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# Guided mode extraction in monolayer colloidal crystals based on the phase variation of reflection and transmission coefficients



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## ABSTRACT

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### 1. Introduction

Controlling the light propagation is possible by periodic modulation of refractive index in structures that their lattice constants are comparable to light wavelengths. Photonic crystals are structures capable of manipulating the flow of light by a property known as photonic band gaps.

Colloidal crystals are periodic arrays of monodisperse colloidal particles, and can be considered as a class of photonic crystals. They can be prepared in self-assembly approaches, in an easier manner and with lower costs compared to photonic crystal fabrication methods, including optical lithography and etching techniques [1,2].

Two-dimensional or three-dimensional periodic colloidal crystals attract great interest due to these challenges in the fabrication of nanoscale photonic crystals. They can find applications in many areas like bio and chemical sensing [3], solar cells [4], display, templates for fabrication of other materials, and miniature diagnostic systems [5]. Also, much progress has been achieved in fabrication of colloidal crystals with point, line and planar defect in recent years [6,7].

Two-dimensional colloidal crystals are monolayer arrays of monodisperse colloidal microspheres or nanospheres which are prepared mostly and commonly in hexagonal close-packed

\* Corresponding author. E-mail address: sah\_nekuee@ee.sharif.edu (S.A.H. Nekuee). patterns by different self-assembly methods such as drop coating, dip-coating, spin-coating, electrophoretic deposition and self-assembly at the gas-liquid interface [8]. Non-close-packed and binary colloidal crystals are other types of two-dimensional colloidal crystals. Monolayer inverse opals as well as two-dimensional periodic arrays of nanobowls, nanocaps and hollow spheres are samples of inverse replicas of monolayer colloidal crystals which have been fabricated recently [9].

An accurate and fast method for guided modes extraction in monolayer colloidal crystals and their in-

verse replicas is presented. These three-dimensional structures are composed of a monolayer of spherical

particles that can easily and simply be prepared by self-assembly method in close packed hexagonal

lattices. In this work, we describe how the guided modes, even or odd modes and light cone boundary

can be easily determined using phase variations of reflection and transmission coefficients. These

coefficients are quickly calculated by Fourier modal method. The band structures are obtained for a

monolayer of polystyrene particles and two-dimensional TiO<sub>2</sub> inverse opal by this proposed method.

The confinement of guided modes in monolayer colloidal crystals and their inverse replicas depend on the refractive index of the dielectric spheres and the substrate which they rest on it. High refractive index contrast in these structures lead to three-dimensional confinement of light similar to the photonic crystal slabs which is acquired by two-dimensional band gaps in the plane of periodicity and total internal reflection in the vertical direction [10,11]. Therefore, these colloidal structures can be used in couplers, wavelength filters and optical interconnects as well as optical sensors. Determining waveguide modes of these colloidal structures are very important in design and optimization of these optical devices.

Extracting the waveguide modes of multilayered structures can be done by solving an eigenvalue equation. Both guided and leaky modes in lossless or lossy structures can be found as solutions of the eigenvalue equation [12]. Reflection pole method is another approach that is used for the determination of mode propagation constants in lossless and lossy planar structures [13]. This approach uses the simple principle that modes are the poles of reflection or transmission coefficients of a multilayered system. The modes and light confinement in monolayer colloidal crystals is studied by full numerical methods, like finite-difference time-domain (FDTD) which are time-consuming [14].

Here we propose a method to determine guided modes of a monolayer of colloidal particles and its inverse replica by following the phase variations of reflection and transmission coefficients. These index-guided modes are poles of reflection and transmission coefficients [13] and based on the Bode diagram theory we demonstrate that these index-guided modes can be obtained efficiently and precisely from phase variations equal to  $\pi$  of (0,0)th reflected and transmitted order. The reflection and transmission coefficients of different diffracted orders are calculated by Fourier Modal Method (FMM). Also, we will show how to distinguish even and odd modes, and how the lower boundary of light cone is determined in the proposed method. The obtained modes form the band structures of these slabs.

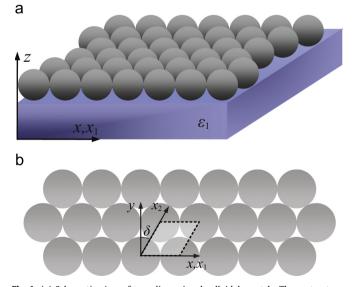
This paper is organized as follows. In Section 2 the brief review about FMM implementation is presented. Then, guided mode extraction from reflection and transmission coefficients is described with more details in Section 3. Band structures are obtained for two different structures in Section 4. Finally, the conclusions of this work are summarized in Section 5.

### 2. FMM implementation

An efficient and accurate calculation method of reflection and transmission coefficients and their subsequent phase is necessary for guided mode extraction in this approach.

In most of two-dimensional colloidal crystals, there is a hexagonal close packed of dielectric spheres between two homogeneous regions. These structures could be analyzed by various numerical methods like rigorous couple wave analysis (RCWA) [15]. Fourier modal method (FMM) is the popular modal method for the analysis of crossed gratings, with simple implementation [16]. Its convergence rate is improved relative to RCWA by applying appropriate factorization rules. In this section only required formulation and necessary details for easy implementation of FMM in 2D colloidal crystals are introduced.

A monolayer of colloidal crystals is two-dimensionally periodic



**Fig. 1.** (a) Schematic view of two-dimensional colloidal crystals. These structures are composed of a monolayer of hexagonal close packed spherical particles. The dielectric constant of the bottom layer is  $\epsilon_1$ . (b) Hexagonal lattice of cylindrical rods that is formed by stair case approximation in  $x_3$  direction. The  $x_1$  and  $x_2$  axes are illustrated in the parallelogramic unit cell.

as shown in Fig. 1. As mentioned above gratings that are uniform in vertical direction could be analyzed by FMM. Consequently, using staircase approximation a monolayer of colloidal crystals is divided into 2l+1 sublayers in the *z* direction. These sublayers of the 2D colloidal crystal are hexagonal lattices of cylindrical rods with various radiuses so that the radius of the middle sublayer is equal to the radius of spherical particles, i.e. *R*.

Due to the symmetry of a sphere in z direction, it is sufficient that only in l+1 regions of 2l+1 sublayer, the main eigenvalue equation of FMM, i.e.

$$[FG - (k_0 k_z \cos \delta)^2] \begin{pmatrix} E_1 \\ E_2 \end{pmatrix} = 0.$$
<sup>(1)</sup>

is solved where *F* and *G* are two square matrices [16]. This eigenvalue problem is acquired in a general nonrectangular coordinate system ( $x_1$ ,  $x_2$ ,  $x_3$ ) which the  $x_1$  and  $x_3$  axes are parallel to the *x* and *z* axes and the angle  $\delta$  is between the  $x_2$  axis and *y* axis. Blocks of these significant matrices are made by applying Fourier factorization rules, i.e. Laurent's and inverse rules to the Fourier series coefficients of permittivity distribution  $\epsilon(x_1, x_2)$  in each sublayer. Note that the calculations of Fourier series coefficients and the angle  $\delta$  depend on the type of selected unit cell. In this equation  $k_0$  is  $2\pi/\lambda$  where  $\lambda$  is the vacuum wavelength and the mediums are assumed to be nonmagnetic ( $\mu = 1$ ). Also,  $k_z$ 's are propagation constants of different orders in the *z* direction and selected such that

$$\operatorname{Re}\left[k_{z}\right] + \operatorname{Im}\left[k_{z}\right] \ge 0 \tag{2}$$

Electric eigenvectors in  $x_1$  and  $x_2$  directions are denoted by  $E_1$  and  $E_2$ , respectively. Magnetic eigenvectors are obtained by

$$\begin{pmatrix} H_1 \\ H_2 \end{pmatrix} = \frac{\sec \delta}{k_0 k_z} G \begin{pmatrix} E_1 \\ E_2 \end{pmatrix}$$
(3)

The obtained eigenvectors and eigenvalues in each sublayer of 2D colloidal crystal form the matrices  $W_1$ ,  $W_2$  and  $\phi$  which are used in the S-matrix algorithm [17]. These matrices can be written as

$$W_{1} = \begin{pmatrix} E_{1mn} \\ E_{2mn} \end{pmatrix}, \quad W_{2} = \begin{pmatrix} H_{1mn} \\ H_{2mn} \end{pmatrix},$$
$$\phi = [\exp(ik_{2mn}h)]$$
(4)

where h = 2R/(2l + 1) demonstrate the thickness of each sublayer. Note that *S*-matrix algorithm is used to match boundary conditions at the interfaces between 2l+1 sublayers and top and bottom homogeneous regions [17].

The electric and magnetic eigenvectors in homogeneous regions, i.e. bottom and top mediums of spherical particles are calculated just by Rayleigh expansion without the need to solve eigenvalue problem. The main matrices for *S*-matrix algorithm in the *p*th region are [18]

$$W_1 = I, \quad W_2 = \begin{pmatrix} F^p & -A^p \\ B^p & -F^p \end{pmatrix}$$
(5)

where  $A^p$ ,  $B^p$  and  $F^p$  have diagonal elements as

$$\begin{aligned} A_{mn}^{p} &= \sec \delta \left[ \frac{k_{0}^{2} \epsilon_{p} - k_{x_{1m}}^{2}}{k_{0} k_{x_{3mn}}^{p}} \right], \\ B_{mn}^{p} &= \sec \delta \left[ \frac{k_{0}^{2} \epsilon_{p} - k_{x_{2n}}^{2}}{k_{0} k_{x_{3mn}}^{p}} \right], \\ F_{mn}^{p} &= \sec \delta \left[ \frac{k_{0}^{2} \epsilon_{p} \sin(\delta) - k_{x_{1m}} k_{x_{2n}}}{k_{0} k_{x_{3mn}}^{p}} \right] \end{aligned}$$
(6)

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