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PAPER

Plasmon dispersion in a multilayer solid torus in terms of three-term vector recurrence relations and matrix continued fractions

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Abstract

Toroidal confinement, which has played a crucial role in magnetized plasmas and Tokamak physics, is emerging as an effective means to obtain useful electronic and optical response in solids. In particular, excitation of surface plasmons in metal nanorings by photons or electrons finds important applications due to the engendered field distribution and electromagnetic energy confinement. However, in contrast to the case of a plasma, often the solid nanorings are multilayered and/or embedded in a medium. The non-simply connected geometry of the torus results in surface modes that are not linearly independent. A three-term difference equation was recently shown to arise when seeking the nonretarded plasmon dispersion relations for a stratified solid torus (Garapati *et al* 2017 *Phys. Rev.* B **95** 165422). The reported generalized plasmon dispersion relations are here investigated in terms of the involved matrix continued fractions and their convergence properties including the determinant forms of the dispersion relations obtained for computing the plasmon eigenmodes. We also present the intricacies of the derivation and properties of the Green's function employed to solve the three term amplitude equation that determines the response of the toroidal structure to arbitrary external excitations.

1. Introduction

A variety of particles are emerging in response to the needs of nanoscale functionality for modifying existing material properties or for creating new properties, see for example the editorial by Roco and Pinna [1]. Apart from the complexity of the material at the atomic, molecular, and cluster scales, both the local geometry and size of the particles have been shown to affect the response of single particles as well as many particle systems. In plasmonics [2], these experimental observations are frequently quite satisfactorily accounted for by theoretically invoking nonretarded electrodynamics. The scattering properties of sub-wavelength structures can thus be obtained in the quasi-static limit, where the field is primarily given by the scalar electric potential. For geometries that permit analytical solutions, such calculations can reveal the resonance behavior of the nanoparticle surface modes in response to electromagnetic excitation [3]. Therefore, surface plasmon dispersion relations may be obtained for the nanoparticles so that experiments can be expedited or measurement results can be better interpreted.

Recently, toroidal nanoparticles such as metal and dielectric nanorings, have gained considerable attention due to their potential use in trapping cold polar molecules [4], levitating and trapping dielectric nanoparticles [5], metamaterials [6–8], soft Coulomb interactions [9], light trapping in energy-harvesting devices [10], and plasmonic nanoantennas [11]. We here suffice by noting that our motivation for studying such structures parallels that for the extensive investigation of cartesian thin film stratified systems for development of optical filters, photonic band gap materials, and metamaterials [12–15]. With reference to the works of Love on the calculation of oscillatory modes of a cold plasma [16, 17], the complete set of the dispersion relations of a single

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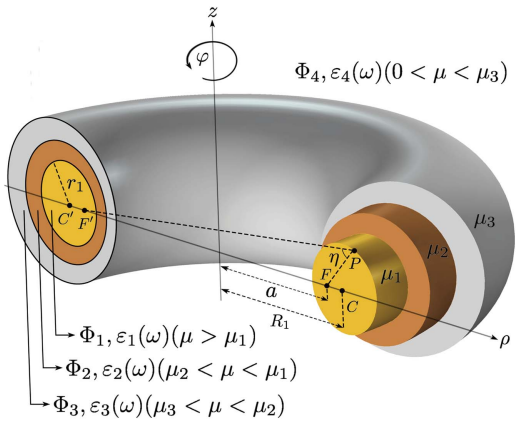

Figure 1. The toroidal coordinates (μ, η, φ) of a point P in space is referred to symmetry axis z and polar axis ρ. C and C' are centers of the minor cross-sections. F and F' are two foci that form the limiting points of a set of coaxial circles, where $\mu = \log(PF'/PF)$ and η is the angle $\angle FPF'$ with the range $[0, 2\pi]$. The angle φ is the azimuthal angle about the z axis. The composite toroid is generated by rotating the circles shown by 180° about the z-axis with fixed focal length a. The coordinate μ_i defines the surface of a composite toroid of major and minor radii R_i and r_i, respectively, where the identity $R_i = r_i \cosh \mu_i$ holds. The scalar potential Φ_i and their associated boundaries μ_i are labeled for typical values of $\cosh \mu_1 = 5$, $\cosh \mu_2 = 3.5$, and $\cosh \mu_3 = 2.7$ considered here.

plasma ring in vacuum and its composite configurations were recently [18] obtained in the quasi-static limit from the separation of variables of the Laplace equation in the toroidal coordinate system, where the surface of a torus is obtained by fixing the value of one of the coordinates. The aim of this article is to rigorously investigate the analytical structure, existence, and convergence properties of the dispersion relations of a system of composite solid tori. Specifically, the derivation and properties of equations (28) and (29) in [18], obtained to analyze a k-layered composite toroidal structure with a single or multiple metal-dielectric interfaces, are presented. In doing so, we consider the confocal toroidal multilayers, shown in figure 1. We here note that for concentric multilayers, as graphically shown in [18], the Laplace equation is not separable [19]. This point was not emphasized in [18], although the analytical treatment pertained to confocal multilayers. The objective there was the experimentally realizable nanostructures of current interest to nanoscience, where the fabrication of multilayer nanorings is practically limited to singly or doubly coated rings such that the ratio of the coating thicknesses to the core ring radius remains small. As a result, the deviation of the confocal rings from concentricity remains negligible.

This article is organized as follows: in section 2, closely following the formulation in [18], we derive a canonical vector three-term recurrence relation that implicitly contains the eigenvalue spectrum corresponding to the quasi-static plasmonic modes of a k-layered toroidal structure. Using a formal argument followed by a rigorous mathematical proof, in section 3, we give the explicit forms of the plasmon dispersion relations for such a geometry in terms of matrix continued fractions (MCFs) and present the determinant forms of the dispersion relations to provide a numerical platform for determination of the resonance values of the involved dielectric functions. In section 4, we introduce the Green's function for the solution of the three term difference equation for an arbitrary continuous toroidal charge distribution. As examples of the application of the analytical results, we visualize the potential for some simple charge distributions. Concluding remarks are provided in section 5.

2. Model of a k-layered torus and the vector three-term recurrence relation

A multilayered torus can be described as a solid torus with toroidal surface $\mu = \mu_1$, dielectric function ε_1 and minor radius r_1, together with $k - 1$ sublayers of confocal toroidal shells, each with dielectric function ε_i, where $i = 2, \ldots, k$ (see figure 1). Thus, a single solid torus corresponds to $k = 1$, with no sublayer between the torus and the outside medium. With distances typically of the order of a few nanometers between the layers embedded in a medium, one can divide the space into $k + 1$ regions based on $\varepsilon_1, \ldots, \varepsilon_{k+1}$, where ε_{k+1} denotes the dielectric function of the outside medium. The first region corresponds to interior of the solid torus and is given by $\mu \geqslant \mu_1$. The remaining $k - 1$ toroidal shells, described by $\mu_i \leqslant \mu \leqslant \mu_{i-1}$ $(i = 2, \ldots, k)$, share the same focal length a with the solid torus via the relations [20]

$$R_i = r_i \cosh \mu_i, \quad a = r_i \sinh \mu_i. \tag{1}$$

Finally, the $(k + 1)$th region, which lies outside the k-layered torus, is described by $0 < \mu \leqslant \mu_k$ (see figure 1 for the case $k = 3$).

Recalling [16, 18] that in the toroidal coordinate system $(\mu,\ \eta,\ \varphi)$ shown in figure 1, solutions of the Laplace equation are given by the harmonics:

$$\begin{cases} f(\mu,\ \eta)\ P^m_{n-\frac{1}{2}}(\cosh\mu)\ \mathrm{e}^{\mathrm{i}n\eta}\ \mathrm{e}^{\mathrm{i}m\varphi} \\ f(\mu,\ \eta)\ Q^m_{n-\frac{1}{2}}(\cosh\mu)\ \mathrm{e}^{\mathrm{i}n\eta}\ \mathrm{e}^{\mathrm{i}m\varphi} \end{cases} n,\ m = 0,\ \pm1,\ \pm2,\ \ldots, \tag{2}$$

where $f(\mu,\ \eta) = \sqrt{\cosh\mu - \cos\eta}$, $P^m_{n-\frac{1}{2}}$ and $Q^m_{n-\frac{1}{2}}$, the so-called toroidal harmonics, denote the associated Legendre functions of first and second kind. It follows that one can use the general form:

$$\begin{aligned}\Phi = f(\mu,\ \eta) \sum_{m,n=-\infty}^{\infty} [&C_{mn} P^m_{n-\frac{1}{2}}(\cosh\mu) \\ &+ D_{mn} Q^m_{n-\frac{1}{2}}(\cosh\mu)]\ \mathrm{e}^{\mathrm{i}n\eta}\ \mathrm{e}^{\mathrm{i}m\varphi},\end{aligned} \tag{3}$$

with constants C_{mn} and D_{mn} to be determined, as a suitable ansatz for the scalar electric potential $\Phi(\mu,\ \eta,\ \varphi)$ of a toroidal structure.

After dividing the space into $k+1$ regions, we denote the associated potential in each region by $\Phi_1,\ \ldots,\ \Phi_{k+1}$, respectively. The general form of the potential given by equations (2) and (3) implies

$$\begin{aligned}\Phi_j = f(\mu,\ \eta) \sum_{m=-\infty}^{\infty} \sum_{n=-\infty}^{\infty} [&C^j_{mn} P^m_{n-\frac{1}{2}}(\cosh\mu) \\ &+ D^j_{mn} Q^m_{n-\frac{1}{2}}(\cosh\mu)]\mathrm{e}^{\mathrm{i}n\eta}\mathrm{e}^{\mathrm{i}m\varphi},\end{aligned} \tag{4}$$

where $j = 1,\ \ldots,\ k+1$. Since the toroidal harmonics $P^m_{n-\frac{1}{2}}(\cosh\mu)$ and $Q^m_{n-\frac{1}{2}}(\cosh\mu)$ become unbounded as $\mu \to \infty$ and $\mu \to 0$; respectively, we must further set

$$C^1_{mn} = 0 \quad \text{and} \quad D^{k+1}_{mn} = 0, \tag{5}$$

for all integers m and n. The continuity of the potential and the normal component of the electric displacement field across each region gives the $2k$-boundary conditions:

$$\Phi_i|_{\mu=\mu_i} = \Phi_{i+1}|_{\mu=\mu_i}, \tag{6}$$

$$\varepsilon_i \frac{\partial\Phi_i}{\partial\cosh\mu}\bigg|_{\mu=\mu_i} = \varepsilon_{i+1} \frac{\partial\Phi_{i+1}}{\partial\cosh\mu}\bigg|_{\mu=\mu_i}, \quad i = 1, \cdots, k. \tag{7}$$

Note that for each fixed j, equation (4) can be written as $\Phi_j = \sum_m \Phi^m_j \cdot \mathrm{e}^{\mathrm{i}m\varphi}$, where Φ^m_j is independent of the azimuthal angle φ. The completeness of the orthogonal system $\{\mathrm{e}^{\mathrm{i}m\varphi}\}$ implies that one can treat equations (6) and (7) separately for each integer m (the potential field has rotational symmetry with respect to the z-axis). With m maintained fixed, we may therefore suppress its notation in upcoming equations. Moreover, we adopt the notations P^i_n, Q^i_n, f_i, C^i_n, D^i_n for $P^m_{n-\frac{1}{2}}(\cosh\mu_i)$, $Q^m_{n-\frac{1}{2}}(\cosh\mu_i)$, $f(\mu_i,\ \eta)$, C^i_{mn}, D^i_{mn}; respectively, and let P'^i_n, Q'^i_n, f'_i denote the derivatives of P^i_n, Q^i_n, f_i with respect to $\cosh\mu$ evaluated at $\mu = \mu_i$.

Introducing the $k \times 1$ coefficient vectors

$$\mathcal{C}_n = \begin{bmatrix} C^2_n \\ C^3_n \\ \vdots \\ C^{k+1}_n \end{bmatrix} \quad \text{and} \quad \mathcal{D}_n = \begin{bmatrix} D^1_n \\ D^2_n \\ \vdots \\ D^k_n \end{bmatrix} \tag{8}$$

and applying the boundary condition equation (6) implies

$$\mathbb{P}_n \mathcal{C}_n = \mathbb{Q}_n \mathcal{D}_n, \tag{9}$$

with $k \times k$ bidiagonal matrices $\mathbb{P}_n$ and $\mathbb{Q}_n$ (see appendix A, equations (A.3) and (A.4)). Both of these bidiagonal matrices have non-zero diagonal entries and hence are invertible. Thus, one can solve, for example, $\mathcal{C}_n$ in terms of $\mathcal{D}_n$ as

$$\mathcal{C}_n = \mathbb{P}^{-1}_n \mathbb{Q}_n \mathcal{D}_n. \tag{10}$$

The application of the second boundary condition equation (7) together with equation (10) gives the vector three-term recurrence

$$\mathcal{W}_{n+1} - R_n \mathcal{W}_n + \mathcal{W}_{n-1} = 0, \tag{11}$$

for $n = 0,\ \pm1,\ \pm2,\ \ldots,$ where

$$\mathcal{W}_n = J_n \mathcal{D}_n, \tag{12}$$

$$J_n = (\mathbb{P}'_n E_2 \mathbb{P}_n^{-1} - \mathbb{Q}'_n E_1 \mathbb{Q}_n^{-1})\mathbb{Q}_n, \tag{13}$$

and

$$R_n = D_\mu + (\mathbb{P}_n E_2 \mathbb{P}_n^{-1} - \mathbb{Q}_n E_1 \mathbb{Q}_n^{-1})(\mathbb{P}'_n E_2 \mathbb{P}_n^{-1} - \mathbb{Q}'_n E_1 \mathbb{Q}_n^{-1})^{-1}. \tag{14}$$

For details regarding the algebraic manipulations resulting in equations (9)–(14) and definitions of the $k \times k$ matrices $\mathbb{P}_n$, $\mathbb{Q}_n$, $\mathbb{P}'_n$, $\mathbb{Q}'_n$, D_μ, E_1, E_2, see appendix A.

Since the normal modes of the system are independent of the chosen set of coefficients, in our case the vector $\mathcal{D}_n$, one is naturally led to ask whether equation (11) would remain invariant with respect to a different choice of a coefficient vector. This is a relevant question and needs to be addressed since the equation system (A.2) can be represented using a different set of coefficient vectors than $\mathcal{C}_n$ and $\mathcal{D}_n$ given by equation (8). We show this invariance under the extra feasibility assumption, which stems from the physical basis of the problem. To see this, we generate a different set of coefficient vectors by rewriting equation (9) as:

$$C_n^2 \vec{p}_{1n} + \cdots + C_n^{k+1} \vec{p}_{kn} = D_n^1 \vec{q}_{1n} + \cdots + D_n^k \vec{q}_{kn}, \tag{15}$$

where $\vec{p}_{1n}$, ..., $\vec{p}_{kn}$ and $\vec{q}_{1n}$, ..., $\vec{q}_{kn}$ denote the column vectors of $\mathbb{P}_n$ and $\mathbb{Q}_n$ in equation (A.3), respectively. A rearrangement of equation (15) can be written in matrix form as:

$$\mathbb{S}_n \mathcal{F}_n = \mathbb{T}_n \mathcal{G}_n, \tag{16}$$

where the columns of the $k \times k$ matrices $\mathbb{S}_n$ and $\mathbb{T}_n$ are a permutation of the set of $2k$ vectors $\{\vec{p}_{1n}, \ldots, \vec{q}_{kn}\}$ with the possibility of a negative sign in case a vector has been moved from one side of equation (15) to the another side, and the coefficient vectors $\mathcal{F}_n$ and $\mathcal{G}_n$ consist of the corresponding coefficients for each chosen column according to equation (15). Similar to equation (9), this is an alternative representation of equation (A.2). In general, neither $\mathbb{S}_n$ nor $\mathbb{T}_n$ has to be invertible. However, in order to obtain the vector three-term recurrence, and thus the dispersion relations, one should be able to solve one set of k variables, chosen from $\{C_n^i\}_{i=2}^{k+1}$ and $\{D_n^i\}_{i=1}^{k}$, in terms of the remaining k variables using the boundary condition equation (6). As a result, we must require that the rearrangement equation (16) is *feasible*; i.e., at least one of the matrices $\mathbb{S}_n$ or $\mathbb{T}_n$, say $\mathbb{S}_n$, is invertible. In this case, we have $\mathcal{F}_n = \mathbb{S}_n^{-1}\mathbb{T}_n\mathcal{G}_n$. It is easily seen that $\mathcal{D}_n$ can be expressed as:

$$\mathcal{D}_n = \mathbb{D}_1 \mathcal{F}_n + \mathbb{D}_2 \mathcal{G}_n, \tag{17}$$

where $\mathbb{D}_1$ and $\mathbb{D}_2$ are diagonal matrices with only zeros or ones in the diagonal such that $\mathbb{D}_1 + \mathbb{D}_2 = I_k$, the identity matrix. Substituting $\mathcal{F}_n$ in equation (17) gives

$$\mathcal{D}_n = (\mathbb{D}_1 \mathbb{S}_n^{-1} \mathbb{T}_n + \mathbb{D}_2)\mathcal{G}_n = \mathbb{L}_n \mathcal{G}_n.$$

Since the coefficients $\{C_n^i\}_{i=2}^{k+1}$ and $\{D_n^i\}_{i=1}^{k}$ are uniquely determined by the boundary condition equations (6) and (7), so are the corresponding three-term recurrence relations. As a result, the substitution $\mathcal{D}_n = \mathbb{L}_n \mathcal{G}_n$ in equation (A.16) gives the vectorial three-term recurrence equation for $\mathcal{G}_n$, which is easily seen to be reduced to equation (11). *Consequently, under the feasibility condition, equations (11) and (14) are the canonical vector three-term recurrence relations for a k-layered toroidal structure.*

Having solidified the form of equation (11), we close this section by considering the limiting case of equation (14), which will be used throughout the rest of the paper. For the proof of theorem 1, see appendix A.

Theorem 1. *Let R_n be defined as in equation (14), then*

$$\lim_{n\to\infty} R_n = D_\mu. \tag{18}$$

Therefore for large n, the vector three-term recurrence relation

$$\mathcal{W}_{n+1} - D_\mu \mathcal{W}_n + \mathcal{W}_{n-1} = 0, \tag{19}$$

with constant diagonal coefficient matrix D_μ, is decoupled in all of its variables, and consists of k scalar three-term recurrences having the general form $A_{n+1} - 2\cosh\mu_i A_n + A_{n-1} = 0$, where, for each $i = 1, \ldots, k$, the roots of the corresponding characteristic equation is given by $e^{\pm\mu_i}$. Since $\mu_1 > \ldots > \mu_k$, all roots of the characteristic equation for the vector three-term recurrence equation (19) are distinct with distinct moduli. This observation in the scalar case, i.e., $k = 1$ in equation (11), implies the utilization of the classical results due to Perron [21] and Pincherle [22] (see also [23]), which prove the convergence of the obtained dispersion relations (see also [17]). Theorem 1 plays the key role in providing the application of Perron–Pincherle type theorem for the multidimensional case $k \geqslant 2$ (see [24–26] for details).

3. Dispersion relations for a *k*-layered torus and MCFs

While much of the discussion on the relevance and applications of the charge density normal modes of nanorings have been covered recently [18], we here continue to provide some of the same equations for

convenience. We start with the facts that the toroidal harmonics $P^m_{n-\frac{1}{2}}(z)$ and $Q^m_{n-\frac{1}{2}}(z)$, and their derivatives with respect to z are symmetric in n, see the appendix in [16]. Therefore, it follows from equation (14) that $R_{-n} = R_n$ holds for all $n = \pm 1, \pm 2, \ldots$.

The symmetric property of R_n together with substitutions:

$$\mathcal{Y}_n = \mathcal{W}_n + \mathcal{W}_{-n} \quad \text{and} \quad \mathcal{Z}_n = \mathcal{W}_n - \mathcal{W}_{-n} \quad (n = 0, 1, \ldots),$$

transforms the bi-infinite vector three-term recurrence equation (11) into semi-infinite vector three-term recurrences:

$$\mathcal{Y}_1 - \frac{1}{2} R_0 \mathcal{Y}_0 = 0, \tag{20}$$

$$\mathcal{Y}_{n+1} - R_n \mathcal{Y}_n + \mathcal{Y}_{n-1} = 0, \quad n = 1, 2, \ldots, \tag{21}$$

and

$$\mathcal{Z}_2 - R_1 \mathcal{Z}_1 = 0, \tag{22}$$

$$\mathcal{Z}_{n+1} - R_n \mathcal{Z}_n + \mathcal{Z}_{n-1} = 0, \quad n = 2, 3, \ldots \tag{23}$$

Recall that for dispersion relation, our goal is not to seek solutions $\{\mathcal{Y}_n\}$ and $\{\mathcal{Z}_n\}$ for equations (20)–(23), but to obtain a relation from which the appropriate set of dielectrics and hence the normal modes of the system can be derived. In the well-known cases of simply connected regions such as plane, sphere, spheroid, cylinder, etc, the dispersion relations are derived from the requirement that the problem must possess non-trivial solution. Here, we do not consider the effects of any nonlinearities or losses in the system that are known to lead to further diversification of the eigenmodes similar to the case of a lossy metallic nanowire [27]. This approach in the more complicated case of a torus, signified by the above equations, fails to yield the desired dispersion relations. To illustrate this idea and as the first natural attempt, one can express equations (20)–(23) as infinite system of linear equations:

$$\begin{bmatrix} \frac{1}{2}R_0 & -I & & & \\ -I & R_1 & -I & & \\ & -I & R_2 & -I & \\ & & \ddots & \ddots & \ddots \end{bmatrix} \begin{bmatrix} \mathcal{Y}_0 \\ \mathcal{Y}_1 \\ \mathcal{Y}_2 \\ \vdots \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ \vdots \end{bmatrix}, \tag{24}$$

$$\begin{bmatrix} R_1 & -I & & & \\ -I & R_2 & -I & & \\ & -I & R_3 & -I & \\ & & \ddots & \ddots & \ddots \end{bmatrix} \begin{bmatrix} \mathcal{Z}_1 \\ \mathcal{Z}_2 \\ \mathcal{Z}_3 \\ \vdots \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ \vdots \end{bmatrix}. \tag{25}$$

At this point, one may be tempted to claim that equations (24) and (25) possess non-trivial solutions if the determinants of the corresponding infinite matrices vanish identically, and thus obtaining the dispersion relations. Statements similar to the above paragraph have appeared in [16, 28]. Unlike systems with finite dimensions where existence of nontrivial solutions are equivalent to the vanishing of the determinant of coefficient matrix of the system, such requirements are not necessarily valid in the infinite dimensional cases. More details regarding the problem with this approach is addressed in appendix B. As we shall see, the correct approach is to employ the theory of MCFs, which is closely related to the vector three-term recurrence relations.

First, note that equations (20)–(23) can be written as a single vector three-term recurrence:

$$\mathcal{X}_{n+1} - R_n \mathcal{X}_n + \mathcal{X}_{n-1} = 0, \quad n = 2, 3, \ldots, \tag{26}$$

with two *initial* conditions:

$$\mathcal{X}_2 - (R_1 - 2R_0^{-1})\mathcal{X}_1 = 0, \tag{27}$$

$$\mathcal{X}_2 - R_1 \mathcal{X}_1 = 0. \tag{28}$$

The usage of the phrase 'initial conditions' is due to the fact that equation (26) can be cast into a first order nonlinear matrix recurrence relation, where equations (27) and (28) serve as initial conditions, see equations (30)–(32).

Next, suppose that the sequence of $k \times k$ nonsingular matrices $\{X_n\}$ is a solution to the matrix three-term recurrence:

$$X_{n+1} - R_n X_n + X_{n-1} = 0, \quad n = 2, 3, \ldots. \tag{29}$$

Assuming $\mathcal{X}_n$ constitutes a single column of X_n, equations (27) and (28) imply the two initial conditions:

$$X_2 X_1^{-1} = R_1 - 2\frac{I}{R_0}, \tag{30}$$

$$X_2 X_1^{-1} = R_1, \tag{31}$$

where I denotes the $k \times k$ identity matrix and the quotient of two $k \times k$ matrices A and B with B non-singular will be denoted by $A/B := B^{-1}A$ throughout the rest of the paper.

Multiplying equation (29) from the right by X_n^{-1} and defining V_n by $V_n = X_{n+1}X_n^{-1}$, we get the following first order nonlinear matrix recurrence:

$$V_{n-1} = \frac{I}{R_n - V_n}, \quad n = 2, 3, \ldots, \tag{32}$$

with $V_1 = X_2 X_1^{-1}$. Successive iteration of equation (32) yields

$$V_1 = \cfrac{I}{R_2 - \cfrac{I}{R_3 - \cfrac{I}{\ddots - \cfrac{I}{R_n - V_n}}}},$$

or written more compactly from now on as:

$$V_1 = \frac{I}{R_2} - \frac{I}{R_3} - \cdots - \frac{I}{R_n - V_n}. \tag{33}$$

Assuming the limit of the right-hand side of equation (33) exists as $n \to \infty$, one gets

$$V_1 = \frac{I}{R_2} - \frac{I}{R_3} - \frac{I}{R_4} - \cdots. \tag{34}$$

Utilization of the initial conditions equations (30) and (31) leads to the formal expressions:

$$R_1 - 2\frac{I}{R_0} = \frac{I}{R_2} - \frac{I}{R_3} - \frac{I}{R_4} - \cdots, \tag{35}$$

$$R_1 = \frac{I}{R_2} - \frac{I}{R_3} - \frac{I}{R_4} - \cdots. \tag{36}$$

It turns out that one can show the following facts.

I. The MCF

$$\frac{I}{R_2} - \frac{I}{R_3} - \frac{I}{R_4} - \cdots \tag{37}$$

converges and its (unique) limit is independent of any specific choice of the dielectric values $\varepsilon_1, \varepsilon_2, \ldots, \varepsilon_{k+1}$.

II. The convergence of the MCF (37) is equivalent to the existence of the minimal solution to the matrix three-term recurrence equation (29).

The proof of the above statements is long and non-trivial and uses many classical results in connection between the theory of continued fractions and linear recurrence relations. For the sake of readability, we therefore have moved the proof to appendix C.

Now, in light of the above results, it follows that equations (35) and (36) are indeed the dispersion relations for the k-layered torus. Clearly since these equations can not hold simultaneously, we have two separate dispersion relations. From the mathematical point of view, however, there is no prior knowledge to assure either of the initial conditions equation (27) or (28) generates a minimal solution. Nevertheless, in view of (II), one can seek for those dielectric values $\varepsilon_1, \varepsilon_2, \ldots, \varepsilon_{k+1}$ which satisfies either of the dispersion relation equations (35) and (36). The two independent sets of k-tuples $(\varepsilon_{1mn}, \varepsilon_{2mn}, \ldots, \varepsilon_{k+1mn})$ and $(\varepsilon'_{1mn}, \varepsilon'_{2mn}, \ldots, \varepsilon'_{k+1mn})$ obtained in this way are the eigenmodes of the system from which the normal modes can be calculated.

Since there is no exact analytical expression for the MCF equation (37), the exact solutions must be calculated using numerical analysis. In order to examine the numerical structure of the dispersion relations equations (35) and (36), we rewrite them as:

$$\frac{1}{2}R_0 - \frac{I}{R_1} - \frac{I}{R_2} - \frac{I}{R_3} - \cdots = 0$$

$$R_1 - \frac{I}{R_2} - \frac{I}{R_3} - \frac{I}{R_4} - \cdots = 0,$$

and make the following trivial observations:

$$\det\left(\frac{1}{2}R_0 - \frac{I}{R_1} - \frac{I}{R_2} - \frac{I}{R_3} - \cdots\right) = 0, \tag{38}$$

and

$$\det\left(R_1 - \frac{I}{R_2} - \frac{I}{R_3} - \frac{I}{R_4} - \cdots\right) = 0, \tag{39}$$

where R_0, R_1, R_2, ... are defined by equation (14).

In attempting to find those $\{\varepsilon_1, \ldots, \varepsilon_{k+1}\}$ which solve equations (38) and (39), we may also obtain extraneous roots. Nevertheless, for numerical calculation, it is preferable to work with equations (38) and (39) instead of equations (35) and (36) due to the fast convergence of determinant in comparison to any matrix-norm method. To illustrate this, consider a sequence of 2×2 matrices $\{F_n\}$ whose asymptotic behavior for large n is given by

$$F_n \simeq \begin{bmatrix} e^{-n} & (\ln n)^{-1} \\ 0 & 1/n \end{bmatrix}.$$

One can easily verify the zero limit by a few iterations of the determinants, while it will be utterly time-consuming to verify this fact utilizing any matrix-norm calculation. The situation described in the above example is also generic in our case by identifying F_n with the nth approximants (see equation (C.2) of the MCF (37)).

The obtained dispersion relation equations (38) and (39) are numerically validated to be in exact agreement with the limiting case results regarding a single-layered torus. More precisely, we obtain the results of a single-layered torus (see figure 3 in [18] or [28] and [16]) using the dispersion relations (38) and (39) for a k-layered torus model (here only $k = 2$ is provided) with the following limiting case justifications:

Case	Limits	Parameter setting	Aspect ratio
1	$\varepsilon_2 = \varepsilon_3$	$-1.5 \leqslant \varepsilon_1 \leqslant -1$ $\varepsilon_2 = 1$	$1.02 \leqslant \cosh\mu_1 \leqslant 5$ $\cosh\mu_2 = 0.99\cosh\mu_1$
2	$\varepsilon_1 = \varepsilon_2$	$-1.5 \leqslant \varepsilon_1 \leqslant -1$ $\varepsilon_3 = 1$	$1.0098 \leqslant \cosh\mu_2 \leqslant 4.95$ $\cosh\mu_1 = 1.01\cosh\mu_2$

It should be mentioned that the associated Legendre functions $Q^m_{n-\frac{1}{2}}(\cosh\mu_i)$, $P^m_{n-\frac{1}{2}}(\cosh\mu_i)$ are numerically evaluated using equation (8.703), equations (8.736-1)–(8.852-2) in [29] as initial seeds respectively for all values of μ. The rest of the associated Legendre function values are evaluated using equations (8.732-3), (8.732-2), (8.731-3) and (8.731-4)(1) in [29].

Thus, having established the properties of the analytical and numerical approaches to obtaining the generalized dispersion relations of the quasi-static normal modes, we now aim to address the properties of the surface modes that arise when the system is subject to electromagnetic perturbation.

4. The Green's function approach

The Green's function approach was employed by Love [17] to solve for the quasi-static response of a dielectric ring to an external uniform field. Unlike the homogenous difference equation (11), describing the normal modes of the multilayer solid torus, the presence of a nonzero external field leads to a source term for the difference equation that ultimately describes the potential distribution of the ring responding to the external field. For a simple (uniform and isotropic) ring, Love obtained a three term difference equation with a source term corresponding to an external uniform axial field (see Love's equation (2.13)). Love's result was generalized by Garapati *et al* [18] to obtain the response of a composite ring to arbitrary external fields created by discrete multipolar charge distributions. This generalization however warrants further consideration with respect to its convergence properties. Here, extending this generalization to also account for continuous charge distributions, we begin by considering a toroidal charge distribution with density ρ that generates a potential Φ_{ap} and expand $\frac{1}{|\mathbf{r}-\mathbf{r}'|}$ in toroidal coordinates [30]:

$$\begin{aligned}\Phi_{\text{ap}} &= \frac{1}{4\pi\varepsilon_0}\iiint_V \frac{\rho(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}h_{\mu'}h_{\varphi'}h_{\eta'}\mathrm{d}\mu'\mathrm{d}\varphi'\mathrm{d}\eta' \\ &= \frac{1}{4\pi\varepsilon_0}\frac{1}{\pi}f(\mu,\eta)\int_{\eta'=0}^{2\pi}\int_{\varphi'=0}^{2\pi}\int_{\mu'=0}^{\infty} f(\mu',\eta')\rho(\mu',\eta',\varphi') \\ &\quad\times\sum_{n=-\infty}^{\infty}\sum_{m=-\infty}^{\infty} H_{mn}\mathrm{e}^{\mathrm{i}m(\varphi-\varphi')}\mathrm{e}^{\mathrm{i}n(\eta-\eta')} \\ &\quad\times h_{\mu'}h_{\eta'}h_{\varphi'}\mathrm{d}\mu'\mathrm{d}\varphi'\mathrm{d}\eta', \\ H_{mn} &= H_{-mn} = (-1)^m\frac{\Gamma(n-m+1/2)}{\Gamma(n+m+1/2)} \\ &\quad\times[\Theta(\mu-\mu')Q^m_{n-\frac{1}{2}}(\cosh\mu)P^m_{n-\frac{1}{2}}(\cosh\mu') \\ &\quad+\Theta(\mu'-\mu)P^m_{n-\frac{1}{2}}(\cosh\mu)Q^m_{n-\frac{1}{2}}(\cosh\mu')],\end{aligned} \tag{40}$$

where ε_0 is the permittivity of free space, Θ is the Heaviside function, and h_μ, h_η, h_φ are scale factors given by

$$h_\mu = h_\eta = \frac{a}{\cosh\mu-\cos\eta}, \quad h_\varphi = \frac{a\sinh\mu}{\cosh\mu-\cos\eta},$$

with $a = R/\coth\mu_k$. The vectors $\mathbf{r}$ and $\mathbf{r}'$, where $\mathbf{r}\neq\mathbf{r}'$, denote the positions of an arbitrary point in the space and a charged particle, respectively. Superposing Φ_{ap} with the exterior potential in equation (4) and fitting the boundary conditions, we can write

$$\begin{aligned}\Phi_j = f(\mu,\eta)\sum_{m=-\infty}^{\infty}\sum_{n=-\infty}^{\infty}&[C^j_{mn}P^m_{n-\frac{1}{2}}(\cosh\mu) \\ &+ D^j_{mn}Q^m_{n-\frac{1}{2}}(\cosh\mu) \\ &+ \delta_{j,k+1}K_{mn}L^m_{n-\frac{1}{2}}(\cosh\mu)]\mathrm{e}^{\mathrm{i}m\eta}\mathrm{e}^{\mathrm{i}m\varphi},\end{aligned} \tag{41}$$

where $j = 1,\ \ldots,\ k+1$ and $\delta_{j,k}$ denotes the Kronecker delta with generalized form of K_{mn} computed through equation (40) as

$$\begin{aligned}K_{mn} = \frac{1}{4\pi^2\varepsilon_0}\int_0^{2\pi}\int_0^{2\pi}\int_{\mu'}^{\infty} &f(\mu',\eta')\rho(\mu',\eta',\varphi')H_{mn,\mu'} \\ &\times(-1)^m\mathrm{e}^{-\mathrm{i}n\eta'}\mathrm{e}^{-\mathrm{i}m\varphi'}h_{\mu'}h_{\eta'}h_{\varphi'}\mathrm{d}\mu'\mathrm{d}\eta'\mathrm{d}\varphi',\end{aligned} \tag{42}$$

with

$$H_{mn,\mu'} = H_{-mn,\mu'} = P^m_{n-\frac{1}{2}}(\cosh\mu')\frac{\Gamma(n-m+1/2)}{\Gamma(n+m+1/2)}, \tag{43}$$

and where $L^m_{n-\frac{1}{2}}(\cosh\mu) = L^{-m}_{n-\frac{1}{2}}(\cosh\mu) = Q^m_{n-\frac{1}{2}}(\cosh\mu)$. Replacing Φ_j in equation (4) with the one given by equation (41) and introducing the $k\times k$ matrix

$$\mathbb{K}^m_n = \begin{bmatrix} 0 & & & 0 \\ & \ddots & & \\ & & 0 & \\ 0 & & & L^k_n \end{bmatrix}, \tag{44}$$

and the $k\times 1$ vector

$$\mathcal{K}^m_n = \begin{bmatrix} 0 \\ \vdots \\ 0 \\ K_{mn} \end{bmatrix}, \tag{45}$$

the boundary conditions equation (6) imply that for each fixed $m = 0,\ \pm1,\ \pm2,\ \ldots,$

$$\mathcal{C}_n = \mathbb{P}_n^{-1}[\mathbb{Q}_n\mathcal{D}_n + \mathbb{K}_n\mathcal{K}_n], \tag{46}$$

where, as in section 2, the index m is suppressed in $\mathbb{K}^m_n$ and $\mathcal{K}^m_n$. Next, applying the boundary conditions equation (7), a similar procedure as illustrated in equations (A.5)–(A.10) with $\mathcal{C}_n$ in equation (10) replaced by equation (46) gives the non-homogeneous three-term vector recurrence equation

$$\mathcal{W}_{n+1} - R_n\mathcal{W}_n + \mathcal{W}_{n-1} = \mathcal{V}_{n+1} - D_\mu\mathcal{V}_n + \mathcal{V}_{n-1}, \tag{47}$$

for $n = 0,\ \pm1,\ \pm2,\ \ldots,$ where

$$\mathcal{V}_n = (\mathbb{K}'_nE_2 - \mathbb{P}'_nE_2\mathbb{P}_n^{-1}\mathbb{K}_n)\mathcal{K}_n, \tag{48}$$

and

$$\mathbb{K}'_n = \begin{bmatrix} 0 & & 0 \\ & \ddots & \\ & 0 & \\ 0 & & L_n'^k \end{bmatrix}. \tag{49}$$

All other used notations, except for $\mathcal{C}_n$ given by equation (46), are the same as those already introduced in section 2.

Despite the fact that the explicit form of homogenous solutions for equation (47) is unknown, it is still possible to find an explicit expression for $\mathcal{W}_n$ with the aid of the Green's functions. As we shall see, the success of Green's method is mostly due to the symmetric property of R_n and that the homogenous part of equation (47) is of Poincaré-type, discussed in section 3. Our method is the generalization of the one described in Love [17], see also [31].

We begin with the simple observation via a direct substitution that

$$\mathcal{W}_n = \sum_{N=-\infty}^{\infty} G_{n,N}\mathcal{V}_N, \tag{50}$$

is the solution of equation (47) if one can find $k \times k$ matrices $\mathbb{G}_{n,N}$ such that for each fixed N, $\mathbb{G}_{n,N}$ satisfies the three-term matrix recurrence

$$\mathbb{G}_{n+1,N} - R_n\mathbb{G}_{n,N} + \mathbb{G}_{n-1,N} = \delta_{n,N+1}I - \delta_{n,N}D_\mu + \delta_{n,N-1}I, \tag{51}$$

where $n = 0, \pm1, \pm2, \ldots$. For each fixed N, we write equation (51) more explicitly as:

$$\mathbb{G}_{n+1,N} - R_n\mathbb{G}_{n,N} + \mathbb{G}_{n-1,N} = 0, \quad \text{for} \quad n \leqslant N-2, \tag{52}$$

$$\mathbb{G}_{n+1,N} - R_n\mathbb{G}_{n,N} + \mathbb{G}_{n-1,N} = 0, \quad \text{for} \quad n \geqslant N+2, \tag{53}$$

and

$$\mathbb{G}_{N,N} - R_n\mathbb{G}_{N-1,N} + \mathbb{G}_{N-2,N} = I, \qquad n = N-1, \tag{54}$$

$$\mathbb{G}_{N+1,N} - R_n\mathbb{G}_{N,N} + \mathbb{G}_{N-1,N} = -D_\mu, \qquad n = N, \tag{55}$$

$$\mathbb{G}_{N+2,N} - R_n\mathbb{G}_{N+1,N} + \mathbb{G}_{N,N} = I, \qquad n = N+1. \tag{56}$$

Suppressing the index N, the recurrence equation (53) can be written in the general form as

$$X_{n+1} - R_nX_n + X_{n-1} = 0, \quad \text{for} \quad n \geqslant N+2. \tag{57}$$

Now, consider the MCF

$$\frac{I}{R_{N+2}} - \frac{I}{R_{N+3}} - \frac{I}{R_{N+4}} - \cdots. \tag{58}$$

For $N \geqslant -1$, the continued fraction equation (58) is the tail of the MCF equation (C.16); whereas, for $N < -1$, equation (C.16) is the tail of equation (58). In either case, convergence of the MCF equation (C.16) (see theorem 5) implies that equation (58) converges as well. By theorem 3, the three-term recurrence equation (57) has a minimal solution. Letting $\mathbb{G}_{n,N}$ denote this minimal solution for $n \geqslant N+2$, it follows from equation (C.20) that

$$\mathbb{G}_{n+1,N}\mathbb{G}_{n,N}^{-1} = \frac{I}{R_{n+1}} - \frac{I}{R_{n+2}} - \frac{I}{R_{n+3}} - \cdots, \quad n \geqslant N+1. \tag{59}$$

To analyze equation (52), we consider the (backward) matrix three-term recurrence:

$$Y_{n+1} - S_nY_n + Y_{n-1} = 0, \quad n = -2, -3, \ldots, \tag{60}$$

with the initial condition $Y_{-1}Y_0^{-1} = C$, where C is a fixed non-singular $k \times k$ matrix. Multiplying equation (60) from the right by Y_n^{-1} and defining $U_n = Y_{n-1}Y_n^{-1}$, we arrive at the first order nonlinear matrix recurrence:

$$U_{n+1} = \frac{I}{S_n - U_n}, \quad n = -1, -2, \ldots. \tag{61}$$

Using a similar argument as in the proof of theorem 3 (see appendix C), it follows that the MCF

$$\frac{I}{S_{-1}} - \frac{I}{S_{-2}} - \frac{I}{S_{-3}} - \cdots, \tag{62}$$

converges if and only if the (backward) matrix three-term recurrence equation (60) has a minimal solution. Moreover, the minimal solution Y_n satisfies

$$Y_{n-1}Y_n^{-1} = \frac{I}{S_{n-1}} - \frac{I}{S_{n-2}} - \frac{I}{S_{n-3}} - \cdots, \tag{63}$$

for $n = 0, -1, -2, \ldots$.

Now going back to the three-term recurrence equation (52) with $S_n = R_n$ in equation (60), it follows from the symmetric property of R_n that equation (62) is the same as $\frac{I}{R_1} - \frac{I}{R_2} - \frac{I}{R_3} - \cdots$, which is convergent. Thus, with a similar argument presented for the case of equation (53), the three-term recurrence equation (52) has a minimal solution. Letting $\mathbb{G}_{n,N}$ denote this minimal solution for $n \leqslant N - 2$, it follows from equation (63) that

$$\mathbb{G}_{n-1,N}\mathbb{G}_{n,N}^{-1} = \frac{I}{R_{n-1}} - \frac{I}{R_{n-2}} - \frac{I}{R_{n-3}} - \cdots, \quad n \leqslant N - 1. \tag{64}$$

Next, we rewrite equations (59) and (64) as:

$$\mathbb{G}_{n+1,N} = \mathfrak{A}_{n+1}\mathbb{G}_{n,N}, \quad n \geqslant N + 1, \tag{65}$$

$$\mathbb{G}_{n-1,N} = \mathfrak{B}_{n-1}\mathbb{G}_{n,N}, \quad n \leqslant N - 1, \tag{66}$$

where $\mathfrak{A}_{n+1}$ and $\mathfrak{B}_{n+1}$ denote the right-hand sides of equations (59) and (64), respectively. Using equations (65) and (66), we can substitute $\mathbb{G}_{N+2,N}$ and $\mathbb{G}_{N-2,N}$ with $\mathfrak{A}_{N+2}\mathbb{G}_{N+1,N}$ and $\mathfrak{B}_{N-2}\mathbb{G}_{N-1,N}$, respectively, in equations (56) and (54). Thus, we can solve for $\mathbb{G}_{N-1,N}$, $\mathbb{G}_{N,N}$, and $\mathbb{G}_{N+1,N}$ from equations (54)–(56) to obtain:

$$\mathbb{G}_{N-1,N} = \mathfrak{B}_{N-1}\frac{D_\mu - R_N}{R_N - \mathfrak{A}_{N+1} - \mathfrak{B}_{N-1}}, \tag{67}$$

$$\mathbb{G}_{N,N} = \frac{D_\mu - \mathfrak{A}_{N+1} - \mathfrak{B}_{N-1}}{R_N - \mathfrak{A}_{N+1} - \mathfrak{B}_{N-1}}, \tag{68}$$

$$\mathbb{G}_{N+1,N} = \mathfrak{A}_{N+1}\frac{D_\mu - R_N}{R_N - \mathfrak{A}_{N+1} - \mathfrak{B}_{N-1}}. \tag{69}$$

Now, for each fixed n, one may use equations (65)–(69) to obtain $\mathcal{W}_n$ from equation (50). Thus one can finally calculate the $k \times 1$ vectors $\mathcal{D}_n$ and $\mathcal{C}_n$ from equations (12) and (46), respectively.

As a final remark regarding the utility of the Green's function, it is illuminating to consider the response of a coated ring to monopoles and dipoles. Other basic cases were treated recently [18]. We consider a k-layered vacuum bounded solid ring in the presence of monopoles and dipoles of charge q_s at $\mathbf{r}_{0,s} = (\mu_{0,s}, \eta_{0,s}, \varphi_{0,s})$ outside the toroidal boundary $\mu = \mu_k > \mu_{0,s}$, with s counting the number of charges. The charge density corresponding to a point charge q_s at $\mathbf{r}_{0,s}$ is

$$\rho_s = q_s\delta(\mathbf{r} - \mathbf{r}_{0,s}), \tag{70}$$

which in the toroidal coordinates reads

$$\begin{aligned}\delta(\mathbf{r} - \mathbf{r}_0) &= \delta[h_\mu(\mu - \mu_0)]\delta[h_\eta(\eta - \eta_0)]\delta[h_\varphi(\varphi - \varphi_0)] \\ &= \frac{1}{h_\mu h_\eta h_\varphi}\delta(\mu - \mu_0)\delta(\eta - \eta_0)\delta(\varphi - \varphi_0).\end{aligned} \tag{71}$$

Using equations (42), (70) and (71) one obtains

$$K_{mn,s} = \frac{1}{4\pi\varepsilon_0\varepsilon_{k+1}}\frac{q_s}{\pi a}(-1)^m f(\mu_{0,s}, \eta_{0,s})H_{mn,\mu_{0,s}} \times \mathrm{e}^{-\mathrm{i}m\eta_{0,s}}\mathrm{e}^{-\mathrm{i}m\varphi_{0,s}} \tag{72}$$

with $1/a$ considered as a scaling factor. Thus, the generalized form of the applied non-uniform external field as in equation (40) may be given as

$$\Phi_{\mathrm{ap}} = f(\mu, \eta)\sum_s \sum_{m,n=-\infty}^{\infty} K_{mn,s}L^m_{n-\frac{1}{2}}(\cosh\mu)\mathrm{e}^{\mathrm{i}n\eta}\mathrm{e}^{\mathrm{i}m\varphi}. \tag{73}$$

Superposing Φ_{ap} with the external potential in equation (4) we obtain

$$\begin{aligned}\Phi_j = f(\mu, \eta)\sum_s \sum_{m,n=-\infty}^{\infty} &[C^j_{mn,s}P^m_{n-\frac{1}{2}}(\cosh\mu)\mathrm{e}^{-\mathrm{i}n\eta^j_{mn,s}} \\ &\times \mathrm{e}^{-\mathrm{i}m\varphi_{0,s}} + D^j_{mn,s}Q^m_{n-\frac{1}{2}}(\cosh\mu)\mathrm{e}^{-\mathrm{i}n\eta'^j_{mn,s}}\mathrm{e}^{-\mathrm{i}m\varphi_{0,s}} \\ &+ \delta_{j,k+1}K_{mn,s}L^m_{n-\frac{1}{2}}(\cosh\mu)]\mathrm{e}^{\mathrm{i}n\eta}\mathrm{e}^{\mathrm{i}m\varphi},\end{aligned} \tag{74}$$

for $j = 1, \ldots, k + 1$. When specialized for $k = 1$, that is, in case of a solid ring, equation (74) reduces to equation (7) in [31], where m runs from 0 to ∞. With rightly chosen K_{mn} for each external charge in equation (74), we present figures 2–4 showing the potential response of the composite (i.e., $k = 2$) nanoring to an external nonuniform field of an electric monopole, and a dipole emitter of charges q_s located at $r_{0,s}$ outside the

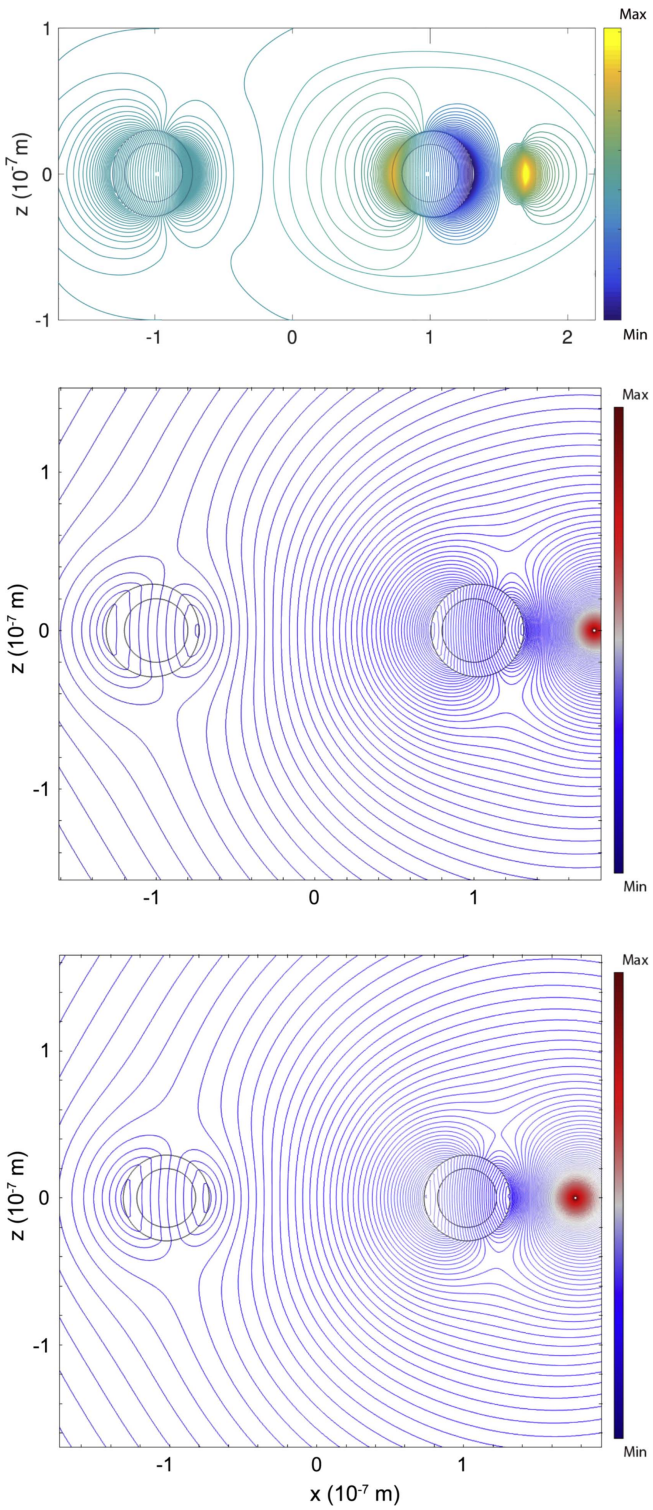

Figure 2. Potential distribution representing the response of a composite nanoring with $a = 0.0980\ \mu$m, $\cosh\mu_1 = 5$, $\cosh\mu_2 = 3.5$, $\epsilon_1 = -1.5$, $\epsilon_2 = -3$, and $\epsilon_3 = 1$ to a non-uniform field of an electric monopole. (*Top*) The result is obtained via equation (74) with $s = 1$ by summation of poloidal and toroidal modes for a coated ring. Computationally determined distribution using FEM for confocal (*Middle*) versus concentric (*Bottom*) rings. Max (Min) signifies the highest (lowest) potential.

toroidal boundary $\mu = \mu_2 > \mu_{0,s}$. To validate the results, we also solved the Laplace equation computationally using finite elements method [32], as shown in figures 2–4. As can be seen, the results are in good agreement.

In case of an uniform field polarized along the z-axis, the generalized form of the applied external potential may be given by (see [17])

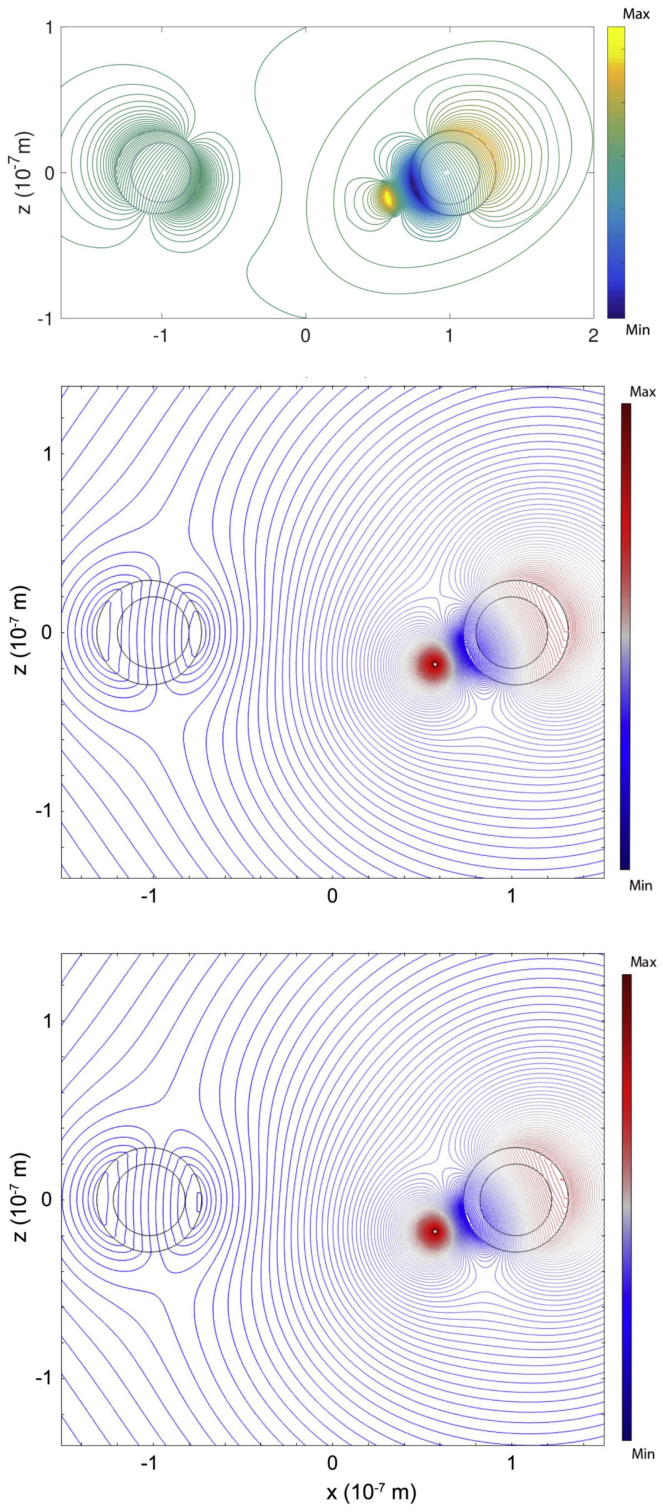

Figure 3. Similar description as in figure 2 but with the monopole placed at an angle. Computationally determined distribution using FEM for confocal (*Middle*) versus concentric (*Bottom*) rings. Max (Min) signifies the highest (lowest) potential.

$$\Phi_{\rm ap} = f(\mu, \eta) \sum_{n=-\infty}^{\infty} K_n Q_{n-\frac{1}{2}} e^{in\eta}, \tag{75}$$

where

$$K_n = \frac{\sqrt{8}\, aE_0}{i\pi} n. \tag{76}$$

Applying the principle of superposition as before we obtain equation (41) but with $m = 0$ considered. As an example we present figure 5 which shows the potential distribution of a coated nanoring in an uniform field with

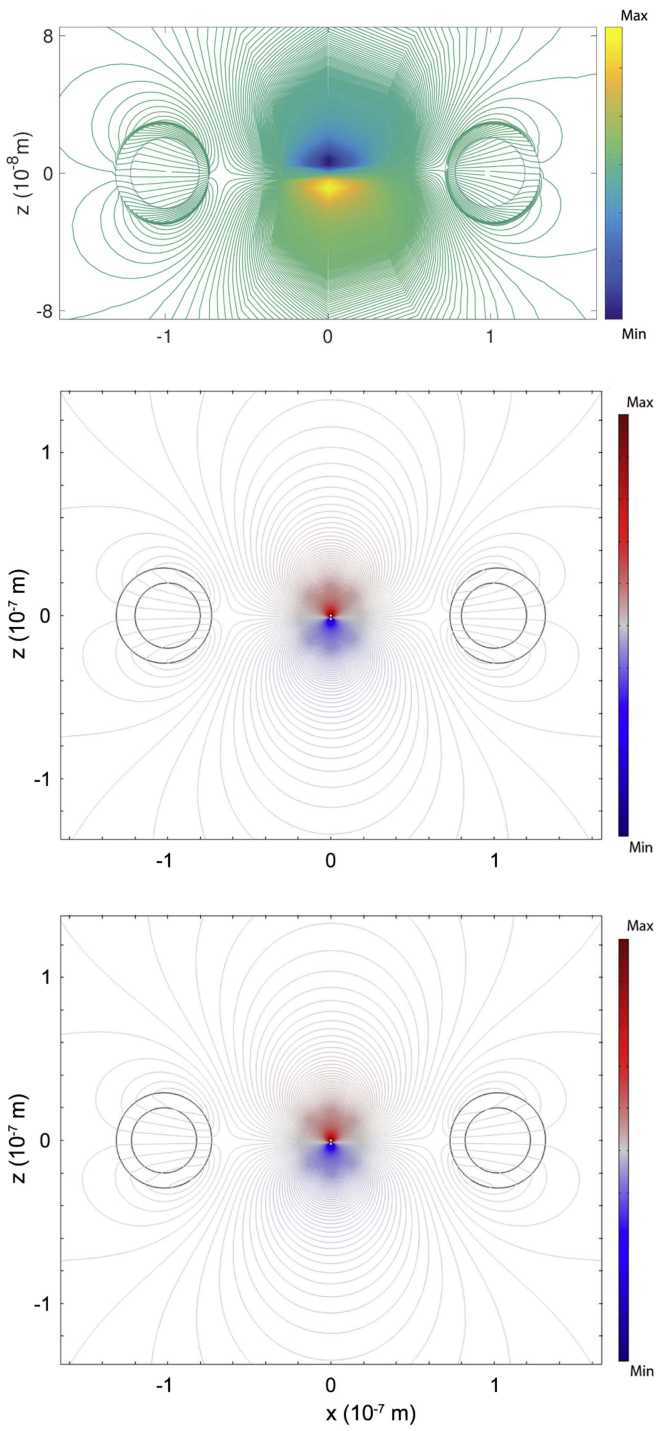

Figure 4. Potential distribution representing the response of a composite nanoring with similar parameters as in figure 2 to a non-uniform field of a dipole emitter located near the origin. (*Top*) The result is obtained via equation (74) with $s = 1, 2$ by summation of poloidal and toroidal modes for a composite ring. Computationally determined distribution using FEM for confocal (*Middle*) versus concentric (*Bottom*) rings. Max (Min) signifies the highest (lowest) potential.

polarization parallel to the symmetry axis of the ring where in the vectors $\mathcal{C}_n$ and $\mathcal{D}_n$ are computed as discussed in the paragraph following equation (69). For comparison, the potential distributions are provided for both confocal and concentric rings, as shown in figure 5. Other relevant cases have been studied in [18].

In closing, regarding the experimental investigation of nanorings, currently within nanophotonics and nanoplasmonics (typical length scale ~ few tens of nm), several (emerging) approaches have been reported for fabrication of these structures [33–40]. The main methods include nanofabrication (electron beam lithography) and chemical synthesis. Single rings, ring arrays, and in-fluid suspended rings (metallic and dielectric) have been attempted. Considering the photon response of the rings, singly and possibly doubly coated metallo-dielectric rings are most conceivable, while it is unlikely that the number of coatings will exceed much beyond a few.

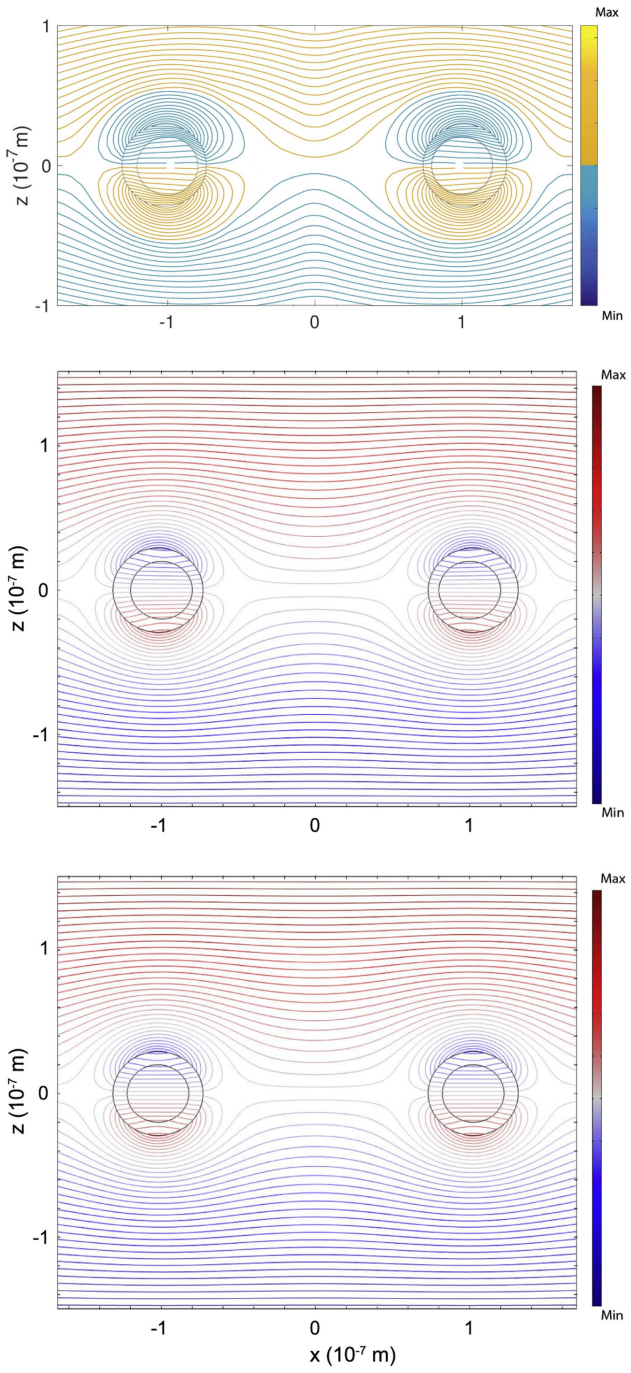

Figure 5. Potential distribution representing the response of a composite metal nanoring with similar parameters as in figure 2 to a uniform field polarized parallel to the ring symmetry axis. (*Top*) The result is obtained via equation (41) with $m = 0$. Computationally determined distribution using FEM for confocal (*Middle*) versus concentric (*Bottom*) rings. Max (Min) signifies the highest (lowest) potential.

Further, we note that typically, the coating thicknesses are only a fraction of the minor radius of the ring. Therefore, for practical purposes, as also seen in figure 1, the deviation from full concentricity is negligible. This is clearly seen also from the comparison of the computationally determined potential distributions for the concentric rings versus those of the confocal rings as shown in figures 2–4.

5. Conclusion

While in general it is recognized that oscillations in the electronic charge density at toroidal interfaces occur at frequencies that can be approximately obtained from the eigenvalues associated with the quasi-static boundary value problem, the scalar three term difference equation that arises when the scalar electric potential is required

to satisfy the boundary conditions across a single toroidal interface is seen to cause significant algebraic complexity. The 'three-term coupling' is due to the quasi-separation of variables in toroidal coordinates while attempting to solve the Laplace equation. This phenomenon is demonstrated in the coupling of the toroidal coordinates μ and η via the function f in equation (2). As a result, the generalization of the scalar three-term difference equations to vector three-term recurrences was shown to be necessary to obtain the plasmon dispersion relations in a multilayered toroidal structure. The structure of the nonretarded surface plasmon dispersion relations for a general multilayer toroidal system may thus be studied following the convergence properties of the MCFs and infinite determinants associated with the vector three-term recurrences. However, contrary to the cases of finite dimensional matrices representing the underlying system of equations, in the toroidal case, as described here, it is reasonable not to simply assume that the vanishing of the matrix determinant would guarantee nontrivial solutions. The convergence properties of the obtained MCFs associated with the vector three-term recurrence relation equations (20)–(23) were shown to provide a numerical platform for computation of the eigenmodes using the determinant forms of the dispersion relations given by equations (38) and (39). The presented results help facilitating numerical analysis of the plasmon dispersion for specific metals such as gold, silver and aluminum assembled, in conjunction with suitable dielectric media such as silicon and quartz, into a complex nanoring. Equations (38) and (39) can be used to obtain the dependence of the plasmon excitation frequency upon the aspect ratio of various nanorings, which enters via the frequency dependence of the dielectric functions of the involved materials. Thus, plasmon dispersion can be investigated in arbitrarily coated toroidal nanoparticles (see also [18]). In addition to the normal mode calculation, the response of a composite ring to arbitrary external fields was shown to be attainable via convergent MCFs.

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Appendix A

In this section, we supply the details in obtaining the vector three-term recurrence equation (11) and give a proof of theorem 1.

First, we apply the boundary condition equation (6) for each $i = 1, \ldots, k$, which relates the coefficients $\{C_n^i\}_{i=2}^{k+1}$ and $\{D_n^i\}_{i=1}^{k}$ via

$$\sum_{n=-\infty}^{\infty} (C_n^i P_n^i + D_n^i Q_n^i) e^{in\eta} = \sum_{n=-\infty}^{\infty} (C_n^{i+1} P_n^i + D_n^{i+1} Q_n^i) e^{in\eta}. \tag{A.1}$$

The completeness of the system $\{e^{in\eta}\}$ implies that, for each fixed n, the corresponding coefficients on both sides of equation (A.1) must agree; i.e.,

$$C_n^i P_n^i + D_n^i Q_n^i = C_n^{i+1} P_n^i + D_n^{i+1} Q_n^i, \tag{A.2}$$

for each $n = 0, \pm 1, \pm 2, \ldots$ and $i = 1, \ldots, k$ with values in equation (5) considered. Using the $k \times 1$-vectors $\mathcal{C}_n$ and $\mathcal{D}_n$ given by equation (8), one can rewrite equation (A.2) as

$$\mathbb{P}_n \mathcal{C}_n = \mathbb{Q}_n \mathcal{D}_n,$$

with $k \times k$ bidiagonal matrices $\mathbb{P}_n$ and $\mathbb{Q}_n$ defined by

$$\mathbb{P}_n = \begin{bmatrix} -P_n^1 & & & 0 \\ P_n^2 & -P_n^2 & & \\ & \ddots & \ddots & \\ 0 & & P_n^k & -P_n^k \end{bmatrix}, \tag{A.3}$$

$$\mathbb{Q}_n = \begin{bmatrix} -Q_n^1 & Q_n^1 & & 0 \\ & \ddots & \ddots & \\ & & -Q_n^{k-1} & Q_n^{k-1} \\ 0 & & & -Q_n^k \end{bmatrix}. \tag{A.4}$$

Similarly, applying the boundary condition equation (7) for each $i = 1, \ldots, k$, we obtain

$$\varepsilon_i \sum_{n=-\infty}^{\infty} [C_n^i(f_i P_n'^i + P_n^i f_i') + D_n^i(f_i Q_n'^i + Q_n^i f_i')]\mathrm{e}^{\mathrm{i}n\eta} = \varepsilon_{i+1} \sum_{n=-\infty}^{\infty} [C_n^{i+1}(f_i P_n'^i + P_n^i f_i')] + D_n^{i+1}(f_i Q_n'^i + Q_n^i f_i')] \times \mathrm{e}^{\mathrm{i}n\eta}. \tag{A.5}$$

Collecting similar terms in equation (A.5) and using the facts that $f_i' = 1/2f_i$ and $f_i^2 = \cosh\mu_i - \cos\eta$, we obtain

$$\begin{aligned}\sum_{n=-\infty}^{\infty} &\{\varepsilon_i[2(\cosh\mu_i - \cos\eta)P_n'^i + P_n^i]C_n^i \\ &- \varepsilon_{i+1}[2(\cosh\mu_i - \cos\eta)P_n'^i + P_n^i]C_n^{i+1}\}\mathrm{e}^{\mathrm{i}n\eta} \\ &= \sum_{n=-\infty}^{\infty} \{\varepsilon_{i+1}[2(\cosh\mu_i - \cos\eta)Q_n'^i + Q_n^i]D_n^{i+1} \\ &- \varepsilon_i[2(\cosh\mu_i - \cos\eta)Q_n'^i + Q_n^i]D_n^i\}\mathrm{e}^{\mathrm{i}n\eta}.\end{aligned} \tag{A.6}$$

The existence of $\cos\eta$ in equation (A.6) prevents the use of the completeness argument for the system $\{\mathrm{e}^{\mathrm{i}n\eta}\}$ directly as in equation (A.2). However, since $\cos\eta = (\mathrm{e}^{\mathrm{i}\eta} + \mathrm{e}^{-\mathrm{i}\eta})/2$, one sees that the $\cos\eta$ term shifts the bi-infinite sequence $\{\mathrm{e}^{\mathrm{i}n\eta}\}$ to the left and right by one unit. Thus, applying the mentioned unilateral backward and forward shifts in equation (A.6) and substituting back $n+1 \mapsto n$ and $n-1 \mapsto n$, we can use the completeness argument presented in equation (A.2) to obtain

$$\begin{aligned}&\varepsilon_i(\alpha_n^i C_n^i - P_{n+1}'^i C_{n+1}^i - P_{n-1}'^i C_{n-1}^i) \\ &- \varepsilon_{i+1}(\alpha_n^i C_n^{i+1} - P_{n+1}'^i C_{n+1}^{i+1} - P_{n-1}'^i C_{n-1}^{i+1}) \\ &= \varepsilon_{i+1}(\beta_n^i D_n^{i+1} - Q_{n+1}'^i D_{n+1}^{i+1} - Q_{n-1}'^i D_{n-1}^{i+1}) \\ &- \varepsilon_i(\beta_n^i D_n^i - Q_{n+1}'^i D_{n+1}^i - Q_{n-1}'^i D_{n-1}^i),\end{aligned} \tag{A.7}$$

for each $n = 0, \pm1, \pm2, \ldots$, and $i = 1, \ldots, k$, where

$$\alpha_n^i = 2\cosh\mu_i P_n'^i + P_n^i, \tag{A.8}$$

$$\beta_n^i = 2\cosh\mu_i Q_n'^i + Q_n^i. \tag{A.9}$$

Using the notations introduced in equations (8), (A.3) and (A.4), one can rewrite equation (A.7) as

$$\mathbb{P}'_{n+1}E_2\,\mathcal{C}_{n+1} - A_n\mathcal{C}_n + \mathbb{P}'_{n-1}E_2\,\mathcal{C}_{n-1} = \mathbb{Q}'_{n+1}E_1\,\mathcal{D}_{n+1} - B_n\mathcal{D}_n + \mathbb{Q}'_{n-1}E_1\,\mathcal{D}_{n-1}, \tag{A.10}$$

for $n = 0, \pm1, \pm2, \ldots$, where

$$\begin{cases} A_n = (\mathbb{P}_n + D_\mu\mathbb{P}'_n)\,E_2, \\ B_n = (\mathbb{Q}_n + D_\mu\mathbb{Q}'_n)\,E_1. \end{cases} \tag{A.11}$$

The $k \times k$ bidiagonal matrices $\mathbb{P}'_n$ and $\mathbb{Q}'_n$ are defined by

$$\mathbb{P}'_n = \begin{bmatrix} -P_n'^1 & & & 0 \\ P_n'^2 & -P_n'^2 & & \\ & \ddots & \ddots & \\ 0 & & P_n'^k & -P_n'^k \end{bmatrix}, \tag{A.12}$$

$$\mathbb{Q}'_n = \begin{bmatrix} -Q_n'^1 & Q_n'^1 & & 0 \\ & \ddots & \ddots & \\ & & -Q_n'^{k-1} & Q_n'^{k-1} \\ 0 & & & -Q_n'^k \end{bmatrix}, \tag{A.13}$$

and the $k \times k$ diagonal matrices D_μ, E_1, E_2 are given by

$$D_\mu = \begin{bmatrix} 2\cosh\mu_1 & & & 0 \\ & 2\cosh\mu_2 & & \\ & & \ddots & \\ 0 & & & 2\cosh\mu_k \end{bmatrix}, \tag{A.14}$$

$$E_1 = \begin{bmatrix} \varepsilon_1 & & 0 \\ & \varepsilon_2 & \\ & \ddots & \\ 0 & & \varepsilon_k \end{bmatrix}, \quad E_2 = \begin{bmatrix} \varepsilon_2 & & 0 \\ & \varepsilon_3 & \\ & \ddots & \\ 0 & & \varepsilon_{k+1} \end{bmatrix}. \tag{A.15}$$

Substituting equation (10) in (A.10) gives

$$J_{n+1}\mathcal{D}_{n+1} - (A_n\mathbb{P}_n^{-1}\mathbb{Q}_n - B_n)\mathcal{D}_n + J_{n-1}\mathcal{D}_{n-1} = 0, \tag{A.16}$$

where J_n is given by equation (13) as

$$J_n = (\mathbb{P}'_n E_2 \mathbb{P}_n^{-1} - \mathbb{Q}'_n E_1 \mathbb{Q}_n^{-1})\mathbb{Q}_n.$$

Using equation (A.11), one can easily see

$$A_n\mathbb{P}_n^{-1}\mathbb{Q}_n - B_n = (\mathbb{P}_n E_2 \mathbb{P}_n^{-1} - \mathbb{Q}_n E_1 \mathbb{Q}_n^{-1})\mathbb{Q}_n + D_\mu J_n.$$

It follows now that the substitution

$$\mathcal{W}_n = J_n\mathcal{D}_n,$$

transforms equation (A.16) into

$$\mathcal{W}_{n+1} - R_n\mathcal{W}_n + \mathcal{W}_{n-1} = 0,$$

for $n = 0, \pm1, \pm2, \ldots$, where

$$R_n = D_\mu + (\mathbb{P}_n E_2 \mathbb{P}_n^{-1} - \mathbb{Q}_n E_1 \mathbb{Q}_n^{-1})(\mathbb{P}'_n E_2 \mathbb{P}_n^{-1} - \mathbb{Q}'_n E_1 \mathbb{Q}_n^{-1})^{-1}.$$

This concludes the algebraic derivation of equation (11).

Proof of theorem 1.

Let $R_n = D_\mu + U_n V_n^{-1}$, where

$$U_n = \mathbb{P}_n E_2 \mathbb{P}_n^{-1} - \mathbb{Q}_n E_1 \mathbb{Q}_n^{-1},$$
$$V_n = \mathbb{P}'_n E_2 \mathbb{P}_n^{-1} - \mathbb{Q}'_n E_1 \mathbb{Q}_n^{-1}.$$

The theorem follows if we can show that $U_n V_n^{-1} \to 0$ as $n \to \infty$. Since $\mathbb{P}_n$ and $\mathbb{Q}_n$ are triangular matrices, one can obtain an explicit formula for their inverses and after some simple algebra, we get

$$[U_n]_{ij} = \begin{cases} \frac{Q_n^i}{Q_n^j}(\varepsilon_{i+1} - \varepsilon_i) & \text{if} \quad i < j, \\ \varepsilon_{i+1} - \varepsilon_i & \text{if} \quad i = j, \\ \frac{P_n^i}{P_n^j}(\varepsilon_{i+1} - \varepsilon_i) & \text{if} \quad i > j, \end{cases}$$

and

$$[V_n]_{ij} = \begin{cases} \frac{Q_n'^i}{Q_n^j}(\varepsilon_{i+1} - \varepsilon_i) & \text{if} \quad i < j, \\ \frac{P_n'^i}{P_n^i}\varepsilon_{i+1} - \frac{Q_n'^i}{Q_n^i}\varepsilon_i & \text{if} \quad i = j, \\ \frac{P_n'^i}{P_n^j}(\varepsilon_{i+1} - \varepsilon_i) & \text{if} \quad i > j, \end{cases}$$

where $i, j = 1, \ldots, k$. From the asymptotic forms of the associated Legendre functions (see appendix in [16]), and their derivatives, using formulas (8.731-1)(1), (8.734-4), and (8.732-1) in [29], we have that for large n

$$P_n^i \simeq \mathrm{e}^{n\mu_i},\ Q_n^i \simeq \mathrm{e}^{-n\mu_i},\ P_n'^i \simeq n\mathrm{e}^{n\mu_i},\ Q_n'^i \simeq n\mathrm{e}^{-n\mu_i}.$$

Thus for large values of n

$$[U_n]_{ij} \simeq \begin{cases} \mathrm{e}^{-n(\mu_i-\mu_j)}(\varepsilon_{i+1} - \varepsilon_i) & \text{if} \quad i < j, \\ \varepsilon_{i+1} - \varepsilon_i & \text{if} \quad i = j, \\ \mathrm{e}^{-n(\mu_j-\mu_i)}(\varepsilon_{i+1} - \varepsilon_i) & \text{if} \quad i > j, \end{cases} \tag{A.17}$$

and

$$[V_n]_{ij} \simeq \begin{cases} n\mathrm{e}^{-n(\mu_i-\mu_j)}(\varepsilon_{i+1} - \varepsilon_i) & \text{if} \quad i < j, \\ n(\varepsilon_{i+1} - \varepsilon_i) & \text{if} \quad i = j, \\ n\mathrm{e}^{-n(\mu_j-\mu_i)}(\varepsilon_{i+1} - \varepsilon_i) & \text{if} \quad i > j, \end{cases} \tag{A.18}$$

where $i, j = 1, \ldots, k$. Since $\mu_i > \mu_j$ whenever $i < j$, it follows from equation (A.18) that all off-diagonal elements of V_n approach zero. Therefore, V_n is nonsingular for large values of n. Moreover, equations (A.17)

and (A.18) imply that $V_n \simeq nU_n$. Thus for sufficiently large n, we have $U_n V_n^{-1} \simeq U_n(nU_n)^{-1} \simeq C/n$, for some (constant) matrix C independent of n. Finally, the last estimate implies $U_n V_n^{-1} \to 0$.

Appendix B

Equations (24) and (25) are special cases of the infinite system of linear equations

$$A\mathcal{X} = 0, \tag{B.1}$$

where $A = [A_{ij}]_{i,j=0}^{\infty}$ is an infinite matrix consisting of block matrices $A_{ij} \in \mathbb{C}^{k\times k}$ and $\mathcal{X} = [\mathcal{X}_0, \mathcal{X}_1, ...]^T$ is the infinite unknown vector consisting of $k \times 1$ vectors $\mathcal{X}_n = [x_1^n, ..., x_k^n]^T$. Letting $A_n := [A_{ij}]_{i,j=0}^{n}$, the infinite determinant is defined by

$$\det(A) = \lim_{n\to\infty} \det(A_n), \tag{B.2}$$

provided such a limit exists, see [41–43]. As mentioned earlier in section 3, statement such as: 'equation (B.1) has non-trivial solutions if and only if $\det(A) = 0$,' which also has appeared in [28, 44], does not hold for infinite system in general. In fact, one can find trivial examples where $\det(A)$, described as in equation (B.2), may not exist but the system still possesses non-trivial solutions, see [18]. On the other hand, one can show the validity of the above statement under certain rather restrictive conditions. One such classic result (see Koch [45] and also [41–43]) states that for a certain class $\mathcal{M}$ of infinite matrices if the moduli of the off diagonal terms are square summable and the infinite product of the diagonal terms converges absolutely, and if the vector $\mathcal{X}$ is also square summable, then $\det(A)$ exists and the infinite system equation (B.1) has a non-trivial solution if and only if $\det(A) = 0$, see Denk [42] for details. As it stands, neither of the infinite block matrices in equations (24) and (25) belongs to the class $\mathcal{M}$. It should also be emphasized that we can not utilize the truncated system method, see [46], where the infinite matrix A has to satisfy similar conditions to those of the class $\mathcal{M}$. Finally, we note that a formal calculation of the determinants for infinite matrices in equations (24) and (25) based on the definition equation (B.2) and the result regarding the determinant of a finite tridigonal matrix [47] does not imply the obtained dispersion relations. This justification, see [48], is beyond the scope of this paper and is therefore omitted.

Appendix C

Here, we prove the claims (I) and (II) of section 3 with regard to the MCF (37) and its relation to the matrix three-term recurrence equation (29).

We start by assessing the convergence of equation (37). Recall that given two sequences of $k \times k$ matrices $\{A_n\}$ and $\{B_n\}$, where B_n are non-singular for large n, the MCF

$$\frac{A_1}{B_1} + \frac{A_2}{B_2} + \frac{A_3}{B_3} + \cdots, \tag{C.1}$$

is said to converge to the $k \times k$ matrix Ω if the sequence of approximants

$$F_n := \frac{A_1}{B_1} + \frac{A_2}{B_2} + \cdots + \frac{A_n}{B_n}, \tag{C.2}$$

converges in $\mathbb{C}^{k\times k}$, in which case we set $\Omega = \frac{A_1}{B_1} + \frac{A_2}{B_2} + \frac{A_3}{B_3} + \cdots$. Matrix F_n is called the nth approximant of the MCF equation (C.1).

The classical approach to continued fractions with the aid of the theory of Möbius or linear fractional transformations is also fruitful in treating MCFs, see Ahlbrandt [24, 25] and references therein. In this paper, however, we only consider and thus explain the portion which is relevant to our special case equation (C.1). So let M be a nonsingular $2k \times 2k$ block matrix

$$M = \begin{bmatrix} \mathbb{C} & \mathbb{D} \\ \mathbb{A} & \mathbb{B} \end{bmatrix}, \tag{C.3}$$

where $\mathbb{A}$, $\mathbb{B}$, $\mathbb{C}$ and $\mathbb{D}$ are $k \times k$ matrices. The matrix linear fractional transformation $T_M : \mathbb{C}^{k\times k} \to \mathbb{C}^{k\times k}$ with the symbol M is defined by

$$T_M(W) = \frac{W\mathbb{C} + \mathbb{A}}{W\mathbb{D} + \mathbb{B}}. \tag{C.4}$$

Note that we will suppress the symbol M from our notation whenever it is understood. It is easily seen that

$$S_1 \circ S_2 \circ \ldots S_n(W) = \frac{A_1}{B_1} + \frac{A_2}{B_2} + \cdots + \frac{A_n}{B_n + W}, \tag{C.5}$$

where the matrix linear fractional transformations S_n are given by

$$S_n(W) = \frac{A_n}{B_n + W}, \quad (n = 1, 2, \ldots), \tag{C.6}$$

with corresponding symbols

$$\theta_n = \begin{bmatrix} 0 & I \\ A_n & B_n \end{bmatrix}. \tag{C.7}$$

As a result, if we let

$$T_n := S_1 \circ S_2 \circ \ldots S_n, \tag{C.8}$$

then it follows from equation (C.5) that $T_n(0) = F_n$, the nth approximant of equation (C.1). Consequently, one can define the convergence of the MCF equation (C.1) as

$$\lim_{n\to\infty} T_n(0), \tag{C.9}$$

provided that the above limit exists. This observation is important. In simple terms, since it is easily verified that the composition of two matrix linear fractional transformations, say $T_K \circ T_L$ with corresponding symbols K and L, is again a linear fractional transformation T_M with the symbol $M = LK$, the definition of T_n in equation (C.4) together with equation (C.7) imply

$$T_n(W) = \frac{W\mathbb{C}_n + \mathbb{A}_n}{W\mathbb{D}_n + \mathbb{B}_n}, \tag{C.10}$$

with the symbol

$$M_n = \begin{bmatrix} \mathbb{C}_n & \mathbb{D}_n \\ \mathbb{A}_n & \mathbb{B}_n \end{bmatrix} = \begin{bmatrix} 0 & I \\ A_n & B_n \end{bmatrix} \cdot \ldots \cdot \begin{bmatrix} 0 & I \\ A_1 & B_1 \end{bmatrix}. \tag{C.11}$$

Now, we can give an alternative definition for the convergence of the MCF equation (C.1). Suppose $\{\mathbb{A}_n\}$ and $\{\mathbb{B}_n\}$ are given by equation (C.11). The MCF equation (C.1) is said to converge if $\mathbb{B}_n$ is nonsingular for large n and

$$\lim_{n\to\infty} \frac{\mathbb{A}_n}{\mathbb{B}_n} \in \mathbb{C}^{k\times k}. \tag{C.12}$$

Writing equation (C.11) in terms of the introduced notations, we get

$$M_n = \theta_n M_{n-1} \quad \text{with} \quad M_0 = I, \tag{C.13}$$

which shows the connection between the theory of continued fractions and linear recurrence relations. To see this, we rewrite equation (29) into a first order recurrence system

$$\begin{bmatrix} X_n \\ X_{n+1} \end{bmatrix} = \begin{bmatrix} 0 & I \\ -I & R_n \end{bmatrix} \begin{bmatrix} X_{n-1} \\ X_n \end{bmatrix}, \quad n \geqslant 2. \tag{C.14}$$

Now if we denote the $2k \times 2k$ block matrix in equation (C.14) by θ_n defined as in equation (C.7); i.e.

$$\theta_n = \begin{bmatrix} 0 & I \\ -I & R_n \end{bmatrix}, \tag{C.15}$$

we are implicitly considering the MCF equation (37) with $A_n = -I$ and $B_n = R_n$, i.e.

$$-\frac{I}{R_2} - \frac{I}{R_3} - \frac{I}{R_4} - \cdots \tag{C.16}$$

Before we can show the connection between equations (C.16) and (C.14), we need some definitions. Two solutions X_n and Y_n of equation (29) are said to be *linearly independent* if their Wronskian (or Casoratian) is nonsingular; that is, the $2k \times 2k$ matrix

$$\begin{bmatrix} X_0 & Y_0 \\ X_1 & Y_1 \end{bmatrix}, \tag{C.17}$$

is nonsingular (see [24] for details).

Definition 1. A solution X_n of the matrix three-term recurrence equation (29) is called minimal if the following conditions hold.

1. X_1 is nonsingular,
2. If Y_n is a solution of equation (29) such that X_n and Y_n are linearly independent, then Y_n is nonsingular for large values of n and

$$\lim_{n\to\infty} \frac{X_n}{Y_n} = 0.$$

Our definition of minimality is based on the notion of *recessive solution* of equation (C.14) introduced in [49] (see also [24]), where it is shown that a recessive solution is unique up to multiplication by a constant matrix. As a result, one could call 'a minimal solution' by 'the minimal solution'. For the purpose of this paper, both terminologies are acceptable and we will not pursue this issue any further. We are now in the position to show the connection between continued fractions and recurrence relations.

Theorem 2. *If the matrix three-term recurrence equation (29) has a minimal solution X_n, then the MCF equation (C.16) converges and its limit is given by $-X_2X_1^{-1}$.*

Proof. Let Y_n be a solution of equation (29) such that X_n and Y_n are linearly independent and put

$$\mathbf{Z}_n = \begin{bmatrix} X_n & Y_n \\ X_{n+1} & Y_{n+1} \end{bmatrix}. \tag{C.18}$$

It follows from equation (C.14) that $\mathbf{Z}_n$ satisfies

$$\mathbf{Z}_n = \theta_n \mathbf{Z}_{n-1}, \quad n = 2, 3, \ldots,$$

where θ_n's are given by equation (C.15). Successive iteration of the above recurrence gives

$$\mathbf{Z}_n = \theta_n\theta_{n-1}\ldots\theta_2\mathbf{Z}_1 = M_n\mathbf{Z}_1,$$

where in the last equality we have used equation (C.11). It is clear that $\det\theta_n = 1$ for all n. So M_n is nonsingular. This observation is important as the symbol of a linear fractional transformation is implicitly assumed to be nonsingular.

Since X_n and Y_n are linearly independent, $\mathbf{Z}_1$ is nonsingular. This implies that we can solve M_n from the last equality as

$$M_n = \mathbf{Z}_n\mathbf{Z}_1^{-1}. \tag{C.19}$$

Since X_n is minimal, X_0 is nonsingular. Therefore, we can write an explicit formula for $\mathbf{Z}_0^{-1}$ as

$$\mathbf{Z}_1^{-1} = \begin{bmatrix} X_1^{-1} + X_1^{-1}Y_1S^{-1}X_2X_1^{-1} & -X_1^{-1}Y_1S^{-1} \\ -S^{-1}X_2X_1^{-1} & S^{-1} \end{bmatrix},$$

where the nonsingular matrix $S = Y_2 - X_2X_1^{-1}Y_1$ is called the Schur complement of X_1 in $\mathbf{Z}_1$, see [50], p 227. Denoting the first row of $\mathbf{Z}_1^{-1}$ by U and V and using the expression for M_n from equation (C.11), the equalty equation (C.19) yields

$$\begin{bmatrix} \mathbb{C}_n & \mathbb{D}_n \\ \mathbb{A}_n & \mathbb{B}_n \end{bmatrix} = \begin{bmatrix} X_n & Y_n \\ X_{n+1} & Y_{n+1} \end{bmatrix}\begin{bmatrix} U & V \\ -S^{-1}X_2X_1^{-1} & S^{-1} \end{bmatrix}.$$

As a consequence

$$\mathbb{A}_n = X_{n+1}U - Y_{n+1}S^{-1}X_2X_1^{-1},$$
$$\mathbb{B}_n = X_{n+1}V + Y_{n+1}S^{-1}.$$

For large values of n, Y_n is nonsingular. Therefore, the last equality gives

$$Y_{n+1}^{-1}\mathbb{B}_n = Y_{n+1}^{-1}X_{n+1}V + S^{-1}.$$

Since S is nonsingular and $\frac{X_{n+1}}{Y_{n+1}} \to 0$, we have that $Y_{n+1}^{-1}\mathbb{B}_n$ and thus $\mathbb{B}_n$ are nonsingular for large n. Moreover,

$$\frac{\mathbb{A}_n}{\mathbb{B}_n} = \frac{\frac{X_{n+1}}{Y_{n+1}}U - S^{-1}X_1X_0^{-1}}{\frac{X_{n+1}}{Y_{n+1}}V + S^{-1}} \to -X_2X_1^{-1}.$$

This completes the proof. □

We should mention that theorem 2 is a generalization of the classic Pincherle's theorem [22], and the proof provided here essentially follows the one given in [26], see theorem 2.1. In fact the converse of theorem 2 also

holds. More precisely, if the MCF equation (C.16) converges, then there exists a solution of equation (C.14), say $\mathbf{Z}_n$ as in equation (C.18), such that both $\mathbf{Z}_0$ and X_0 are nonsingular, Y_n is nonsingular for large n, and $\lim_{n\to\infty} \frac{X_n}{Y_n} = 0$. Such a $\mathbf{Z}_n$ is called a *fundamental system of solutions* of equation (C.14). In our case, it is easily seen that the definition of minimality and fundamental system of solutions are equivalent. Therefore, one can state the following extension of theorem 2 (see also [26], theorem 2.1).

Theorem 3. *The MCF equation (C.16) converges if and only if the matrix three-term recurrence equation (29) has a minimal solution. Moreover, the minimal solution X_n satisfies*

$$X_{n+1}X_n^{-1} = \frac{I}{R_{n+1}} - \frac{I}{R_{n+2}} - \frac{I}{R_{n+3}} - \cdots, \quad n = 1, 2, \ldots. \tag{C.20}$$

We note that equation (C.20) follows from equation (32) together with the convergence of the MCF equation (C.16). The full version of this theorem is not needed for this part; however, in section 4, the converse of theorem 3 and the identity equation (C.20) play crucial roles in obtaining the Green's function for an arbitrary applied external potential field.

At this point, we have only been able to show that the convergence of the continued fraction equation (C.16) is equivalent to the existence of a minimal solution for equation (29). The next theorem is a combination of original results given by Perron [51], Máté and Nevai [52], and completes this picture. For the full version of this theorem see [26].

Theorem 4. *Consider the first order recurrence*

$$Z_n = \theta_n Z_{n-1}, \quad n = 2, 3, \ldots, \tag{C.21}$$

where $Z_n \in \mathbb{C}^{2k\times k}$, $\theta_n \in \mathbb{C}^{2k\times 2k}$, and all θ_n's are nonsingular. If $\lim_{n\to\infty}\theta_n = \theta$ and if all eigenvalues of θ are different in modulus, then equation (C.21) has a fundamental system of solutions.

We point out that the recurrence equation (C.21) with the property $\lim_{n\to\infty}\theta_n = \theta$ is said to be of *Poincaré-type* and the corresponding MCF is called *limit periodic*. In view of theorem 4, we can give our last theorem of this section, which concludes what we ought to show.

Theorem 5. *The MCF equation (C.16) converges. Moreover,*

$$X_2X_1^{-1} = \frac{I}{R_2} - \frac{I}{R_3} - \frac{I}{R_4} - \cdots,$$

where X_n denotes a minimal solution of equation (29).

Proof. First of all we have $\det\theta_n = 1$ for all $n \geqslant 2$, as mentioned in theorem 2. So all θ_n are nonsingular. Next, in view of theorem 1, we have

$$\theta_n = \begin{bmatrix} 0 & I \\ -I & R_n \end{bmatrix} \to \begin{bmatrix} 0 & I \\ -I & D_\mu \end{bmatrix} \quad \text{as} \quad n \to \infty.$$

Denoting the above limiting matrix by θ, the characteristic polynomial of θ is given by

$$\det(\theta - \lambda I) = \det\begin{bmatrix} -\lambda I & I \\ -I & D_\mu - \lambda I \end{bmatrix}.$$

Since I and $D_\mu - \lambda I$ commute, we can write

$$\begin{aligned}\det(\theta - \lambda I) &= \det((-\lambda I)(D_\mu - \lambda I) + I) \\ &= \det(\lambda^2 I - \lambda D_\mu + I).\end{aligned}$$

Using the fact that D_μ is a diagonal matrix, see equation (A.14), the above expression gives

$$\det(\theta - \lambda I) = \prod_{j=1}^{k} (\lambda^2 - 2\cosh\mu_j\,\lambda + 1).$$

Each factor of the above product has two distinct zeros e^{μ_j} and $e^{-\mu_j}$. Since μ_j's are all distinct, it follows that the $2k$ eigenvalues of θ, given by $\{e^{-\mu_1}, e^{\mu_1}, \ldots, e^{-\mu_k}, e^{\mu_k}\}$, are all different in modulus. In view of theorem 4, we conclude that the recurrence relation equation (C.21) has a fundamental system of solutions $\mathbf{Z}_n$; or equivalently, the matrix three-term recurrence equation (29) has a minimal solution X_n. Therefore, the proof follows from an application of theorem 2. □

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