonant frequency. For the same radius $a = 7.5$ nm and the same material, silver, for the both $A$ and $B$ nanorods we get $L_A = 150$ nm and $L_B = 139$ nm for the previously mentioned desired resonant frequencies (see Fig. 6-3). (The observation point is at $r = 3 \mu m \hat{z}$, assuming the nanorod is located along the $y$-axis).

Having the two designed nanorods $A$ and $B$, we can construct the $13 \times 13$ Fibonacci quasi-lattice of order 6, demonstrated in Fig. 4. The arrangement of the $A$ and $B$ nanorods located in the first row and column of the array in Fig. 4 is according to $F_6$ in (2). For other columns and rows, depending on the first element ($A$ or $B$) with which the column or row starts, the arrangement is either $F_6$ or $\overline{F}_6$ (the complement of $F_6$ for which $A$ and $B$ are simply interchanged).
Fig. 6-3: The magnitude of the scattered field by the designed A and B plasmonic nanorods to get the resonance at $f_A=260$ THz and $f_B=1.05f_A=273$ THz.

Fig. 6-4: Fibonacci quasi-lattice of order 6, 13×13. The array comprises of two different plasmonic nanorods, blue nanorod with lower resonant and red with higher resonant frequencies.
The optical performance of the 13×13 Fibonacci quasi-lattice of nanorods is illustrated in Fig. 6-5 by using the CBFM, described before. The result is also compared with the 13×13 alternative array which instead of \( F_6 \) it uses the alternative sequence \( S = \text{ABABABABABABA} \), of the length 13, and its complement \( \bar{S} \). The inter-element spacing in both x- and y-directions is \( \Lambda_x = \Lambda_y = 200 \text{ nm} \). For both of the Fibonacci and the alternative arrays, the frequency response can be described as a blend of two resonant response illustrated in Fig. 6-3. For the Fibonacci case the second resonance is slightly wider-band and closer to the first resonance. Moreover, in Fig. 6-5, we characterize the optical performance of the 53×13 alternative array, in which we bring the elements closer along the x-direction, \( \Lambda_x = 50 \) and \( \Lambda_y = 200 \) nm, but we increase the number of elements in x-direction to have approximately the same aperture size as the 13×13 alternative array. By bringing the elements closer to each other the two resonances are merged and a wider bandwidth is demonstrated.

Fig. 6-5: The optical performance of the Fibonacci and alternative quasi-lattices of plasmonic nanorods. Bringing the elements closer to each other can merge the two resonances.
We need to stress again that our model can characterize the performance of the finite arrays (disorder or Fibonacci) extremely fast and accurate. The modeling of the large arrays presented here takes about 6 min/40 frequency samples on the machine Alienware i7-3.47 GHz CPU with 8.00 GB RAM over the entire frequency band. Our technique can be used as a powerful engine for efficient analysis and novel design optimization of large and non-periodic plasmonic configurations.
Chapter 7

Conclusions and Possible Future Works

In chapter 2, Array of dielectric-plasmonic core-shell nanoparticles is developed to engineer the near-field pattern and enable subwavelength optical focusing. Dipolar mode equations along with the dyadic Green’s function formulation for the interaction between the elements are applied to summarize the required equations. Point matching method is used and a non-linear inverse scattering problem is determined to design the geometry of each array nanoparticle and establish the desired focusing pattern. Levenberg-Marquardt technique is successfully employed to solve the obtained set of nonlinear equations and find the polarizability of each element. The closed form formula for the polarizability of a concentric core-shell nanoparticle is then employed to find the geometry configuration (the core and shell radii) for each element (with the use of magnitude and phase contours of the polarizability).

Arrays of $5 \times 5$ and $11 \times 11$ nanoparticles are developed to focus the optical beam in a specified focal plane, successfully. The physical meanings of the numerical results are highlighted. The subwavelength focusing is achieved by proper superposition of shifted beams in near field of each of the nanoparticles. Our theoretical model is compared well with a full-wave
analysis based on the CST commercial software. Any component of the electromagnetic fields can be manipulated with the proper arrangements of the plasmonic nanoparticles. The proposed technique in chapter 2 enables a capable approach for near-field engineering of the optical patterns with the use of novel array of plasmonic nanoparticles.

Chapter 3 presents a fast and accurate computational scheme for characterizing complex elements structures. The focus has been on PEC cross-shaped elements but the applicability of the method is very broad. Macro Basis Functions approach is introduced to represent the physics of the structure with a simple and low-rank matrix equation. The accuracy is validated excellently by comparing the results with FEKO data. The required memory is reduced considerably and the computational time is expedited by orders of magnitude. We anticipate MBF method to be a capable and powerful paradigm for characterizing complex electromagnetic and antenna structures.

Physics-based MBFs are employed in chapter 4 to develop a computational scheme for accurate and efficient analysis of the scattering characteristics of plasmonic nanorod antennas. It is shown that the polarization current induced on the nanorod can be expressed in terms of very few Macro Basis Functions, for which either closed-form expressions can be derived, or can be rapidly computed by using an eight-point Gaussian integration scheme. The accuracy of the method has been validated via a comparison with the corresponding results derived by using the full-wave FDTD numerical technique. The frequency response of the plasmonic nanorod is investigated, both for the normal and oblique incidence case, by examining the induced currents and scattered fields. It is demonstrated that the proposed MBF scheme generates results with comparable accuracy, but requires only a small fraction of the time needed by the FDTD algorithm. It is also shown that the MBF-based method leads to small and well conditioned
matrices, which is not the case in conventional MoM formulation for problems of this type involving plasmonic nanorods, that are very difficult to handle by using existing commercial codes. Finally, we mention that the proposed technique is well suited for modeling other types of nanorods, such as Carbon Nano Tubes (CNTs) that have even longer aspect ratios, and are made of dispersive materials. In addition, the method is capable of handling much larger problems such as clusters of nanoparticles and arrays of plasmonic nanorods that are highly computer-intensive, both in terms of CPU memory and time.

A numerically efficient computational scheme, which is based on the CBFM, has been introduced in chapter 5 to characterize the performance of an array of plasmonic nanorods illuminated by an arbitrary plane wave. The SVD is applied to downselect a few basis functions representing the polarization current along the rod, thereby reducing the number of unknowns for different angles of incidence and different polarization states. A relatively small truncated array, comprising a few rings, is used to capture the shape of macro-CBF, and their levels are computed efficiently by applying the Parseval’s theorem. Closed-form formulas for reflection and transmission coefficients are derived, and are related to the FT of the macro-CBF at a wave-number dictated by the incident plane wave. The accuracy of the model is validated through comparison of full wave FDTD simulations. The proposed method is computationally efficient, and typically orders of magnitude faster than alternate approaches. Finally, the methodology is general and is well-suited for the task of characterizing other large clusters of metamaterials.

In chapter 6, we formulate and investigate the optical performance of finite arrays of plasmonic nanorod antennas in randomly tilted disordered and Fibonacci configurations. To efficiently model the scattering performance of a nanorod we take advantage of Characteristic Basis Function Method (CBFM) in conjunction with Macro Basis Functions. We study how
random rotations of the nanorods, as a disorder, may affect their electromagnetic response. Also, the impact of quasi-periodic order on the performance of the array in the form of two-dimensional Fibonacci quasi-lattice comprising of plasmonic nanorods with two different lengths is studied. Our technique can be used as a powerful engine for efficient analysis and novel design optimization of large and non-periodic plasmonic configurations.
Appendix

A.I. Levenberg-Marquardt Algorithm

Levenberg-Marquardt Algorithm [70,74], LMA, is an elegant and heuristic method for solving simultaneous nonlinear equations. It is indeed a nonlinear least-squares algorithm. Let us assume that there is a set of N nonlinear equations with N unknowns which can be written as

$$F(x) = 0,$$ \hspace{1cm} (A.I.1)

where $F=(F_1, F_2, F_3, ..., F_N)$ and $x=(x_1, x_2, x_3, ..., x_N)$. Instead of solving (A.I.1) directly, the summation of the squares, $s(x)$, defined as below, will be minimized:

$$s(x) = \frac{1}{2} \sum_{n=1}^{N} F_n^2(x).$$ \hspace{1cm} (A.I.2)

Hence, the efforts should be focused on obtaining the minimum of $s(x)$ which satisfies equation

$$\nabla s(x) = 0.$$ \hspace{1cm} (A.I.3)

There are two common iterative algorithms for minimizing $s(x)$, Gradient Descent Algorithm (GDA) and Gauss-Newton Algorithm (GNA). As we illustrate in this appendix, LMA is just a blend of these two algorithms.
In GDA, which is actually the most intuitive technique to find the minima of a function, state update is performed by adding the negative scaled gradient at each step:

\[ x_{i+1} = x_i - \gamma_i \nabla s(x_i), \quad (A.I.4) \]

where \( \gamma_i > 0 \) is the step size. When the gradient is small we would like to take large steps (large \( \gamma_i \)); conversely, small steps should be taken when the slope is not gentle (large gradient). The search direction \( d_i = -\gamma_i \nabla s(x_i) \) causes a convergent problem when the surface has a long and narrow valley. In this case, GDA is just rattling out the minima as the search direction is very small at the base of the valley and very large along the valley walls. To provide a successful LMA solver, the GDA’s bottle-neck and its advantage must be weighted properly (as will be seen later).

In GNA, the gradient of the function is expanded around the current state, \( x_i \), given by the Taylor series:

\[ \nabla s(x_{i+1}) = \nabla s(x_i) + [H(x)](x_{i+1} - x_i) + \text{Higher Order Terms}, \quad (A.I.5) \]

where \([H(x)]\) is the Hessian matrix defined by

\[ [H(x)]_{m,n} = -\frac{\partial^2 s}{\partial x_m \partial x_n}, \quad (A.I.6) \]

As long as \( s(x) \) has a quadratic behavior around the minima, higher order terms of \( (x_{i+1} - x_i) \) can be neglected and the state update is found for GNA as

\[ x_{i+1} = x_i - [H(x_i)]^{-1} \nabla s(x_i). \quad (A.I.7) \]

A closed form formula for Hessian can be obtained by taking a double gradient of (A.I.2) as follows
\[
\n\n\frac{\partial s(x)}{\partial x} = \sum_{n=1}^{N} F_n(x) \frac{\partial F_n(x)}{\partial x} = [J(x)]^T F(x), \tag{A.I.8}
\]

\[

[H(x)] = \nabla^2 s(x) = [J(x)]^T [J(x)] + \sum_{n=1}^{N} F_n(x) \nabla^2 F_n(x), \tag{A.I.9}
\]

where \( [J(x)] \) is the Jacobian defined as, \( [J(x)]_{m,n} = \frac{\partial F_m}{\partial x_n} \). According to (A.I.1), it is possible to assume each nonlinear function, \( F_m(x) \), small near the solution so that an approximation for Hessian can be determined as given below

\[

[H(x)] = [J(x)]^T [J(x)]. \tag{A.I.10}
\]

When around the minima \( s(x) \) has a quadratic behavior, GNA converges rapidly. So GNA and GDA are complementary in the advantages they provide. Levenberg proposed an algorithm whose update rule is a blend of GNA and GDA which is given by

\[
x_{i+1} = x_i - ([H(x_i)] + \gamma_i [I])^{-1} \nabla s(x_i), \tag{A.I.11}
\]

where \([I]\) is the identity matrix. Following an update, if the error is reduced, it implies that the quadratic assumption on \( s(x) \) is working and we reduce \( \gamma_i \) (usually by a factor of 10) to reduce the influence of GDA. On the other hand, if the error is increased, GDA is more prior to be followed; and hence \( \gamma_i \) is increased by the same factor.

When the value of \( \gamma_i \) is large, larger movement should be taken along the directions where the curvature is low, this crucial insight was provided by Marquardt. Since the diagonal terms of the Hessian are proportional to the curvature of \( s(x) \), Marquardt replaced the identity matrix in (A.I.10) with the diagonal terms of Hessian, resulting to the well-known Levenberg-Marquardt update rule (after we replace the gradient by (A.I.8)).
\[ x_{i+1} = x_i - ([H(x_i)] + \gamma \text{diag}[H(x_i)])^{-1} [J(x)]^T F(x). \]  
(A.I.12)

LMA works extremely well in practice and has become the standard of nonlinear least-squares solvers.

**A.II. Computing the Level of Macro-CBF**

In this appendix, we derive a closed form formula for the level of macro-CBF introduced in (5.22). If we replace the macro-CBF given by (5.22) in the polarization current equation in (5.12), we get

\[ j \omega \epsilon_0 (\epsilon_r - 1)(E_y^{\text{inc}} + CE_y^{\text{shape}}) = CI_{\text{shape}}(y)/(\pi a^2), \quad -L/2 \leq y \leq L/2 \]  
(A.II.1)

where \( E_y^{\text{shape}} \) is the y-component of the electric field radiated by the infinite elements of the array when the \( pq \)-element carries the current \( e_{pq} \times I_{\text{shape}}(y) \), and \( e_{pq} \) is the inter-element phasing factor introduced in (5.11). Indeed \( E_y^{\text{shape}} \) can be written in a closed form as follows:

\[ E_y^{\text{shape}} = \sum_{n=1}^{N_n} I_n^{\text{CBF}(M)} \sum_{p,q=0}^{+\infty} e_{pq} G_{pq}^{\text{CBF},n}, \]  
(A.II.2)

and \( I_n^{\text{CBF}(M)} \) is the coefficient of CBF\#n at stage\#M, after M rings. To find the only unknown, \( C \), we test (A.II.1) by \( I_{\text{shape}}(y) \) at the top of the central element, \((x,y,z) = (0,y,a)\), to obtain:

\[ C = \frac{-V_{\text{tot}}}{\text{Int}_G - \text{Int}_{\text{res}}}, \]  
(A.II.3)

where

\[ V_{\text{tot}} = \int_{-L/2}^{L/2} E_y^{\text{inc}}(y)I_{\text{shape}}(y)dy, \]  
(A.II.4)

\[ \text{Int}_G = \int_{-L/2}^{L/2} E_y^{\text{shape}}(y)I_{\text{shape}}(y)dy, \]  
(A.II.5)
\[ \text{Int}_{\text{res}} = \frac{-j\eta}{\pi a^2 k_0 (\epsilon_r - 1)} \int_{-L/2}^{L/2} (l_{\text{shape}}(y))^2 \, dy. \]  

(A.II.6)

we can rewrite \( V_{\text{tot}}, \text{Int}_G, \) and \( \text{Int}_{\text{res}} \) in terms of \( [I^{\text{CBF}}]^{M_3}, N \times 1 \) matrix including the CBFs coefficients after \( M \) rings for \( l_{\text{shape}}(y) \), after we replace the expressions for \( l_{\text{shape}}(y) \) and \( E_y^{\text{shape}} \), given by (5.22) and (A.II.2), respectively, into (A.II.4- A.II.6), to obtain the following expressions by using the definitions for voltage and impedance matrices in (5.16-5.18):

\[
\begin{align*}
V_{\text{tot}} &= \left( [I^{\text{CBF}}]^{M_3} \right)^T \left[ V^{\text{CBF}} \right] \\
\text{Int}_G &= \left( [I^{\text{CBF}}]^{M_3} \right)^T \left[ Z^{\text{CBF}} \right] \left( [I^{\text{CBF}}]^{M_3} \right), \\
\text{Int}_{\text{res}} &= \left( [I^{\text{CBF}}]^{M_3} \right)^T \left[ Z^{\text{res}}_{\text{CBF}} \right] \left( [I^{\text{CBF}}]^{M_3} \right). 
\end{align*}
\] 

(A.II.7) \hspace{1cm} (A.II.8) \hspace{1cm} (A.II.9)

Notice that \( T \) denotes matrix transpose (and not conjugate transpose). Replacing the matrix expressions for \( V_{\text{tot}}, \text{Int}_G, \) and \( \text{Int}_{\text{res}} \) given by (A.II.7- A.II.9) in (A.II.3) will get the closed form expression for the level of macro-CBF brought in (5.23).

**A.III. Useful Identities in Fourier Transform**

This Appendix shows the definitions for required Fourier transforms (FTs) used in chapter 5. For \( f(r) \), a scalar function in spatial domain, we use the following definition for its FT, \( \tilde{f}(k) \):

\[
\tilde{f}(k) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} f(r) e^{-jkr} \, dx \, dy \, dz,
\] 

(A.III.1)

where \( k = (k_x, k_y, k_z) \), and \( r = (x, y, z) \). Then the inverse FT of \( \tilde{f}(k) \) gets the following formula

\[
f(r) = \frac{1}{(2\pi)^3} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \tilde{f}(k) e^{+jkr} \, dk_x \, dk_y \, dk_z.
\] 

(A.III.2)
The Parseval theorem for two scalar functions \( f(\mathbf{r}) \) and \( g(\mathbf{r}) \) is as follows [96]:

\[
\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} f(\mathbf{r}) g(\mathbf{r}) \, d\mathbf{r} = \frac{1}{(2\pi)^3} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \hat{f}(\mathbf{k}) \hat{g}(\mathbf{k}) e^{-j\mathbf{k}\cdot\mathbf{r}} \, dk_x \, dk_y \, dk_z,
\]

where symbol tilde, \( \sim \), denotes the FT. The other useful formula used in the paper, is the impulse-train identity [96], which is

\[
\sum_{p=-\infty}^{+\infty} e^{-jwp} = 2\pi \sum_{p=-\infty}^{+\infty} \delta(A - 2\pi p),
\]

where \( A \) is a constant. And finally, the FT of a convolution of \( f(\mathbf{r}) \) and \( g(\mathbf{r}) \) can be written as the multiplication of their FTs:

\[
\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} f(\mathbf{r}) g(\mathbf{r} - \mathbf{r}') \, d\mathbf{r} d\mathbf{r}' \rightarrow \hat{f}(\mathbf{k}) \hat{g}(\mathbf{k}).
\]

**A.IV. Physics Based Residual Calculus to Evaluate an Integral**

In this appendix, we will evaluate, in closed form, the integral given by (5.36), which can be rewritten as

\[
\text{Int}(k_{\rho}, \mathbf{r}) = e^{jk_{\rho} \cdot \mathbf{r}} \int_{-\infty}^{\infty} \frac{e^{j k_z z}}{k_z^2 + k_{\rho}^2 - k_0^2} \, dk_z.
\]

(A.IV.1)

For \( k_{\rho}^2 < k_0^2 \), the integrand has real poles, \( k_z = \pm \sqrt{k_0^2 - k_{\rho}^2} \), lie on the real \( k_z \)-axis, rendering the integral in (A.IV.1) undefined [24]. If we assume a very small conductivity \( \sigma \) for the free space, instead of \( k_0 \), a complex \( k_0 \angle -\delta \) is used, where \( \tan(\delta) = \sigma \eta / k_0 \) is the very small loss tangent. Such a physical assumption makes the poles become off the real axis by a small angle \( \delta \) as
shown in Fig. A-1(a) and render the integral in (A.IV.1) well-defined. When $z>0$, because of $\exp(jk_z z)$ in the numerator of the integrand, to apply the Cauchy’s theorem with Jordan’s lemma [26], the infinite semi-circular contour must be closed in upper half-$k_z$-plane, for which the Im($k_z$)>0. The lower contour is used for $z<0$. Then by applying the Cauchy’s theorem with Jordan’s lemma [26], (A.IV.1) becomes the following

$$Int(k_\rho, r) = -j\pi e^{jk_\rho \rho} e^{-j|k_\rho^2-k_0^2|z} \frac{k_0^2 > k_\rho^2}{\sqrt{k_0^2 - k_\rho^2}}.$$  \hspace{1cm} (A.IV.2)

When $k_\rho^2 > k_0^2$, the two poles are pure imaginary complex conjugates as depicted in Fig. A-1(b) and by using the proper contour for the proper sign of $z$, as discussed above, we get the following for $Int(k_\rho, r)$:

$$Int(k_\rho, r) = \pi e^{jk_\rho \rho} e^{-j|k_\rho^2-k_0^2|z} \frac{k_0^2 > k_\rho^2}{\sqrt{k_0^2 - k_\rho^2}}.$$  \hspace{1cm} (A.IV.3)
Fig. A-1: The proper infinite semi-circular contours to evaluate the integral in (A.IV.1), (a) For $k_0^2 < k_0^2$, (b) For $k_0^2 < k_0^2$.

**A.V. Closed Form Formula for the FT of the CBFs**

The Fourier Transform (FT) of the half and full triangular sinusoidal MBFs, and the resultant CBF are discussed in this appendix. Referring to Fig. 5-3(d), the right half-MBF can be written as follows

$$b_{\text{right}}(y; H) = \begin{cases} \sin(k_0(-y + H)) & 0 < y < H \\ 0 & \text{oth.} \end{cases}$$

(A.V.1)

If we take the FT from (A.V.1), by using (A.III.1), we get

$$\tilde{b}_{\text{right}}(k_y; H) = -\frac{k_0}{k_0 + k_y} \left\{ j \frac{\sin(k_0H)}{k_0} + \frac{e^{-jk_yH} - e^{-jk_0H}}{k_y - k_0} \right\}.$$ 

(A.V.2)

For the left MBF, because $b_{\text{left}}(y; H) = b_{\text{right}}(-y; H)$, by using the FT properties we get
\[ \tilde{b}_{\text{left}}(k_y;H) = \tilde{b}_{\text{right}}(-k_y;H). \] 
(A.V.3)

And for the full MBF we have, \[ \tilde{b}_{\text{full}}(k_y;H) = \tilde{b}_{\text{left}}(k_y;H) + \tilde{b}_{\text{right}}(k_y;H). \] For a CBF, \( f(y) \), one can express it as a summation of shifted MBFs (see Fig. 5-3(c)) as follows

\[
 f(y) = I_1^{MBF} b_{right}(y + L/2) + I_{N_{MBF}}^{MBF} b_{left}(y - L/2) \\
+ \sum_{n=2}^{N_{MBF}-1} I_n^{MBF} b_{full}(y + L/2 - (n-1)H). 
\] 
(A.V.4)

By using the FT properties, the FT of the CBF gets the following closed form

\[
 \tilde{f}(k_y) = I_1^{MBF} e^{jk_y L/2} \tilde{b}_{right}(k_y) + I_{N_{MBF}}^{MBF} e^{-jk_y L/2} \tilde{b}_{left}(k_y) \\
+ \sum_{n=2}^{N_{MBF}-1} I_n^{MBF} e^{jk_y (L/2-(n-1)H)} \tilde{b}_{full}(k_y). 
\] 
(A.V.5)
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Note: Chapters 2-6 have been taken from my PhD papers which are: [6], [102], [57], [97] and [101], respectively.