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Optical absorption for parallel cylinder arrays

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We study the long-wavelength electromagnetic resonances of interacting cylinder arrays. By using a normal-modes expansion where the effects of geometry and material are separated, it is shown that two parallel cylinders with different radii have electromagnetic modes distributed symmetrically about depolarization factor $\frac{1}{2}$. Both sets couple to longitudinal and transverse components of the external field, but amplitudes of symmetric depolarization factors become exchanged when considering longitudinal or transverse polarization. We also find that amplitudes satisfy sum rules that depend on the ratio of the cylinders radii. The main effect of the difference in radii is a spectral shift towards the isolated cylinder resonance as this difference increases.

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I. INTRODUCTION

The optical properties of ordered cylinder arrays has become a subject of much recent interest mainly because of their potential use as photonic crystals [1–3] and their occurence in carbon nanotube bundles [4]. Theoretical research once done for spherical particles [5–8] has lately been applied to cylinders [9–12]. It is well known that in the long-wavelength limit, the optical properties of a dilute composite of microscopic spherical particles are well described by mean-field theories such as Claussius-Mosotti or Maxwell-Garnett. These theories are essentially based on a dipolar approximation assuming that the particles are sufficiently far apart so that it is possible to neglect contributions from higher-order multipoles. As particles become closer, however, this approach is no longer valid. Several models have been presented to overcome this difficulty, among which the theory of normal modes has been shown to be particularly convenient since it makes possible an expansion of the system response in terms of resonance terms, where dielectric properties appear separate from geometrical factors [13,14]. The simplest system exhibiting the effects of interactions is a pair of identical particles very close to each other. A pair of particles of the same material and form but different size is the simplest nonsymmetric system of interacting particles [8].

Recently, a model to study arbitrary cylinder arrays made of the same material has been constructed and applied in detail to a pair of identical cylinders [11]. The response of periodic arrays of identical parallel cylinders including proximity effects is also easily treated within that formalism. The method follows a normal-modes description appropriate to the long-wavelength limit first proposed by Bergmann [13,14], and makes use of a basis of cylindrical harmonics solutions to Laplace's equation. Modes are characterized by depolarization factors and strengths, defined in such a way that an isolated cylinder exhibits a depolarization factor $\frac{1}{2}$ and unit strength. We here follow a similar procedure to study a pair of non-touching parallel cylinders of the same material but different radii, for different polarizations of the external field. We show that a difference in radii does not alter the property that depolarization factors are symmetric about $\frac{1}{2}$, although while in the equal radii case only modes with all depolarization factors either smaller or larger than $\frac{1}{2}$ are excited for a given polarization, mixing now occurs. We find that all normal modes are active for an external field perpendicular to the cylinders axis, whether parallel or perpendicular to the plane containing the axis. Furthermore, strengths of modes with depolarization factors smaller than $\frac{1}{2}$ are exchanged with those of depolarization modes bigger than $\frac{1}{2}$, when the direction of the electric field changes from parallel to perpendicular.

In Sec. II, we get the multipolar moments and the absorption cross section for a pair of unequal cylinders. In Sec. III, we present and discuss our numerical results. Finally, in Sec. IV, we summarize our conclusions.

II. THEORY

We consider a set of N parallel, infinite, uncharged cylinders of dielectric function ε_1 placed in a homogeneous medium of dielectric function ε_2, excited by an external electric field whose wavelength is much longer than the cylinder radii or separation between cylinders. The charge distribution they acquire may be described in terms of individual multipole moments q_{mj} obeying the equations, [6]

$$q_{mj} = -\alpha_{mj}\left(V_m + \sum_{m'j'} A_{mj}^{m'j'} q_{m'j'} \right). \qquad (1)$$

Here, m is a positive or negative integer labeling the angular momentum component along the cylinder axes, $j = 1,2,\ldots,N$ is a particle index, $\alpha_{mj} = |m| a_j^{2|m|}(\varepsilon_1 - \varepsilon_2)/(\varepsilon_1 + \varepsilon_2)$ are the multipolar polarizabilities of cylinder

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j of radius a_j, and V_m are the coefficients in the expansion of the external potential in terms of cylindrical harmonics. The coupling coefficients are given by [11]

$$A_{mj}^{m'j'} = \begin{cases} 0 & \text{if } mm'>0, \\ \dfrac{(-1)^{m'}(|m|+|m'|-1)!}{|m|!|m'|!}\dfrac{e^{i(m'-m)\theta_{jj'}}}{\rho_{jj'}^{|m|+|m'|}} & \text{if } mm'<0, \end{cases} \tag{2}$$

where $(\rho_{jj'},\theta_{jj'})=\vec{\rho}_{j'}-\vec{\rho}_j$ are polar coordinates in the x-y plane giving the relative position of cylinder j' with respect to cylinder j.

As discussed in Ref. [11], if the cylinders are of the same material, one can separate in Eq. (1) terms depending on the material susceptibility χ from those involving the geometry of the array. We intend here to follow the same procedure and write Eq. (1) as

$$\sum_{\mu'} (\chi^{-1}\delta_{\mu\mu'}+H_{\mu}^{\mu'})x_{\mu'}=f_{\mu}, \tag{3}$$

where μ represents the pair of indices (m,j), and

$$H_{mj}^{m'j'}=2\pi(\delta_{mm'}\delta_{jj'}+|mm'|^{1/2}a_j^{|m|}a_{j'}^{|m'|}A_{mj}^{m'j'}), \tag{4}$$

$$f_{mj}=-2\pi|m|^{1/2}a_j^{|m|}V_{mj}, \tag{5}$$

$$x_{mj}=\frac{q_{mj}}{|m|^{1/2}a_j^{|m|}}. \tag{6}$$

Note the important feature that matrix H depends on geometry only and its eigenvalues $\{4\pi n_\mu\}$ define the depolarization factors $\{n_\mu\}$ of the array. For later convenience, we write $\mathbf{H}=2\pi(\mathbf{I}+\mathbf{B})$, with $\mathbf{I}$ the unit matrix and $B_{mj}^{m'j'}=|mm'|^{1/2}a_j^{|m|}a_{j'}^{|m'|}A_{mj}^{m'j'}$, so that the depolarization factors $\{n_\mu\}$ and eigenvalues $\{\lambda_\mu\}$ of $\mathbf{B}$ satisfy the relation,

$$n_\mu=\tfrac{1}{2}(1+\lambda_\mu). \tag{7}$$

Because of the property $B_{mj}^{m'j'}=0$ if $mm'>0$ [see Eq. (2)], we write rows and columns of matrix $\mathbf{B}$ with indexes m and m' following the sequence $1,2,\ldots,-1,-2,\ldots$, resulting in matrix $\mathbf{B}$ written in terms of a real matrix $\mathbf{b}$ of half its dimension, as

$$\mathbf{B}=\begin{bmatrix} 0 & b \\ b & 0 \end{bmatrix}. \tag{8}$$

From now on, we use index m and m' as positive integers, and write the elements of matrix $\mathbf{b}$ as follows:

$$b_{mj}^{m'j'}=(-1)^{m'}\sqrt{mm'}\frac{(m+m'-1)!}{m!m'!}\frac{a_j^m a_{j'}^{m'}e^{i(m+m')\theta_{jj'}}}{\rho_{jj'}^{m+m'}}. \tag{9}$$

It can be shown that the eigenvalues of matrix $\mathbf{B}$ come in pairs with opposite sign $\lambda_\mu=\pm\ell_\mu$, where ℓ_μ are the eigenvalues of $\mathbf{b}$ (see the Appendix). As follows from Eq. (7), the depolarization factors are then symmetric about the value 1/2. The components of vector x_μ can de written in terms of the eigenvalues of matrix $\mathbf{b}$ and elements of matrix $\mathbf{u}$ that diagonalizes $\mathbf{b}$,

$$\mathbf{u}^{-1}\mathbf{b}\mathbf{u}=\ell. \tag{10}$$

In the case of a uniform electric-field E_0 parallel to the plane containing the cylinder axes and perpendicular to the latter-(parallel field geometry), $x_{mj}=\{x_{-mj}\}$. Vector $\mathbf{x}_+=x_{mj}$ is then given by

$$\mathbf{x}_+=(\mathbf{u}\mathbf{s}^{-1}\mathbf{u}^{-1})\mathbf{f}^+, \tag{11}$$

where

$$s_{mj}^{m'j'}=\delta_{mm'}\delta_{jj'}[\chi^{-1}+2\pi(1+\ell_{mj})], \tag{12}$$

$$f_{mj}^{+}=\delta_{m1}\pi a_j E_0. \tag{13}$$

In the case of an electric field perpendicular to the plane containing the cylinder axes (perpendicular field geometry), $x_{mj}=-x_{-mj}$. Vector $\mathbf{x}_-=\{x_{-mj}\}$ is then given by

$$\mathbf{x}_-=(\mathbf{u}\mathbf{r}^{-1}\mathbf{u}^{-1})\mathbf{f}^-, \tag{14}$$

where now

$$r_{mj}^{m'j'}=\delta_{mm'}\delta_{jj'}[\chi^{-1}+2\pi(1-\ell_{mj})], \tag{15}$$

$$f_{-mj}^{-}=\delta_{m1}i\pi a_j E_0. \tag{16}$$

For a pair of unequal parallel cylinders with radii a_1 and a_2, and axis at a distance R, we define dimensionless parameters $\beta=a_2/a_1$ and $\delta=R/a_1$. Because of the properties $b_{mj}^{m'j}=0$ and $b_{m2}^{m'1}=(-\beta)^{m-m'}b_{m1}^{m'2}$, we write rows (columns) of matrix $\mathbf{b}$ with particle index j (j') in the sequence 1,2 resulting in matrix $\mathbf{b}$ written in terms of a smaller array $\mathbf{g}$ as follows:

$$\mathbf{b}=\begin{bmatrix} 0 & \mathbf{g} \\ \bar{\mathbf{g}} & 0 \end{bmatrix}, \tag{17}$$

where $\bar{\mathbf{g}}$ is the transpose of $\mathbf{g}$, and the elements of matrix $\mathbf{g}$ are given by

$$g_m^{m'}=(-1)^{m'}\sqrt{mm'}\frac{(m+m'-1)!}{m!m'!}\frac{\beta^{m'}}{\delta^{m+m'}}. \tag{18}$$

Results for a pair of cylinders with an external field in the parallel or perpendicular configuration can be written in terms of a single normal-modes expansion as

$$x_{\pm mj}=\sum_{m'j'}\frac{C_{mj}^{m'j'}f_{\pm}}{\chi^{-1}+4\pi n_{\pm m'j'}}. \tag{19}$$

In this expression, the upper (lower) sign corresponds to the parallel (perpendicular) configuration, with (m',j') labeling the excitation modes of the pair as a coupled system. It gives just half of the multipoles; the others are obtained from the corresponding symmetry property as given in the paragraph preceding Eqs. (11) and (14). We have defined the depolarization factors of modes,

$$n_{\pm m'j'} = \tfrac{1}{2}(1 \pm \ell_{m'j'}), \qquad (20)$$

and coefficients corresponding to strength of modes,

$$C_{mj}^{m'j'} = u_{mj}^{m'j'}(u_{1,1}^{m'j'} + \beta u_{1,2}^{m'j'}). \qquad (21)$$

We have also defined

$$f_+ = f_{1,1}^{+}, \qquad (22)$$

$$f_- = f_{-1,1}^{-}. \qquad (23)$$

We find that coefficients $C_{mj}^{m'j'}$ satisfy the sum rules

$$\sum_{m'j'} C_{m1}^{m'j'} = \delta_{m1}, \qquad (24)$$

$$\sum_{m'j'} C_{m2}^{m'j'} = \beta\delta_{m1}. \qquad (25)$$

It can be shown that, as with the original matrix **B**, eigenvalues $\{\ell_{mj}\}$ of matrix **b** come also in pairs with an opposite sign; therefore, the sets of depolarization factors $\{n_{+mj}\}$ and $\{n_{-mj}\}$ are identical (see the Appendix). A given depolarization factor exhibits a different strength depending on the direction of the external field. As seen in the normal-modes expansion given by Eq. (19) the same strength coefficients $C_{mj}^{m'j'}$ appear for depolarization factor $n_{m'j'}$ in the parallel field response and for $n_{-m'j'}$ in the perpendicular field response. Then, strenghts corresponding to depolarization factors symmetric around value 1/2 are exchanged between responses corresponding to fields parallel or perpendicular.

The magnitude of the electric dipole moment for the pair can be written as

$$p_{\pm} = \pi a_1^2 \sum_{m'j'} \frac{C_{11}^{m'j'} + \beta C_{12}^{m'j'}}{\chi^{-1} + 4\pi n_{\pm m'j'}} E_0, \qquad (26)$$

where $p_+(p_-)$ corresponds to a parallel (perpendicular) field. The absorption cross section is proportional to the imaginary part of the factor accompanying E_0 in the previous expression, a quantity we identify as the complex effective polarizability of the pair. Thus, we arrive at a normal-modes decomposition for the absorption cross section of two parallel cylinders,

$$\sigma_{\pm} \sim \mathrm{Im}\left\{ \sum_{m'j'} \frac{C_{11}^{m'j'} + \beta C_{12}^{m'j'}}{\chi^{-1} + 4\pi n_{\pm m'j'}} \right\} \qquad (27)$$

where $\sigma_+(\sigma_-)$ corresponds to a parallel (perpendicular) field. Notice that, as follows from Eq. (21), the numerator in the previous sum can be written as

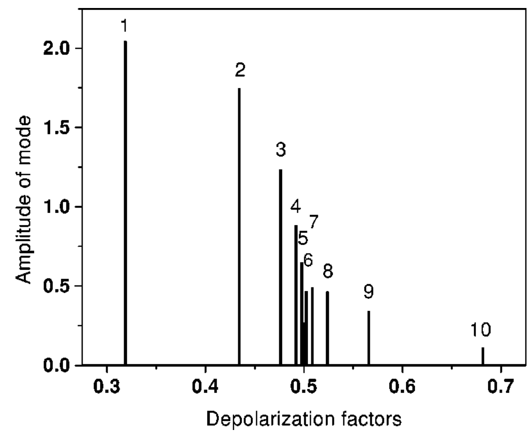

FIG. 1. Mode amplitudes for a pair of unequal cylinders under a uniform electric field in the parallel field configuration. The radii ratio equals $\beta = 3$, and the separation parameter is $\sigma = 1.1$.

$$(u_{1,1}^{m'j'} + \beta u_{1,2}^{m'j'})^2, \qquad (28)$$

and is always positive definite. According to the sum rules given by Eqs. (24) and (25), the sum of the numerators in expansions (26) and (27) is $1+\beta^2$, a feature we use in calculating the normalized strength of modes in the following section.

III. NUMERICAL RESULTS

We have solved numerically the eigenvalue equation for matrix **b** for the case of a pair of parallel cylinders of different radii a_1 and a_2, and have calculated the depolarization factors $n_{m'j'}$ and strength coefficients $C_{mj}^{m'j'}$ using Eqs. (20) and (21). We have studied in detail the normal-modes expansion for the dipole moment of the pair as given by Eq. (26). Our most important finding is that when the radii are not equal, modes with depolarization factors above and below the value $\frac{1}{2}$ mix for all orientations of the external field. This is known not to happen when cylinders are equal [11].

In obtaining numerical results, we use the dimensionless parameters $\sigma = R/(a_1+a_2)$ that measures the center-to-center distance, $\beta = a_2/a_1$ which characterizes how disimilar the radii are, and $\mu = (R - a_1 - a_2)/a_1$ measuring the border to border distance. In Fig. 1, we plot modes for very close cylinders ($\sigma = 1.10$) with one radius three times the other ($\beta = 3$). Modes are for the parallel configuration, while those for the perpendicular case are obtained by mirror reflection about depolarization factor $\frac{1}{2}$. Note that modes are placed symmetrically about this central value so that, as far as position is concerned, they are indistinguishable in both configurations. The figure shows the modes with largest amplitude, while weaker modes cluster around $n = \frac{1}{2}$ adding up to a significant strength around this value. The total sum of amplitudes is 10, as required by the sum rule mentioned after Eq. (28). Labels, included in order to match with labeling in Fig. 2, are arbitrary.

Figure 2 shows depolarization factors (a) and normalized strengths (b) in terms of the parameter β, at fixed $\sigma = 1.1$. The sum over all strengths is unity, having been normalized

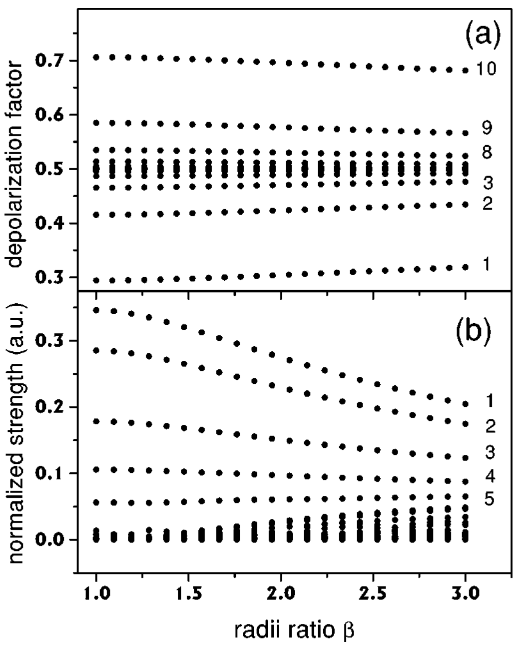

FIG. 2. Depolarization factors (a) and normalized strengths (b) as a function of size parameter β, for a pair of unequal cylinders with fixed separation parameter $\sigma=1.1$ under a uniform electric field. Labels correspond to those in Fig. 1.

by the factor $1+\beta^2$. Thus, the results at $\beta=3$ correspond to amplitudes shown in Fig. 1 with the normalization factor 10. In changing β, we keep constant the parameter σ by changing the center-to-center distance R accordingly. Note that modes with essentially zero strength at $\beta=1$ become important when increasing this ratio. Labels are arbitrary and are used just to relate the data in different figures.

Results shown in Fig. 3 were obtained by changing β and the center-to-center separation R, but keeping constant the border-to-border distance at the fixed value $\mu=0.4$. It is known that for spheres, this distance is the relevant parameter in determining the position of the modes. We note that the depolarization factors move appart with increasing β, while at constant σ [Fig. 2(a)] they get closer. This is because the relation between the edge-to-edge and center-to-center parameters is $\mu=(\sigma-1)(1+\beta)$, indicating that as β goes to infinity, so does μ if σ is kept constant. Thus, all modes should converge to the isolated cylinder value $n=1/2$ in this case, while if μ is kept constant, the modes converge to those of a cylinder in front of a plane at the same distance.

Figure 4 shows the absorption coefficient for a pair of silver cylinders in the parallel configuration, for the cases $\beta=3$ and $\beta=9$, keeping the border to border distance μ fixed at the value 0.4. Up to 45 moments (M=45) were necessary in order to achieve convergence. The dielectric function used had the Drude form

$$\varepsilon(\omega)=\varepsilon_b-\frac{\omega_p^2}{\omega(\omega+i\gamma)},$$

with $\varepsilon_b=3.6$, $\omega_p=75\,256\ \text{cm}^{-1}$ and $\gamma=486\ \text{cm}^{-1}$ [15].

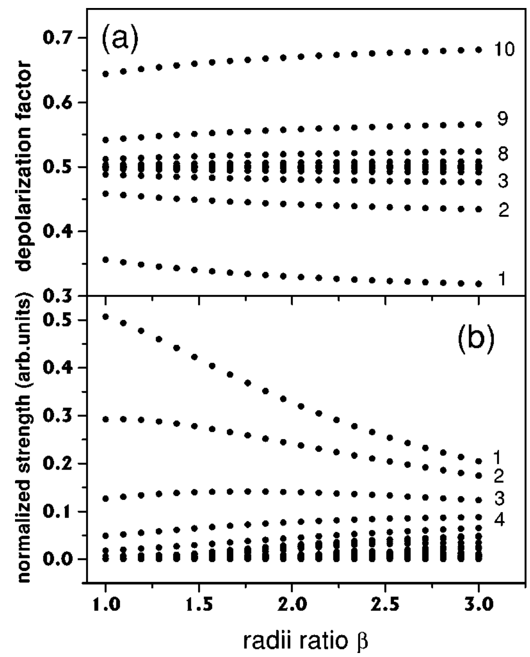

FIG. 3. Same as Fig. 2, but with fixed border to border parameter $\mu=0.4$.

From this expression, and Eq. (27), it follows that resonances occur at frequencies given approximately by

$$\Omega_\mu=\frac{\omega_p}{\sqrt{\frac{1}{n_\mu}+(\varepsilon_b-1)}}.$$

Using the above equation and Fig. 3, one can verify the approximate position of the various peaks in Fig. 4. In the figure, the equal radii case ($\beta=1$) has been included for comparison. It is apparent from the figure that as the radii become more disimilar, the spectral weight is shifted to

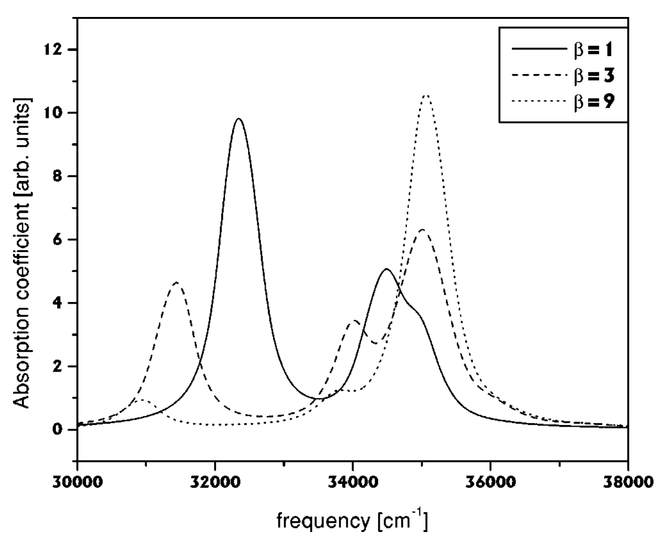

FIG. 4. Absorption coefficient for a pair of silver cylinders with radii ratios $\beta=1$, 3, and 9.

higher frequencies, clustering around the isolated cylinder resonance at $\Omega_\mu = \omega_p/\sqrt{1+\varepsilon_b}$, a result already suggested by Fig. 3(b).

IV. CONCLUSIONS

In summary, we have shown that the absorption cross section of a pair of parallel cylinders of the same material but different radii contains modes whose depolarization factors are symmetrically distributed around $\frac{1}{2}$, with amplitudes depending on the direction of the external field. When the field changes from the parallel to the perpendicular configuration, amplitudes corresponding to symmetric depolarization factors about the central value 1/2 are exchanged. The main effect of the difference in radii is a shift of the spectral weight towards this central value, which characterizes the resonance of an isolated cylinder.

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APPENDIX

We consider the eigenvalue equation for operator **T**,

$$\mathbf{T}\mathbf{x} = \lambda \mathbf{x}, \tag{A1}$$

in a basis of dimension $2M$. Here, **T** has the form

$$\mathbf{T} = \begin{bmatrix} 0 & A \\ B & 0 \end{bmatrix}, \tag{A2}$$

where **A**, **B** each has dimension M. In writing the eigenvectors **x** in terms of two smaller vectors w and v of dimension M the eigenvalue equation is cast into the form,

$$\begin{bmatrix} 0 & \mathbf{A} \\ \mathbf{B} & 0 \end{bmatrix} \begin{bmatrix} w \\ v \end{bmatrix} = \lambda \begin{bmatrix} w \\ v \end{bmatrix} \tag{A3}$$

or

$$\mathbf{A}v = \lambda w, \tag{A4}$$

$$\mathbf{B}w = \lambda v. \tag{A5}$$

From there we get the separate eigenvalue problems,

$$(\mathbf{AB})w = \lambda^2 w, \tag{A6}$$

$$(\mathbf{BA})v = \lambda^2 v, \tag{A7}$$

both having the same eigenvalues λ^2. In solving for the corresponding eigenvectors and writing them as columns, we get matrices **w** and **v** that diagonalize matrices **AB** and **BA**. They can be used to form a matrix **U** as,

$$\mathbf{U} = \frac{1}{\sqrt{2}} \begin{bmatrix} \mathbf{w} & \mathbf{w} \\ \mathbf{v} & -\mathbf{v} \end{bmatrix}, \tag{A8}$$

which diagonalizes matrix **T** according to the relation

$$\mathbf{U}^{-1}\mathbf{T}\mathbf{U} = \mathbf{\Lambda}, \tag{A9}$$

with matrix $\mathbf{\Lambda}$ given by

$$\mathbf{\Lambda} = \begin{bmatrix} \boldsymbol{\lambda} & 0 \\ 0 & -\boldsymbol{\lambda} \end{bmatrix}. \tag{A10}$$

Here, $\boldsymbol{\lambda}(-\boldsymbol{\lambda})$ is a diagonal matrix formed by the positive (negative) square root of the eigenvalues of matrices **AB** or **BA**. Therefore, the eigenvalues of matrix **T** come in pairs with opposite sign. In the case of a pair of cylinders, we find the previous feature two times. It first happens because coupling coefficients $A_{mj}^{m'j'}$ are zero if m and m' have the same sign, and then occurs also because they are zero for $j = j'$. The dimensionality $(4M)\times(4M)$ of the original eigenvalue problem is seen to be reduced to $M\times M$ dimensions.

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