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Multipole methods for Nano-antennas design : applications to Yagi-Uda configurations

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Abstract

We present a detailed formalism allowing analytical calculations of the radiative properties of nano-antennas. This formalism does not rely on dipole approximations and utilizes multipolar multiple-scattering theory. The improvement in both accuracy and calculation speeds offered by this formulation provides significant advantages that are used in this work to study Yagi-Uda type nano-antennas. We provide a study which questions the necessity of the reflector particle in nano-antennas.

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I. INTRODUCTION

There is an increasing interest in using nano-antennas to extract[1-12] and redirect light[13-23] from quantum emitters such as single molecule fluorophores and quantum dots. Although the emission processes under consideration are intrinsically quantum phenomena, the decay rates of a quantum system depend on the modifications of the local electromagnetic environment induced by the antenna structure. Given that the structures of typical optical antennas, although small, are generally large with respect to the atomic scale (nano to micro-meter scales overall), semi-classical electromagnetic calculations are usually the most convenient method available for calculating modifications to decay rates and radiation patterns.

In semi-classical calculations, the quantum emitter is replaced by a radiating dipole, and one calculates the modifications to the emitted power, the radiated power, and the radiation distribution that are induced by the antenna structure. These properties in turn allow one to deduce the modifications to the decay rate and radiation pattern of a quantum emitter. Such calculations require precise information on both near and far-fields, and generally tend to be quite time-consuming even for modern computers. A notable exception to the previous statement are Mie-type calculations of quantum emission properties in the neighborhood of a single spherical particle. In that case, the multipole approach of the Mie theory allows one to formulate the physical quantities of interest in terms of analytical formulas which are both highly accurate and rapid to calculate.[24–27]

Generalized Mie theory, [28–30] has well established advantages for studying the scattering by multiple-particle systems, including orders of magnitude reductions in computation times. Nevertheless, even in the multipole context, the calculation of nano-antenna properties previously required laborious numerical integrations of the Poynting vector in both the near and far-field. In this work, we derive multipole formulas for analytically evaluating theses integrals when a quantum emitter is placed in the neighborhood of an antenna structure. Although such multiple scattering techniques can be applied to systems in which the antenna components are non-spherical, [31] we will restrict ourselves in this work to examples of antennas with spherical components where they can be most readily applied.

In the interest of completeness, section II presents a brief overview of the Green function and multiple-scattering formulations for treating electromagnetic sources and scattering. Exact multipole formulas for decay rate enhancements and directivity are derived in section III.

Despite their accuracy, the complexity of multipole techniques can make it difficult to analyze their physical content. Modeling the antenna particles as induced dipoles allows more intuitive physics, and in certain situations can provide relatively good estimations of the electromagnetic response provided that the radiation damping effects are accurately modeled. An alternative coupled dipole formulation incorporating new analytic formulas for the radiative properties of nano-antennas is formulated in section IV.

In section V, we use these multipolar and dipolar formulations to study the influence of number of particles and the presence of reflector particles in nano-antenna designs of the Yagi-Uda type. More precisely, we show that the negative role of the reflector particle on both radiation properties and quantum efficiencies is not always outweighed by gains in directivity.

II. GREEN FUNCTION FORMULATION

Given the large quantity and variety of physical information that one wishes to treat during antenna calculations, it proves advantageous to formulate the problem in terms of Green functions. The complexity of the antenna Green function is the chief obstacle to such calculations. We will see below and in section III however that the multipole formulation makes this problem tractable.

A fundamental assumption of this work (which can be relaxed) is that the quantum emitter is sufficiently small with respect to both the antenna structure and the field variations to be approximated as a point dipole. The antenna is considered to consist of particles immersed in a homogeneous medium described by a (possibly complex) relative dielectric function $\varepsilon_b(\omega)$. With these assumptions, we model the currents in the quantum emitter, \mathbf{j}_e , by a time harmonic point dipole with strength \mathbf{p}_e , located at a point \mathbf{x}_e within the homogeneous media. The polarization current for such a point dipole is given by $\mathbf{j}_e(\mathbf{x}) = -i\omega\mathbf{p}_e\delta^3(\mathbf{x}-\mathbf{x}_e)$.

The dyadic Green function, $\overleftarrow{\mathbf{G}}$, of the antenna contains the information necessary for electromagnetic calculations in that it yields the electric field everywhere via the integral

formula[28]:

$$\mathbf{E}(\mathbf{x}) = i\omega\mu_0 \int d\mathbf{x}' \,\overleftrightarrow{\mathbf{G}}(\mathbf{x} - \mathbf{x}') \,\mathbf{j}_e(\mathbf{x}') \quad . \tag{1}$$

We simplify matters by restricting $\overleftarrow{\mathbf{G}}(\mathbf{x} - \mathbf{x}')$ to situations where both the source current positions, \mathbf{x}' , and 'receptor' positions, \mathbf{x} , are located within the host medium. The Green function can then be separated into an 'unperturbed' Green function of the homogeneous exterior medium Green function, $\overleftarrow{\mathbf{G}}_{0}$, plus a 'scattering' contribution, $\overleftarrow{\mathbf{G}}_{s}[28, 32]$:

$$\overleftrightarrow{\mathbf{G}}(\mathbf{x}, \mathbf{x}') = \overleftrightarrow{\mathbf{G}}_{0}(\mathbf{x}, \mathbf{x}') + \overleftrightarrow{\mathbf{G}}_{s}(\mathbf{x}, \mathbf{x}') \quad .$$
⁽²⁾

The homogeneous 'unperturbed' Green function is translationally invariant and satisfies the equation

$$\nabla \times \nabla \times \overleftrightarrow{\mathbf{G}}_{0}(\mathbf{x} - \mathbf{x}') - k_{b}^{2} \overleftrightarrow{\mathbf{G}}_{0}(\mathbf{x} - \mathbf{x}') = \overleftrightarrow{\mathbb{I}} \delta^{3}(\mathbf{x} - \mathbf{x}') , \qquad (3)$$

where $k_b = (\omega/c)\sqrt{\varepsilon_b}$ is the wavenumber of the exterior medium. A technical difficulty is that $\overleftarrow{\mathbf{G}}_0$ is singular at the origin, but this has been studied in detail and one can show that $\overleftarrow{\mathbf{G}}_0$ can be well defined provided that we treat it as a distribution and take care in treating the limit $\mathbf{x} \to \mathbf{x}'$.[28] Expressing $\overleftarrow{\mathbf{G}}_0$ in direct space with $\mathbf{r} \equiv \mathbf{x} - \mathbf{x}'$, one has[28, 32]:

$$\overleftarrow{\mathbf{G}}_{0}\left(\mathbf{r}\right) = \frac{e^{ik_{b}r}}{4\pi k_{b}^{2}r^{3}} \mathrm{P.V.}\left\{\left(1 - ik_{b}r\right)\left(3\widehat{\mathbf{r}}\widehat{\mathbf{r}} - \overleftarrow{\mathbf{I}}\right) + k_{b}^{2}r^{2}\left(\overleftarrow{\mathbf{I}} - \widehat{\mathbf{r}}\widehat{\mathbf{r}}\right)\right\} - \frac{\overleftarrow{\mathbf{I}}}{3k_{b}^{2}}\delta^{3}\left(\mathbf{r}\right) ,\quad (4)$$

where P.V. stands for principal value and $\overleftrightarrow{\mathbb{I}}$ is the unit dyadic. As explained in ref.[28], the 3D delta function term depends on the exclusion volume chosen for the principal value. The formula presented here corresponds to a principal value chosen as either a spherical or cubic infinitesimal value around the source point. Replacing the total Green function in eq.(1) with the homogeneous Green function of (4) yields the electric field, \mathbf{E}_0 , produced by an isolated point dipole:

$$\mathbf{E}_{0}\left(\mathbf{x}\right) = \frac{e^{ik_{b}r}}{4\pi\varepsilon_{b}\epsilon_{0}r^{3}}\left\{\left(1 - ik_{b}r\right)\left[3\widehat{\mathbf{r}}\left(\widehat{\mathbf{r}}\cdot\mathbf{p}_{e}\right) - \mathbf{p}_{e}\right] + k_{b}^{2}r^{2}\left[\mathbf{p}_{e} - \widehat{\mathbf{r}}\left(\widehat{\mathbf{r}}\cdot\mathbf{p}_{e}\right)\right]\right\} - \frac{\mathbf{p}_{e}}{3\varepsilon_{b}\epsilon_{0}}\delta^{3}\left(\mathbf{r}\right) .$$
 (5)

The information coming from the antenna structure is embodied in the scattering part of the total Green function, $\overleftarrow{\mathbf{G}}_{s}$. The scattering Green function, $\overleftarrow{\mathbf{G}}_{s}$, must take into account the multiple scattering of the emitter radiation from all the N components of the antenna structure. For the purpose of calculation, it is advantageous to express the scattering Green function in terms of a multiple scattering T-matrix which we define in operator notation as:

$$\overleftrightarrow{\mathbf{G}}_{s} = \overleftrightarrow{\mathbf{G}}_{0} \left(\sum_{i=1,j=1}^{N} \overleftrightarrow{\mathbf{T}}^{(i,j)} \right) \overleftrightarrow{\mathbf{G}}_{0}$$
(6)

where *i* and *j* are particle labels. The multiple scattering T-matrix in this equation has thus been split up into N^2 operators, $\overleftarrow{\mathbf{T}}^{(i,j)}$. From a multiple scattering viewpoint, one can visualize each $\overleftarrow{\mathbf{T}}^{(i,j)}$ as representing all multiple scattering events in which the first particle encountered by incident radiation is *j* and the last particle to be encountered is *i*.[29]

The $\overleftarrow{\mathbf{T}}^{(i,j)}$ can be manageably calculated in the vector partial-wave (VPW) basis:

$$\overleftarrow{\mathbf{T}}^{(i,j)} = \sum_{q=1,q'=1}^{2} \sum_{n=1;n'=1}^{\infty} \sum_{m=-n}^{m=n} \sum_{m'=-n'}^{m'=n'} |\Psi_{q,n,m}\rangle T_{q,n,m;q',n',m'}^{(i,j)} \langle \Psi_{q'n',m'}|$$
(7)

where $|\Psi_{q,n,m}\rangle$ are the vector partial wave states (see the appendix A 2 for explicit representations) and are specified by the 3 discrete 'quantum' numbers: $q = 1, 2; n = 1, 2, ...\infty$; and m = -n, ..., n (which for the purpose of numerical computations can be combined into a single discrete index[30, 34]). The great advantage of the VPW basis, is that the $\overleftarrow{\mathbf{T}}^{(i,j)}$ operator is determined as an infinite dimensional matrix in the VPW space that can be calculated from the T-matrices of the isolated particles, denoted $t^{(j)}$ (j = 1, ..., N), and the pairwise translation-addition matrices, $H^{(i,j)}$, between particle centers (see eq.(8) below). The $T^{(i,j)}$ matrices, henceforth referred to as body-centered T-matrices, can be rendered finite by truncating the orbital quantum numbers, n, to some finite dimension, n_{max} (whose value depends on particle sizes and interaction strengths).

A number of different methods for calculating the $T^{(i,j)}$ matrices exist in the literature (generally formulated within the Foldy-Lax framework[30, 33, 34]). Probably one of the simplest methods (both conceptually and numerically) is to extract the $T^{(i,j)}$ as the submatrices obtained after inversion of the following system matrix, *i.e.*,

$$\begin{bmatrix} T_N^{(1,1)} & T_N^{(1,2)} & \cdots & T_N^{(1,N)} \\ T_N^{(2,1)} & T_N^{(2,2)} & \cdots & T_N^{(2,N)} \\ \vdots & \vdots & \ddots & \vdots \\ T_N^{(N,1)} & T_N^{(N,2)} & \cdots & T_N^{(N,N)} \end{bmatrix} = \begin{bmatrix} \begin{bmatrix} t^{(1)} \end{bmatrix}^{-1} & -H^{(1,2)} & \cdots & -H^{(1,N)} \\ -H^{(2,1)} & \begin{bmatrix} t^{(2)} \end{bmatrix}^{-1} & \cdots & -H^{(2,N)} \\ \vdots & \vdots & \ddots & \vdots \\ -H^{(N,1)} & -H^{(N,2)} & \cdots & \begin{bmatrix} t^{(N)} \end{bmatrix}^{-1} \end{bmatrix}^{-1}$$
(8)

where $H^{(j,l)} \equiv H(k_b (\mathbf{x}_j - \mathbf{x}_l))$ are irregular translation matrices (analytical expressions for the matrix elements of $H(k\mathbf{x})$ as well as those of the regular translation matrix, $J(k\mathbf{x})$, are given in references[28, 29, 35]).

It should be remarked that such direct matrix inversions were for a long time disregarded in 3D calculations due to the fact that matrices like the one on the right hand side of eq.(8) were numerically ill-conditioned for matrix inversion. However, it has been recently pointed out that such direct matrix inversions work quite well provided that one employs analytical matrix balancing techniques.[30] In lieu of employing matrix balancing, many multiple-scattering codes privilege iterative techniques where the ill-conditioning of the problem can also be handled via conjugate gradient techniques. Although numerically performant, iterative techniques pose the disadvantage of having an additional convergence parameter and not all iterative formulations determine the $T^{(i,j)}$ matrices.

Once the on-shell T-matrices has been determined using eq.(8) or an alternative technique, we can derive analytic expressions for the electromagnetic properties of the antenna system such as decay rates, local fields and far-field emission. Notably, the total emitted power is evaluated by time averaging $P_{\rm t} \equiv -\mathbf{E}_{\rm t} \cdot \mathbf{j}_{\rm src}$ over a period where $\mathbf{E}_{\rm t}$ is the electric field produced by the source current while taking into account interactions with the antenna structure. Averaging this power over a period, $T = 2\pi/\omega$, we obtain[32]:

$$\Gamma_{\rm t} \equiv -\frac{1}{T} \int_0^T dt \int d\mathbf{x} \, \mathbf{E}_{\rm t}\left(\mathbf{x}, t\right) \cdot \mathbf{j}_e\left(\mathbf{x}, t\right) = \frac{\omega^3}{2} \mu_0 \, \mathrm{Im} \left\{ \mathbf{p}_e^*\left(\mathbf{x}_j\right) \cdot \overleftarrow{\mathbf{G}}\left(\mathbf{x}_j, \mathbf{x}_j\right) \cdot \mathbf{p}_e\left(\mathbf{x}_j\right) \right\} \tag{9}$$

Some of the power emanating from the dipole emitter will be dissipated by the antenna. The rest will be radiated off into the far field where it can be detected. The calculation of the radiated power proceeds by first taking the far-field limit of the electric field given by eq.(1). The electric field is transverse in the far-field limit, and we can readily obtain the **H** field from the electric field via the relation[36]:

$$\lim_{r \to \infty} \mathbf{H}_{t}(\mathbf{r}) = \frac{k_{b}}{\mu_{0}\omega} \widehat{\mathbf{r}} \wedge \mathbf{E}_{t}$$
(10)

In the $r \to \infty$ limit, the time averaged Poynting vector is thus:

$$\lim_{r \to \infty} \langle \mathbf{S} \rangle = \lim_{r \to \infty} \frac{1}{2} \operatorname{Re} \left\{ \mathbf{E}_{t}^{*} \wedge \mathbf{H}_{t} \right\} = \frac{1}{2} \frac{k_{b}}{\omega \mu_{0}} \widehat{\mathbf{r}} \left\| \mathbf{E}_{t} \right\|^{2}$$
(11)

The far-field irradiance, $I_r(\theta, \phi)$, and total radiated power are defined respectively by:

$$I_{\rm r}\left(\theta,\phi\right) \equiv \lim_{r \to \infty} r^2 \left< \mathbf{S} \right> \cdot \hat{\mathbf{r}} \qquad \text{and} \qquad \Gamma_{\rm r} \equiv \int d\Omega \, I_{\rm r}\left(\theta,\phi\right) \tag{12}$$

In order to determine the modifications to Γ_t , $I_r(\theta, \phi)$, and Γ_r induced by the antenna, we will need to normalize these values with respect to the corresponding quantities of an isolated emitter placed inside the homogeneous background. In this case, the analytical expressions for the field and homogeneous Green function of eqs.(4) and (5) yield the textbook results for dipole emission in a homogeneous medium. Notably, the power emitted in a homogeneous dielectric medium is:

$$\Gamma_{\mathbf{t},0} = \frac{\omega^3}{2} \mu_0 \operatorname{Im} \left\{ \mathbf{p}_e^*(\mathbf{x}_j) \cdot \overleftarrow{\mathbf{G}}_0(\mathbf{x}_j, \mathbf{x}_j) \cdot \mathbf{p}_e(\mathbf{x}_j) \right\} = \left| \mathbf{p}_e \right|^2 \frac{\omega^3}{12\pi\epsilon_0 c^2} \operatorname{Re} \left\{ k_b \right\}$$
(13)

The classic far-field radiation pattern and radiated power, Γ_0 , are readily obtained from eq.(5) applied to eqs.(11) and (12):

$$I_{\mathrm{r},0}\left(\widehat{\mathbf{r}}\right) = \frac{\omega^{3}k_{b}}{32\pi^{2}\epsilon_{0}c^{2}}\left(1 - \left(\widehat{\mathbf{r}}\cdot\widehat{\mathbf{p}}_{e}\right)^{2}\right)\left|\mathbf{p}_{e}\right|^{2}, \qquad \Gamma_{0} \equiv \int d\Omega I_{\mathrm{r},0}\left(\theta,\phi\right) = \left|\mathbf{p}_{e}\right|^{2}\frac{\omega^{3}k_{b}}{12\pi\epsilon_{0}c^{2}} \qquad (14)$$

This concludes the review of the background material necessary in order to derive the multipole antenna formulas of the next section.

III. MULTIPOLE FORMULAS FOR DECAY RATE ENHANCEMENTS

The purpose of this section is to generalize the analytic expressions for emitted and radiated powers to the case in which the emitter is located near a nano-antenna structure. We saw in the previous section that the multiple-scattering T-matrix of eq.(8) determines the scattering Green function of eq.(6). The scattering Green function can then be expressed on the VPW basis provided that we also express the homogeneous Green function on the VPW basis. Taking advantage of the translational invariance of $\mathbf{G}_0(\mathbf{x}, \mathbf{x}')$, it can be written [28]:

$$\overleftrightarrow{\mathbf{G}}_{0}(\mathbf{r},\mathbf{0}) = ik_{b}\sum_{m=-1}^{1} \mathbf{N}_{1m}(k_{b},\mathbf{r}) Rg\left\{\widetilde{\mathbf{N}}_{1m}(\mathbf{0})\right\} - \frac{\widehat{\mathbf{r}}\widehat{\mathbf{r}}}{k_{b}^{2}}\delta\left(\mathbf{r}\right)$$
(15)

where $\mathbf{N}_{1,-1}$, $\mathbf{N}_{1,0}$ and \mathbf{N}_{11} are the three outgoing electric dipolar partial wave functions (**N** functions correspond to the q = 2 VPWs detailed in appendix A 2). Employing this expression in eq.(1), the unperturbed electric field created by an isolated point dipole, denoted \mathbf{E}_0 , is then expressed:

$$\mathbf{E}_{0}(\mathbf{x}) = \omega^{2} \mu_{0} \int d\mathbf{x}' \overleftrightarrow{\mathbf{G}}_{0}(\mathbf{x}, \mathbf{x}') \cdot \mathbf{p}_{e} \,\delta^{3}(\mathbf{x}') = \frac{ik_{b}\omega^{2}p_{e}}{\epsilon_{0}c^{2}} \sum_{m=-1}^{1} \mathbf{N}_{1m}(k_{b}\mathbf{x}) \,f_{2,1,m}$$
(16)

where we define the outgoing dipole field coefficients, $f_{q=2,n=1,m}$, to be given by:

$$f_{2,1,m} \equiv \widetilde{\mathbf{N}}_{1m} \left(\mathbf{0} \right) \cdot \widehat{\mathbf{n}} = \langle \Psi_{2,n,m} | \mathbf{0} \rangle \cdot \widehat{\mathbf{n}}$$
(17)

and $\hat{\mathbf{n}}$ is the unit vector in the direction of the emitter dipole moment, defined such that $\mathbf{p}_e = p_e \hat{\mathbf{n}}$. All other emitter multipoles, n > 1 or $q \neq 2$, are taken to be zero.

Utilizing the analytical expression for $\widetilde{\mathbf{N}}_{1m}(\mathbf{0})$, we obtain the following expressions for the emitter field coefficients:

$$f_{q,n,0} = \delta_{q,2}\delta_{n,1}\sqrt{\frac{1}{6\pi}}\widehat{\mathbf{z}}\cdot\widehat{\mathbf{n}}, \qquad f_{q,n,1} = \frac{\delta_{q,2}\delta_{n,1}}{2\sqrt{3\pi}}\left(-\widehat{\mathbf{x}} + i\widehat{\mathbf{y}}\right)\cdot\widehat{\mathbf{n}}, \qquad f_{q,n,-1} = \frac{\delta_{q,2}\delta_{n,1}}{2\sqrt{3\pi}}\left(\widehat{\mathbf{x}} + i\widehat{\mathbf{y}}\right)\cdot\widehat{\mathbf{n}}$$
(18)

Employing expression (15) for $\overleftarrow{\mathbf{G}}_0$ in eqs.(6), (2) and (1) of the previous section and invoking the translation-addition theorem, we obtain an entirely multipolar expression for the field radiated by a dipole emitter interacting with an antenna structure:

$$\mathbf{E}_{t}(\mathbf{r}) = \mathbf{E}_{0} + \mathbf{E}_{s} = \frac{ip_{e}k_{b}\omega^{2}}{\epsilon_{0}c^{2}} \left[\mathbf{N}(\mathbf{r}) f + \sum_{j,l=1}^{N} \left[\mathbf{M}(k\mathbf{r}_{j}), \mathbf{N}(k\mathbf{r}_{j}) \right] T^{(j,l)} H^{(l,e)} f \right]$$
$$\equiv \frac{ip_{e}k_{b}\omega^{2}}{\epsilon_{0}c^{2}} \widetilde{\mathbf{E}}_{t}(\mathbf{r})$$
(19)

where f denotes a column matrix containing the emitter coefficients in the multipole space (with only electric dipole elements non-zero) and $H^{(l,e)} \equiv H(k_b(\mathbf{x}_l - \mathbf{x}_e))$ are the irregular translation-addition matrices between the position of particle l and the emitter position.

In the second line of eq.(19), we defined a dimensionless field, $\widetilde{\mathbf{E}}_{t}$, proportional to the total electric field. This definition of $\widetilde{\mathbf{E}}_{t}$ proves convenient when normalizing the antenna irradiance, $I_{r}(\theta, \phi)$, with respect to $\Gamma_{0}/(4\pi)$ of the isolated emitter. Using the definition of eq.(19) in eqs.(11) and (12), the normalized irradiance is given by:

$$\widetilde{I}_{\rm r} \equiv \frac{4\pi I_{\rm r}\left(\theta,\phi\right)}{\Gamma_0} = 24\pi^2 \lim_{r\to\infty} \left(k_b r\right)^2 \left\|\widetilde{\mathbf{E}}_{\rm t}\left(\mathbf{r}\right)\right\|^2 \tag{20}$$

The electric field of eq.(19), can then be utilized in equation (9) to obtain the decay rate enhancement factor (valid even in an absorbing host medium):

$$\widetilde{\Gamma_{t}} \equiv \frac{\Gamma_{t}}{\Gamma_{t,0}} = 1 + \frac{\operatorname{Re}\left\{6\pi k_{b}\sum_{j,l=1}^{N} f^{\dagger} H^{(e,j)} T^{(j,l)} H^{(l,e)} f\right\}}{\operatorname{Re}\left\{k_{b}\right\}}$$
(21)

Likewise, for an absorption free host medium, the enhancement in radiative decay rate is obtained by inserting eq.(19) into eqs.(11) and (12). Utilizing the translation-addition theorem and the orthogonality properties of the vector spherical harmonics, one obtains for the radiative decay rate enhancement:

$$\widetilde{\Gamma}_{\mathbf{r}} \equiv \frac{\Gamma_{\mathbf{r}}}{\Gamma_{0}} = 1 + 6\pi \sum_{i,j,k,l=1}^{N} \left[T^{(j,i)} H^{(i,e)} f \right]^{\dagger} J^{(j,k)} T^{(k,l)} H^{(l,e)} f + 12\pi \operatorname{Re} \left[\sum_{j,l=1}^{N} f^{\dagger} J^{(e,j)} T^{(j,l)} H^{(l,e)} f \right]$$
(22)

where we see that eqs.(22) and (21) required the use of both regular, J, and irregular, H, translation-addition matrices[28, 29, 35].

The multiple-scattering results of eqs.(21) and (22) simplify considerably when a single antenna particle is present:

$$\widetilde{\Gamma}_{t} = 1 + \frac{\operatorname{Re}\left\{6\pi k_{b}f^{\dagger} H^{(e,j)} t H^{(j,e)} f\right\}}{\operatorname{Re}\left\{k_{b}\right\}}$$
(23)

and

$$\widetilde{\Gamma}_{\mathbf{r}} = 1 + 6\pi \left[H^{(j,e)} f \right]^{\dagger} t^{\dagger} t H^{(j,e)} f + 12\pi \operatorname{Re} \left[f^{\dagger} J^{(e,j)} t H^{(j,e)} f \right]$$
(24)

where t is the single-particle T-matrix. If the T-matrix is that of a spherical (Mie) scatterer, then eqs.(23) and (24) are equivalent to expressions that were derived previously for Mie scatterers.[24-27]

IV. INDUCED DIPOLE FORMULATION FOR YAGI-UDA DESIGNS

In the Yagi-Uda type designs considered in section V below, the emitting dipole and the spherical antenna elements are all positioned along the same axis, henceforth denoted the x axis (see Fig. 1(a)). We furthermore consider the emitting dipole to be perpendicular to the x axis, henceforth denoted the z axis. For sufficiently small antenna particles and sufficiently large separations, it is possible for electric dipole excitations to dominate the antenna response. Dipole couplings have been widely studied and can lead to more intuitive physics than multipole couplings. We therefore derive in this section coupled dipole analogues to eqs.(21) and (22) for the antenna geometries studied in section V in order to compare with multipole calculations.

A. Coulped dipole formalism

We follow the terminology of dielectric polarizability usually employed when dealing with dipole approximations. In this context, the dipole moment induced in a material particle immersed in a material medium of relative dielectric constant ε_b is proportional to the excitation field via the relation:

$$\mathbf{p}(\omega) = \epsilon_0 \varepsilon_b \alpha(\omega) \mathbf{E}_{\text{exc}}(\omega)$$
(25)



FIG. 1. (a) Yagi-Uda antenna design with a silver reflector element 120nm in diameter and a collector array of 8 silver spheres 100nm in diameter. b) Radiation pattern, $\tilde{I}(\theta, \phi)$ of this antenna in the far-field for an emitter operating at a vacuum wavelength of $\lambda_{\rm v} = 618$ nm.

where $\alpha(\omega)$ is the frequency dependent polarizability characterizing the particle.

We denote the field strength of an arbitrary $\hat{\mathbf{z}}$ polarized 'incident' field at each particle position as $\mathbf{E}_{\text{inc},j} = E_{\text{inc},j}\hat{\mathbf{z}}$, and the excitation fields as $\mathbf{E}_{\text{exc},j} = E_{\text{exc},j}\hat{\mathbf{z}}$. Using the dipole field expression of eq.(5), the excitation field of the j^{th} particle in the finite chain of coupled dipoles can then be written:

$$E_{\text{exc},j} = E_{\text{inc},j} - \sum_{l \neq j} e^{ik_b d_{j,l}} \frac{a_l^3}{d_{j,l}^3} \left(1 - ik_b d_{j,l} - k_b^2 d_{j,l}^2 \right) \widetilde{\alpha}_l \left(\omega \right) E_{\text{exc},l}$$
$$= E_{\text{inc},j} + \sum_{l \neq j} \gamma_{j,l} \widetilde{\alpha}_l \left(\omega \right) E_{\text{exc},l}$$
(26)

where in order to simplify the notation, we defined dimensionless 'polarizability' functions $\widetilde{\alpha}_{j}(\omega)$:

$$\widetilde{\alpha}_{j}\left(\omega\right) \equiv \frac{\alpha_{j}\left(\omega\right)}{4\pi a_{j}^{3}} \tag{27}$$

with a_j , as the radius of the j^{th} sphere. We also define for eq.(26) and formulas below, dimensionless field coupling factors, $\gamma_{j,l}$, between particles l and j, and couplings, $\gamma_{j,e}$, between the emitter and a particle j:

$$\gamma_{j,l} \equiv -e^{ik_b d_{j,l}} \left(\frac{a_l}{d_{j,l}}\right)^3 \left(1 - ik_b d_{j,l} - k_b^2 d_{j,l}^2\right) \qquad \gamma_{j,e} \equiv -e^{ik_b d_{j,e}} \left(\frac{a_j}{d_{j,e}}\right)^3 \left(1 - ik_b d_{j,e} - k_b^2 d_{j,e}^2\right)$$
(28)

with $d_{j,l} \equiv |x_j - x_l|$ and $d_{j,e} \equiv |x_j - x_e|$ being respectively the distances between different particle centers and the distance of particles from the emitter.

Defining also quantities \tilde{p}_j with the dimension of electric field:

$$\widetilde{p}_j \equiv \widetilde{\alpha}_j \left(\omega \right) E_{\text{exc},j} , \qquad (29)$$

the coupled equations in (26) can then be solved via matrix inversion:

$$\begin{bmatrix} \widetilde{p}_1 \\ \vdots \\ \widetilde{p}_N \end{bmatrix} = \begin{bmatrix} \widetilde{\alpha}_1^{-1} & -\gamma_{1,2} & \cdots & -\gamma_{1,N} \\ -\gamma_{2,1} & \widetilde{\alpha}_2^{-1} & \cdots & -\gamma_{2,N} \\ \vdots & \cdots & \ddots & \vdots \\ -\gamma_{N,1} & -\gamma_{N,2} & \cdots & \widetilde{\alpha}_N^{-1} \end{bmatrix}^{-1} \begin{bmatrix} E_{\text{inc},1} \\ \vdots \\ E_{\text{inc},N} \end{bmatrix}$$
(30)

The matrix inversion in eq.(30) is the dipole analogue of the multipole T-matrix evaluation of eq.(8). One can next define 'effective' dimensionless polarizabilities, $\tilde{\alpha}_{j}^{\text{eff}}$, that contain all multiple scattering effects:

$$\widetilde{\alpha}_{j}^{\text{eff}}\left(\omega\right) \equiv \frac{\widetilde{p}_{j}}{E_{\text{inc},j}} \tag{31}$$

The field incident on each particle from the dipolar emitter in the absence of an antenna is:

$$E_{\text{inc},j} = -e^{ik_b d_{j,e}} \left(\frac{1}{d_{j,e}}\right)^3 \left(1 - ik_b d_{j,e} - k_b^2 d_{j,e}^2\right) \frac{p_e}{4\pi\epsilon_0\varepsilon_b}$$
(32)

Once the $\widetilde{\alpha}_j^{\text{eff}}$ of eq.(31) have been calculated, the total electric field can be written:

$$\mathbf{E}_{t}\left(\mathbf{r}\right) = \frac{1}{4\pi\epsilon_{0}\varepsilon_{b}}\sum_{j=0}^{N}\frac{e^{ik_{b}r_{j}}}{r_{j}^{3}}\left\{\left(1-ik_{b}r_{j}\right)\left[3\widehat{\mathbf{r}}_{j}\left(\widehat{\mathbf{r}}_{j}\cdot\mathbf{p}_{j}\right)-\mathbf{p}_{j}\right]+k_{b}^{2}r_{j}^{2}\left(\mathbf{p}_{j}-\widehat{\mathbf{r}}_{j}\left(\widehat{\mathbf{r}}_{j}\cdot\mathbf{p}_{j}\right)\right)\right\}$$
(33)

where $\mathbf{r}_j = r_j \hat{\mathbf{r}}_j \equiv \mathbf{r} - \mathbf{x}_j$ are the relative positions with respect to the particle centers, \mathbf{x}_j , with j = 0 designating the dipole emitter (*i.e.* $\mathbf{x}_0 \equiv \mathbf{x}_e$ and $\mathbf{p}_0 \equiv \mathbf{p}_e$).

Utilizing the expressions of eqs.(31)-(33) and invoking the definitions of dimensionless fields and intensities of eqs.(19) and (20), we obtain relatively simple expressions for the far field and the irradiance:

$$\lim_{r \to \infty} \widetilde{\mathbf{E}}_{t} \left(r, \theta, \phi \right) = \frac{e^{ik_{b}r}}{4\pi i k_{b}r} \sin \theta \, \widehat{\theta} \left[1 + \sum_{j=1}^{N} \gamma_{j,e} \widetilde{\alpha}_{j}^{\text{eff}} e^{-ik_{b}d_{j,e}\sin\theta\cos\phi} \right]$$
$$\widetilde{I}_{r} \left(\theta, \phi \right) \equiv \frac{4\pi I_{r} \left(\theta, \phi \right)}{\Gamma_{0}} = \frac{3}{2} \sin^{2}\theta \left| 1 + \sum_{j=1}^{N} \gamma_{j,e} \widetilde{\alpha}_{j}^{\text{eff}} e^{-ik_{b}d_{j,e}\sin\theta\cos\phi} \right|^{2}$$
(34)

where θ and ϕ are respectively the angles with respect to z and x axes.

As with the multipole approach, the enhancement in radiative decay rate is obtained by inserting eq.(33) into eqs.(11) and (12). We can calculate emission and radiative enhancement factors in a manner analogous to that carried out in section III. After some algebra and integrations, we obtain the following formulas for the dipolar enhancement factors:

$$\widetilde{\Gamma}_{t} \equiv \frac{\Gamma_{t}}{\Gamma_{t,0}} = 1 + \frac{3}{2} \sum_{j=1}^{N} \frac{\operatorname{Im}\left\{ \left(\frac{\gamma_{j,e}}{k_{b}a_{j}} \right)^{2} \widetilde{\alpha}_{j}^{\text{eff}} \right\}}{\operatorname{Re}\left\{ k_{b}a_{j} \right\}}$$
(35)

and

$$\widetilde{\Gamma}_{\mathbf{r}} \equiv \frac{\Gamma_{\mathbf{r}}}{\Gamma_{0}} = 1 + \sum_{j=1}^{N} \left| \widetilde{\alpha}_{j}^{\text{eff}} \gamma_{j,e} \right|^{2} + \sum_{j=1}^{N} 3 \operatorname{Re} \left[\widetilde{\alpha}_{j}^{\text{eff}} \gamma_{j,e} \right] \left[\frac{\left(k_{b} d_{j,e} \right)^{2} - 1}{\left(k_{b} d_{j,e} \right)^{3}} \sin\left(k_{b} d_{j,e} \right) + \frac{\cos\left(k_{b} d_{j,e} \right)}{\left(k_{b} d_{j,e} \right)^{2}} \right] + \sum_{l>j}^{N} 3 \operatorname{Re} \left[\gamma_{l,e}^{*} \widetilde{\alpha}_{l}^{\text{eff},*} \widetilde{\alpha}_{j}^{\text{eff}} \gamma_{j,e} \right] \left[\frac{\left(k_{b} d_{l,j} \right)^{2} - 1}{\left(k_{b} d_{l,j} \right)^{3}} \sin\left(k_{b} d_{l,j} \right) + \frac{\cos\left(k_{b} d_{l,j} \right)}{\left(k_{b} d_{l,j} \right)^{2}} \right]$$
(36)

which are respectively the electric dipole analogues of eqs.(21) and (22).

B. Time harmonic polarizability

In order to evaluate the formulas in eqs.(35) and (36), we need an accurate model of the frequency dependent dipole polarizability $\alpha(\omega)$ of the plasmonic antenna components. The commonly adopted quasi-static approximation, or even the more sophisticated pointlike models[37–39] can introduce inaccuracies associated with the model rather than actual defaults of the dipole approximation *per se*. To avoid such problems, we adopted the unconventional choice of using the dipole polarizability prescribed by Mie theory.

Taking into account the differences in formalism between the multipole framework and the polarizability picture, we find that the electric dipole polarizability of a sphere is:

$$\alpha\left(\omega\right) = \frac{6\pi}{ik_b^3} t_{2,1}\left(\omega\right) \tag{37}$$

where $t_{q=2,n=1}(\omega)$ is the electric dipole element of the (diagonal) Mie T-matrix[36] (nondependent on *m* due to spherical symmetry). This gives us a fully analytic frequency dependent polarizability corresponding to the electric dipolar response from Mie theory:

$$\widetilde{\alpha}(\omega) = \frac{\alpha(\omega)}{4\pi a^3} = \frac{3}{2i(ak_b)^3} \frac{j_1(ak_b)}{h_1(ak_b)} \frac{\varepsilon_s \varphi_1(ak_b) - \varepsilon_b \varphi_1(ak_s)}{\varepsilon_b \varphi_1(ak_s) - \varepsilon_s \varphi_1^{(1)}(ak_b)}$$
(38)

where ε_s and k_s are the relative dielectric function and wavenumber associated with the spherical particle. The functions φ_1 and $\varphi_1^{(1)}$ are expressed in terms of first order spherical Bessel and Hankel functions:

$$\varphi_1(z) \equiv \frac{[zj_1(z)]'}{j_1(z)} \qquad \varphi_1^{(1)}(x) \equiv \frac{[zh_1(z)]'}{h_1(z)} \tag{39}$$

It is important to underline the importance of using a frequency dependent polarizability like that of eq.(38) in order to reliably include radiation damping effects in dipole simulations. To date, radiative effects in dipole calculations were typically handled by invoking the socalled 'point-scatterer' model[37–39]. Although one can arrange point scattering models to approximate the polarizability function of eq.(38) for sufficiently small values of ak_b , our choice of using Mie theory to determine the polarizability seems to be more reliable for larger values of the ak_b parameter.

Now that dipole and multipole simulations are in hand, the next section aims to illustrate the utility of the dipolar and multipolar modeling techniques by simulating a few realistic antenna designs.

V. YAGI-UDA NANO-ANTENNA DESIGN WITH SPHERICAL ELEMENTS

It has recently been shown that Yagi-Uda type optical antenna designs[10, 14–16, 18, 22, 23] can be achieved by a chain of plasmonic spheres serving as a 'collector' chain and a somewhat larger sphere serving as a 'reflector' element. A study of such Yagi-Uda designs appeared as an interesting means for demonstrating the utility of the formulation derived in this work. The goal of this section is to show how the formulas developed in the previous sections provide insights into established nano-antenna designs and indicate possible design modifications. We will also argue, that one must be careful in specifying 'optimal' nano-antenna characteristics.

Let us consider the design illustrated in Fig. 1(a) consisting of a collector made of 8 silver spheres 100nm in diameter combined with a silver reflector sphere 120nm in diameter. The antenna is taken to be immersed in a dielectric medium of index $n_b = 1.5$. The

emitting dipole is positioned at d = 30nm equidistantly between the reflector particle and the collector chain. Its dipole moment is taken to be oriented perpendicular to the antenna axis. The radiation pattern of this antenna, illustrated in Fig. 1(b) for a quantum dipole emitter operating at a vacuum wavelength of $\lambda_{\rm v} = 618$ nm, clearly illustrates the desired strong directivity along the collector direction. We remark that the radiation pattern along the collector axis is relatively axi-symmetric, with little radiation leaking into the backward hemisphere.

In order to quantitatively study antenna directivity, we inspired ourselves from analogous radio frequency quantities and chose a directivity parameter of $\mathcal{D} \equiv 10 \log_{10}(4\pi I_{\text{axis}}/\Gamma_{\text{r}}) =$ $10 \log_{10}(\tilde{I}_{\text{axis}}/\tilde{\Gamma}_{\text{r}})$. In other words, directivity is measured in decibels of the intensity along the collector axis divided by the steradian average of total radiated power. Quantum efficiency was also calculated from its usual definition of $\eta = \Gamma_{\text{r}}/\Gamma_{\text{t}}$ (for perfect emitters). All multipole simulations in this section were carried out with a multipole cutoff of $n_{\text{max}} = 10$ which proved amply sufficient for convergence in the studied configurations.



FIG. 2. (a) Antenna schematic: 4 silver spheres $D_{Ag} = 100$ nm in diameter with or without a $D_{R} = 120$ nm 'reflector' particle). (b) Directivity parameter $10 \log_{10}(4\pi I_{axis}/\Gamma_r)$ as a function of vacuum wavelength. (c) Radiative enhancement, Γ_r/Γ_0 . (d) Quantum efficiency, $\eta = \Gamma_r/\Gamma_{tot}$.

An important design property is the number of particles necessary in the collector chain. We therefore begin with multipole simulations of a Yagi-Uda design with a 4-particle collector chain in Fig. 2. The principal characteristic of this antenna, as seen in Fig. 2(b), is that it becomes highly directive for vacuum wavelengths $\lambda_{\rm v} \gtrsim 600$ nm. Due to the transverse coupling, radiation enhancements are low and even inferior to 1 for long wavelengths, as shown in Fig. 2(c). These low radiative enhancements are a direct consequence of the fact that this antenna design is optimized for directivity (if emission enhancements are also required, one must add a super-emitter to the design (see refs.[4, 10, 21] and the discussion of Fig. 8 below). Simulations were carried out both with and without a reflector particle. Although it is clear from Fig. 2(b) that the reflector does indeed enhance directivity, this comes at a considerable cost to the radiative decay rate and quantum efficiency as can be seen by inspection of Figs. 2(c) and 2(d).



FIG. 3. (a) Antenna schematic: same characteristics as in Fig. 2 but with an 8-particle collector array. (b) Directivity parameter $10 \log_{10}(4\pi I_{\text{axis}}/\Gamma_{\text{r}})$ as a function of vacuum wavelength. (c) Radiative enhancement, $\Gamma_{\text{r}}/\Gamma_{0}$. (d) Quantum efficiency, $\eta = \Gamma_{\text{r}}/\Gamma_{\text{tot}}$.

Next, we carried out multipole simulations for the more technically complex design of 8 aligned collector particles in Fig. 3 (all other properties are the same as those in Fig. 2). The results were quite similar to those of the 4-particle collector Yagi-Uda except for a significant increase in directivity accompanied by additional losses in quantum efficiency.

In order to better visualize the net effect of a reflector particle, the emission power along the collector axis, normalized by that of an isolated emitter, is plotted as a function of wavelength in Fig. 4 for the 4 and 8-particle collector configurations studied above. It is clear from this figure that the reflector particle decreases the radiation intensity along the



FIG. 4. Power emitted along the collector axis for emitters at 30nm from the first collector particle in configurations with and without a reflector particle. Full squares: 8-particle collector without reflector. Full circle: 4-particle collector without reflector. White squares: 8-particle collector with reflector. White circle: 4-particle collector with reflector.

detector axis. The detrimental effect of the reflector particle could of course be decreased in this design by adopting larger spacings, d, between the emitter and the antenna particles as it has been done in other antenna designs in the literature. For instance, if we increased the reflector-collector separation from 60 to 100nm, we would arrive at a design very similar to that considered by Koenderink.[10]

The quantum efficiency and radiative decay rate enhancement with different reflectorcollector separations is presented in Fig. 5 (for the sake of simplicity, the emitter is always taken to lie in the center of the gap). The curve labeled with diamonds is that of an emitter located at d = 50nm from the collector, but without a reflector element. As we can see from this figure, increasing gap size does indeed improve the radiative decay rates and quantum efficiency, but further gains to both quantities can still be obtained by removing the reflector. This behavior was expected, and must be balanced against the advantage of a reflector element which is to enhance emission directivity. However, the issue of directivity, (and how it is defined) is directly related to our choice of reduced emitter-antenna separation distances, d, which we discuss below.

Let us recall that in this work we chose to define directivity, \mathcal{D} , as the radiation along



FIG. 5. Quantum efficiency, (a), and radiative enhancement, (b), as functions of the wavelength for a 9-particle Yagi-Uda with the same parameters as in Fig. 1, with varying reflector-collector separations (emitter equidistant from reflector and first collector particles: 2d = 60, 70, 80, 100 nm).

the collector chain divided by average emitted power. Optimizing \mathcal{D} differs from optimizing the normalized radiated power along the collector axis which, unlike the directivity, has contributions from the radiation enhancement factor. Directivity enhancement and on-axis power enhancement as functions of wavelength and emitter-collector distance are plotted in Fig. 6 for both the 4 and 8-particle collector antennas (without reflectors). As we can see from the figure, optimizing directivity favors somewhat smaller emitter-collector distances, d, than does an optimization of the on-axis power enhancement, which explains the choices of this work. One can perhaps better visualize the situation, by examining the radiation diagrams of the chains at their optimum parameters for directivity and power respectively for both 4 and 8-particle chains which are presented in Fig. (7).

Another design consideration that seems appropriate to mention is that of orienting the dipole emitter perpendicular to the antenna chain. As can be seen from Fig. 8, the





FIG. 6. Figs.(a)-(b) Directivity, \mathcal{D} , and Figs.(c)-(d) on-axis normalized radiative power enhancement as functions of wavelength and distance, d, of the emitter to the first collector. (a)-(c) 4-particle collector, (b)-(d) 8-particle collector.

directivity drops rapidly with variation of the emitter axis from the perpendicular orientation (falling by $\simeq 3$ dB at $\simeq 10^{\circ}$ from a perpendicular orientation). For randomly oriented dipoles, this poses significant limitations to antenna properties. However, dipole emissions perpendicular to the collector axis can be privileged by an on-axis super-emitter around the quantum emitter[10, 20, 21] or off-axis longitudinal couplings of an emitter to an antenna particle[16, 19, 23]. In such cases, the longitudinal couplings induce strong decay rate enhancements that can largely outweigh the relatively modest decay rate damping resulting from small emitter-collector separations.

The last issue that we wish to address in this section is the feasibility of purely electric dipole modeling of these antennas. Although it has already been pointed out that multipoles are quite important in quantitative studies of the longitudinal couplings of 'super-emitter' designs, the Yagi-Uda design relies on the much weaker transverse couplings and one expects



FIG. 7. Radiation diagrams at the 'optimal' parameters obtained from Fig. 6. (Irradiance is normalized such that 1 corresponds to the intensity of maximum free-space radiation). Optimal directivity for a : (a) 4-particle collector at $\lambda = 617$ nm and emitter-collector separation of d = 40nm ; (b) 8-particle collector at $\lambda = 626$ nm with d = 35nm. Optimal on-axis irradiance for a : (c) 4particle collector at $\lambda = 630$ nm with d = 90nm ; (d) 8-particle collector at $\lambda = 638$ nm with d = 85nm.

the dipolar model developed in section IV to be approximately valid in this case.

The results obtained using the coupled dipole formulas of section IV A coupled with the Mie based polarizability of section IV B, are compared with multipole calculations in Fig. 9 for an 8-particle collector antenna. Although there are significant differences between the dipolar and multipolar results at shorter wavelengths, the coupled dipole calculations correspond rather well to the quasi-exact results at the larger wavelengths, *i.e.* $\lambda_{\rm v} \gtrsim 600$ nm, for which the antenna is designed. There are of course some differences between the coupled dipole calculations and the exact multipole result at all wavelengths, but these can largely be attributed to the proximity of the emitter to plasmonic antenna particles, a situation which excites higher order modes in the neighboring plasmonic particles.



FIG. 8. Directivity, in decibels, plotted as a function of the angle of the emitter with the direction perpendicular to the collector chain for a 4-particle and 8-particle collector chain (without reflector), and emitter-collector separations of d = 30nm (respective operating wavelengths of $\lambda = 615$ nm, and $\lambda = 626$ nm selected respectively for high directivities).

VI. CONCLUSIONS

An important result of this work was to derive analytic multipole formulas for calculating the quantum emission properties of nano-antennas in a manner that avoided numerical integrations of energy flow. The gain in speed and accuracy provides significant advantages to nano-antenna design. We also derived new analytical formulas in the coupled dipole approximation which permit the integration-free calculation of quantum decay rates of quantum emitters in Yagi-Uda type designs.

In the last section of this work, we performed an in-depth study of the radiative and directive properties of Yagi-Uda antennas. We studied therein a variety of antenna design properties, including the number of particles in the collector chain, the quantum emitter's orientation and position, and the utility of a reflector particle in optical Yagi-Uda antennas. Concerning this last point, we showed that the improvements in beam directivity provided by a reflector particle come at a considerable expense to the radiative decay rate and quantum yield. We propose that reflector-free antennas may prove to be an interesting alternative design.



FIG. 9. (a) Comparison between coupled electric dipole results and multipole calculations for an 8-particle collector array antenna. (b) Directivity parameter $10 \log_{10}(4\pi I_{\text{axis}}/\Gamma_{\text{r}})$. (c) Radiative enhancement, $\Gamma_{\text{r}}/\Gamma_{0}$. (d) Quantum efficiency $\eta = \Gamma_{\text{r}}/\Gamma_{\text{tot}}$.

Appendix A: Appendix

1. Vector Spherical Harmonics

The Vector Spherical Harmonics (VSHs) are described in a number of works [35, 40–42], but the notations and definitions vary with authors. They form a complete orthogonal basis set for describing the angular variations of any vector field. We define the spherical VSHs as follows :

$$\mathbf{Y}_{nm}(\theta,\phi) \equiv \hat{\mathbf{r}} Y_{nm}(\theta,\phi) \tag{A1}$$

$$\mathbf{Z}_{nm}(\theta,\phi) \equiv \frac{r \mathbf{\nabla} Y_{nm}(\theta,\phi)}{\sqrt{n(n+1)}} \tag{A2}$$

$$\mathbf{X}_{nm}(\theta,\phi) \equiv \mathbf{Z}_{nm}(\theta,\phi) \wedge \widehat{\mathbf{r}}$$
(A3)

All the VSHs are mutually orthogonal in the sense that taking $\mathbf{W}_{nm}^{(i)}$ (i = 0, 1, 2) to

respectively denote the VSHs \mathbf{Y}_{nm} , \mathbf{X}_{nm} , or \mathbf{Z}_{nm} , we have:

$$\left\langle \mathbf{W}_{nm}^{(i)} \mid \mathbf{W}_{\nu\mu}^{(j)} \right\rangle \equiv (-)^m \int_0^{4\pi} \mathbf{W}_{n,-m}^{(i)} \cdot \mathbf{W}_{\nu\mu}^{(j)} \, d\Omega = \delta_{ij} \delta_{n\nu} \delta_{m\mu} \tag{A4}$$

2. Vector Partial Waves

The vector partial waves are often referred to as *regular* spherical vector waves, $Rg \{\mathbf{M}_{nm}(k\mathbf{r})\}$ and $Rg \{\mathbf{N}_{nm}(k\mathbf{r})\}$ [35], which are respectively the direct space representations of the Vector Partial Waves (VPWs) $\langle \mathbf{r} | \Psi_{q=1,n,m} \rangle$ and $\langle \mathbf{r} | \Psi_{q=2,n,m} \rangle$. Their analytical expressions are given by:

$$\langle \boldsymbol{\Psi}_{1,n,m} | \mathbf{r} \rangle \equiv Rg \left\{ \widetilde{\mathbf{M}}_{n,m} \left(k\mathbf{r} \right) \right\} \equiv (-)^{m} j_{n} \left(kr \right) \mathbf{X}_{n,-m} (\widehat{\mathbf{r}})$$

$$\langle \boldsymbol{\Psi}_{2,n,m} | \mathbf{r} \rangle \equiv Rg \left\{ \widetilde{\mathbf{N}}_{nm} \left(k\mathbf{r} \right) \right\} \qquad n = 1, 2, ... \infty \qquad m = -n, ..., n$$

$$\equiv \frac{(-)^{m}}{kr} \left\{ \sqrt{n \left(n+1 \right)} j_{n} \left(kr \right) \widehat{\mathbf{r}} Y_{n,-m} (\widehat{\mathbf{r}}) + \left[kr j_{n} \left(kr \right) \right]' \mathbf{Z}_{n,-m} (\widehat{\mathbf{r}}) \right\}$$

$$(A5)$$

The total field in the antenna problem satisfies outgoing boundary conditions. Consequently, when evaluating the total fields like in eq.(19) for example, the fields were developed in terms of VPWs satisfying the outgoing boundary conditions, traditionally labeled \mathbf{M}_{nm} and \mathbf{N}_{nm} [35], which are analogous to the regular waves of eq.(A5) with the spherical Bessel functions being replaced by spherical Hankel functions:

$$\mathbf{N}_{nm}\left(k\mathbf{r}\right) \equiv \frac{1}{kr} \left\{ \sqrt{n\left(n+1\right)} h_n\left(kr\right) \hat{\mathbf{r}} Y_{nm}(\hat{\mathbf{r}}) + \left[krh_n\left(kr\right)\right]' \mathbf{Z}_{nm}(\hat{\mathbf{r}}) \right\}$$
$$\mathbf{M}_{nm}\left(k\mathbf{r}\right) \equiv h_n\left(kr\right) \mathbf{X}_{nm}(\hat{\mathbf{r}}) \tag{A6}$$

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