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Exact S-matrix for N-disc systems and various boundary conditions: I. Generalization of the Korringa–Kohn–Rostoker–Berry method

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Abstract. Scattering of waves and particles from N discs fixed in a plane is studied. Various boundary conditions on the scatterers, corresponding to mesoscopic quantum physics, acoustics or electromagnetism, are considered. An exact formalism allowing us to calculate the S-matrix, its scattering resonances and far-field form functions is developed for systems with discrete $\mathcal{C}_{2v}$, $\mathcal{C}_{3v}$ and $\mathcal{C}_{4v}$ symmetries. It extends the Korringa–Kohn–Rostoker method developed in the context of solid state physics and generalizes the works of Berry and of Gaspard and Rice in quantum chaos.

1. Introduction

Recently, scattering of a point particle from N hard discs fixed in a plane has been extensively studied in the context of 'quantum chaos'. For reviews on the subject, see [1–4] and for some recent papers, see [5–10]. In these works, the exact calculations are performed from the S-matrix formalism developed by Gaspard and Rice [11]. These two authors have presented the exact quantum mechanics of the scattering of a point particle from a three-disc scatterer by emphasizing the role of the symmetries of the system. Their method is inspired by the work of Berry on the quantization of a bounded classically chaotic system [12]. Berry's quantum formalism was based on the Korringa–Kohn–Rostoker (KKR) method developed in the context of solid state physics [13–15]. In the perspective of the study of chaotic scattering in more realistic problems such as scattering of waves in acoustics or electromagnetism and of particles in mesoscopic quantum physics, it is useful to generalize the Gaspard and Rice approach. In such situations, it will be possible and interesting to experimentally confirm the theoretical results and the new physical effects expected.

In this paper, we are concerned with scattering by N discs presenting various boundary conditions. In section 2, the S-matrix is defined and obtained from two sets of coefficients defining the partial waves and their gradients on the boundaries of the N discs. Then we construct the associated far-field form functions. In section 3, we consider some particular boundary conditions:

—Dirichlet boundary condition in quantum mechanics, in acoustics and in electromagnetism (particle scattering by hard discs [1–11], ultrasonic wave scattering by soft discs and microwave scattering by metallic conductors [16]),

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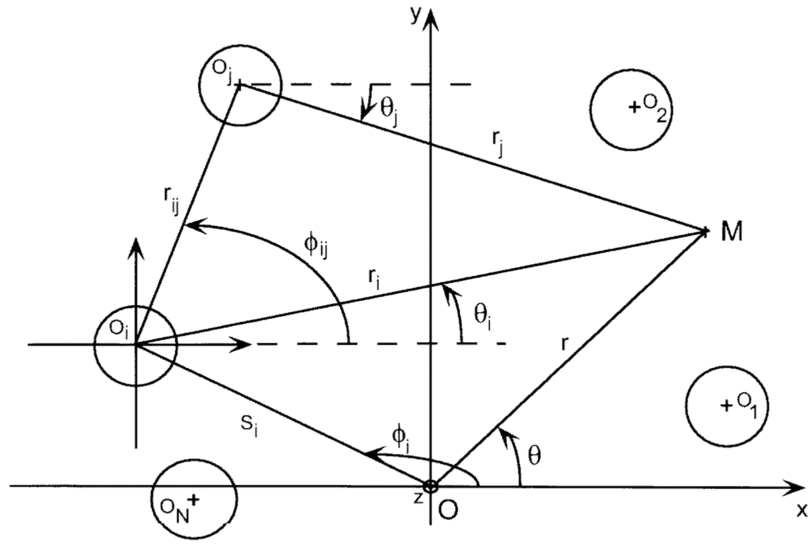

Figure 1. N-discs system geometry: various coordinates for an arbitrary point M.

—Neumann boundary condition in acoustics (ultrasonic wave scattering by hard discs),

—impedance boundary conditions in electromagnetism (transverse magnetic (TM) and transverse electric (TE) scattering by conductors with a given constant impedance),

—mixed boundary conditions in quantum mechanics (particle scattering by a square well and by a square barrier in the 'overdense' and 'underdense' cases),

—elastic boundary conditions in acoustics (ultrasonic wave scattering by elastic cylinders immersed in water).

In section 4, we examine special configurations presenting discrete $\mathcal{C}_{2v}$, $\mathcal{C}_{3v}$ and $\mathcal{C}_{4v}$ symmetries. The Korringa–Kohn–Rostoker–Berry (KKRB) method permits us to easily integrate symmetry considerations and to expand the S-matrix on the irreducible representations of symmetry groups [11–17]. In a short appendix, the properties of the S-matrix (unitarity and reciprocity) are linked to the properties of the coefficients defining the partial waves and their gradients on the boundaries of the discs.

2. S-matrix: general theory

2.1. Geometry of the N-discs system. Definition of the S-matrix

We consider a set of N identical and parallel cylinders of radius a. Cylinders are parallel to the Oz axis so that the system can be seen as a set of N non-overlapping discs in the plane Oxy. The geometry of the system as well as the notations used are shown in figure 1. In particular, we denote O_i the centre of scatterer i, (r_i, θ_i) the system of polar coordinates centred on O_i and (r, θ) the system centred on O. Furthermore, s_i is the distance OO_i, r_{ij} the distance O_iO_j, ϕ_i the angle between Ox and OO_i, and ϕ_{ij} the angle between Ox and O_iO_j.

We consider the partial wave solution ϕ_m of the following problem:

(i) ϕ_m satisfies the Helmholtz equation (or time-independent Schrödinger equation)

$$(\Delta + k^2)\phi_m = 0 \tag{1}$$

where Δ is the two-dimensional Laplacian,

(ii) ϕ_m and its gradient $\nabla\phi_m$ are given on the boundaries of the N discs by

$$\phi_m(\boldsymbol{x}) = \sum_{p=-\infty}^{+\infty} A_{mp}^{(i)} \mathrm{e}^{\mathrm{i}p\theta_i(\boldsymbol{x})} \tag{2}$$

$$\boldsymbol{n}_i \cdot \nabla\phi_m(\boldsymbol{x}) = \sum_{p=-\infty}^{+\infty} B_{mp}^{(i)} \mathrm{e}^{\mathrm{i}p\theta_i(\boldsymbol{x})} \tag{3}$$

where $A_{mp}^{(i)}$ and $B_{mp}^{(i)}$ are two sets of unknown matrices, $\boldsymbol{x}$ is an arbitrary point on the boundary of disc i, $\boldsymbol{n}_i$ is a unit normal vector directed into disc i at the point $\boldsymbol{x}$ and $\theta_i(\boldsymbol{x})$ the angular coordinate of the point $\boldsymbol{x}$,

(iii) at large distance, ϕ_m has the asymptotic behaviour

$$\phi_m(r,\theta) \underset{r\to\infty}{\sim} \frac{1}{\sqrt{2\pi kr}} \sum_{p=-\infty}^{+\infty} [\mathrm{e}^{-\mathrm{i}(kr-p\pi/2-\pi/4)}\delta_{mp} + \mathrm{e}^{\mathrm{i}(kr-p\pi/2-\pi/4)} S_{mp}]\mathrm{e}^{\mathrm{i}p\theta}. \tag{4}$$

The last equation defines the elements S_{mp} of the S-matrix [18].

The far-field form function is expressible directly in terms of the S-matrix and is given by [11]

$$f_\infty(\theta,\alpha) = \frac{1}{\sqrt{\pi ka}} \sum_{m=-\infty}^{+\infty} \sum_{p=-\infty}^{+\infty} \mathrm{e}^{-\mathrm{i}m(\alpha-\frac{\pi}{2})}(S_{mp}-\delta_{mp})\mathrm{e}^{\mathrm{i}p(\theta-\frac{\pi}{2})} \tag{5}$$

where α and θ respectively denote the angles of incidence and observation. We shall be equally interested in the total scattering cross section averaged over all the angles α and θ and given by

$$\overline{\sigma}_{tot} = \frac{4}{\pi ka} \sum_{m=-\infty}^{+\infty} \sum_{p=-\infty}^{+\infty} |S_{mp}-\delta_{mp}|^2. \tag{6}$$

2.2. Calculation of the S-matrix. Extension of the KKRB method

2.2.1. The KKRB method. Let us consider an arbitrary closed domain D of the plane and its boundary ∂D. Green's theorem (see for example [19])

$$\int_D \mathrm{d}V\,(f\Delta g - g\Delta f) = \int_{\partial D} \mathrm{d}\boldsymbol{S}\cdot(f\nabla g - g\nabla f) \tag{7}$$

taking for g the partial wave ϕ_m and f the free space Green's function

$$G_k(\boldsymbol{x},\boldsymbol{x}') = \frac{\mathrm{i}}{4}H_0^{(1)}(k|\boldsymbol{x}-\boldsymbol{x}'|) \tag{8}$$

which satisfies $(\Delta_{\boldsymbol{x}}+k^2)G_k(\boldsymbol{x},\boldsymbol{x}') = -\delta(\boldsymbol{x}-\boldsymbol{x}')$, permits us to express $\phi_m(\boldsymbol{x})$ in terms of the values of ϕ_m and G_k on the boundary ∂D. We obtain

$$\phi_m(\boldsymbol{x}) = \int_{\partial D} \mathrm{d}\boldsymbol{S}_{\boldsymbol{x}'}\cdot[G_k(\boldsymbol{x},\boldsymbol{x}')\nabla_{\boldsymbol{x}'}\phi_m(\boldsymbol{x}') - \phi_m(\boldsymbol{x}')\nabla_{\boldsymbol{x}'}G_k(\boldsymbol{x},\boldsymbol{x}')] \tag{9}$$

where $\mathrm{d}\boldsymbol{S}_{\boldsymbol{x}'}$ denotes the surface element pointing away from the interior of the domain D. In the following, we shall use the particular contour ∂D shown in figure 2 and defined by

$$\partial D = \partial D_\infty \cup \left(\bigcup_{i=1}^{N} \partial D_i\right) \tag{10}$$

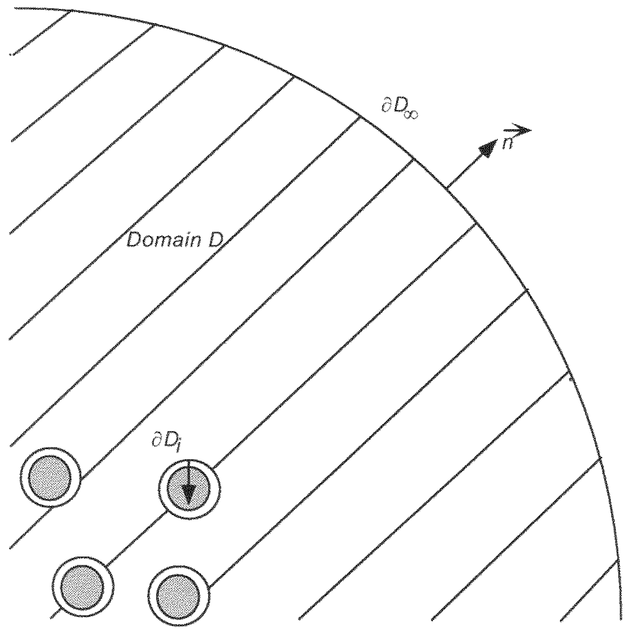

Figure 2. Domain D and its boundary ∂D.

where ∂D_∞ is a circle at large distance from the N-discs system and ∂D_i is one circle centred on disc i but a little larger than the disc itself.

We use equation (9) in two steps:

—first, we choose for the extremity of the vector $\boldsymbol{x}$ a point belonging to the surface of a scatterer and we calculate the line integral over ∂D. We thus obtain an equation linking the two sets of coefficients $A_{mp}^{(i)}$ and $B_{mp}^{(i)}$,

—then, we choose for the extremity of the vector $\boldsymbol{x}$ a point belonging to the domain D at large distance from the system composed by the N discs. We then express the matrix elements S_{mp} in terms of the two sets of coefficients $A_{mp}^{(i)}$ and $B_{mp}^{(i)}$.

The reader who simply wishes to calculate the S-matrix and is not especially interested in following the derivation can directly use equation (37)–(42) and (54)–(56).

2.2.2. First step: $\boldsymbol{x}$ belongs to the surface of scatterer i_0. In this part of the study, $\boldsymbol{x}$ lies on the surface of scatterer i_0. Because $\boldsymbol{x}$ does not belong to the domain D, $\phi_m(\boldsymbol{x}) = 0$, and equation (9) reads

$$0 = I_\infty(\boldsymbol{x}) + I_{i_0}(\boldsymbol{x}) + \sum_{j=1(j\neq i_0)}^{j=N} I_j(\boldsymbol{x}) \tag{11}$$

with $I_\infty(\boldsymbol{x})$ the integral over ∂D_∞, $I_{i_0}(\boldsymbol{x})$ the integral over ∂D_{i_0}, and $I_j(\boldsymbol{x})$ the one over ∂D_j defined by

$$I_\infty(\boldsymbol{x}) = \int_{\partial D_\infty} \mathrm{d}\boldsymbol{S}_{\boldsymbol{x}'} \cdot [G_k(\boldsymbol{x}, \boldsymbol{x}')\boldsymbol{\nabla}_{\boldsymbol{x}'}\phi_m(\boldsymbol{x}') - \phi_m(\boldsymbol{x}')\boldsymbol{\nabla}_{\boldsymbol{x}'}G_k(\boldsymbol{x}, \boldsymbol{x}')] \tag{12}$$

$$I_{i_0}(\boldsymbol{x}) = \int_{\partial D_{i_0}} \mathrm{d}\boldsymbol{S}_{\boldsymbol{x}'} \cdot [G_k(\boldsymbol{x}, \boldsymbol{x}')\boldsymbol{\nabla}_{\boldsymbol{x}'}\phi_m(\boldsymbol{x}') - \phi_m(\boldsymbol{x}')\boldsymbol{\nabla}_{\boldsymbol{x}'}G_k(\boldsymbol{x}, \boldsymbol{x}')] \tag{13}$$

$$I_j(\boldsymbol{x}) = \int_{\partial D_j} \mathrm{d}\boldsymbol{S}_{\boldsymbol{x}'} \cdot [G_k(\boldsymbol{x}, \boldsymbol{x}')\boldsymbol{\nabla}_{\boldsymbol{x}'}\phi_m(\boldsymbol{x}') - \phi_m(\boldsymbol{x}')\boldsymbol{\nabla}_{\boldsymbol{x}'}G_k(\boldsymbol{x}, \boldsymbol{x}')]. \tag{14}$$

We first evaluate the line integral at large distance $I_\infty(\boldsymbol{x})$. In this case, $\boldsymbol{x} = (r, \theta)$ belongs to ∂D_{i_0} and $\boldsymbol{x}' = (r', \theta')$ to ∂D_∞, so that $r' > r$. Consequently, from Graf's theorem [20], $G_k(\boldsymbol{x}, \boldsymbol{x}')$ can be written in the form

$$G_k(\boldsymbol{x}, \boldsymbol{x}') = \frac{\mathrm{i}}{4} \sum_{p=-\infty}^{+\infty} J_p(kr) H_p^{(1)}(kr') \mathrm{e}^{\mathrm{i}p(\theta-\theta')} \tag{15}$$

with

$$H_p^{(1)}(kr') \underset{r'\to\infty}{\sim} \sqrt{\frac{2}{\pi k r'}} \mathrm{e}^{\mathrm{i}(kr'-p\pi/2-\pi/4)}. \tag{16}$$

Therefore we have

$$\boldsymbol{n}' \cdot \boldsymbol{\nabla}_{\boldsymbol{x}'} G_k(\boldsymbol{x}, \boldsymbol{x}') = \mathrm{i}k G_k(\boldsymbol{x}, \boldsymbol{x}') + \mathrm{O}_{r'\to\infty}\left(\frac{1}{(r')^{3/2}}\right) \tag{17}$$

where $\boldsymbol{n}'$ is an unit vector normal to ∂D_∞. Furthermore, from equation (4), we obtain

$$\frac{\partial \phi_m(\boldsymbol{x}')}{\partial r'} - \mathrm{i}k\phi_m(\boldsymbol{x}') = \frac{1}{\sqrt{2\pi k r'}}(-2\mathrm{i}k)\mathrm{e}^{-\mathrm{i}(kr'-m\pi/2-\pi/4)}\mathrm{e}^{\mathrm{i}m\theta'} + \mathrm{O}_{r'\to\infty}\left(\frac{1}{(r')^{3/2}}\right). \tag{18}$$

We finally find

$$I_\infty(\boldsymbol{x}) = J_m(kr)\mathrm{e}^{\mathrm{i}m\theta}. \tag{19}$$

$I_\infty(\boldsymbol{x})$ has been expressed in terms of the coordinates (r, θ) of $\boldsymbol{x}$. In order to express it in terms of the coordinates centred on scatterer i_0 (see figure 3), we use Graf's addition theorem [19]

$$J_m(kr)\mathrm{e}^{\mathrm{i}m(\phi_{i_0}-\theta)} = \sum_{p=-\infty}^{+\infty} J_{m+p}(ks_{i_0}) J_p(ka) \mathrm{e}^{\mathrm{i}p(\pi-\phi_{i_0}+\theta_{i_0})} \tag{20}$$

and we obtain

$$I_\infty(\boldsymbol{x}) = \mathrm{e}^{\mathrm{i}m\phi_{i_0}} \sum_{p=-\infty}^{+\infty} J_{m-p}(ks_{i_0}) J_p(ka) \mathrm{e}^{\mathrm{i}p(\theta_{i_0}-\phi_{i_0})}. \tag{21}$$

We then evaluate the line integral $I_{i_0}(\boldsymbol{x})$. We can write $I_{i_0}(\boldsymbol{x}) = I_{i_0}^{(1)}(\boldsymbol{x}) - I_{i_0}^{(2)}(\boldsymbol{x})$ with

$$I_{i_0}^{(1)}(\boldsymbol{x}) = \int_{\partial D_{i_0}} \mathrm{d}\boldsymbol{S}_{\boldsymbol{x}'} \cdot [G_k(\boldsymbol{x}, \boldsymbol{x}')\boldsymbol{\nabla}_{\boldsymbol{x}'}\phi_m(\boldsymbol{x}')] \tag{22}$$

and

$$I_{i_0}^{(2)}(\boldsymbol{x}) = \int_{\partial D_{i_0}} \mathrm{d}\boldsymbol{S}_{\boldsymbol{x}'} \cdot [\phi_m(\boldsymbol{x}')\boldsymbol{\nabla}_{\boldsymbol{x}'}G_k(\boldsymbol{x}, \boldsymbol{x}')]. \tag{23}$$

As far as the calculation of $I_{i_0}^{(1)}(\boldsymbol{x})$ is concerned, we directly obtain

$$I_{i_0}^{(1)}(\boldsymbol{x}) = \frac{\mathrm{i}\pi a}{2} \sum_{p=-\infty}^{+\infty} B_{mp}^{(i_0)} J_p(ka) H_p^{(1)}(ka) \mathrm{e}^{\mathrm{i}p\theta_{i_0}} \tag{24}$$

by expressing $G_k(\boldsymbol{x}, \boldsymbol{x}')$ in the coordinate system $(O_{i_0}xy)$. The calculation of $I_{i_0}^{(2)}(\boldsymbol{x})$ is not so obvious because it is only at the end of the calculation that we shall take the limit in which ∂D_{i_0} tends to the boundary of disc i_0 (see figure 4).

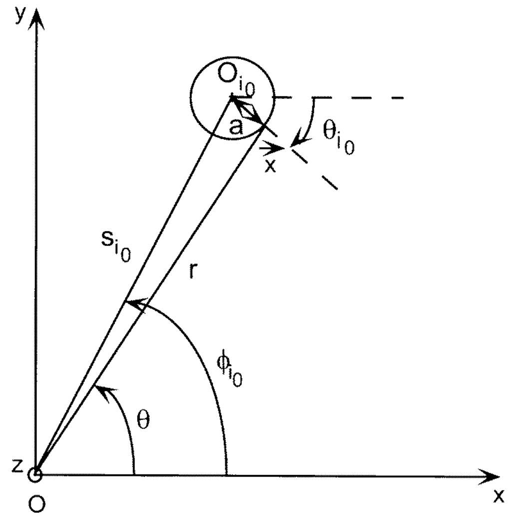

Figure 3. From the coordinate system (r, θ) to the coordinate system $(r_{i_0} = a, \theta_{i_0})$.

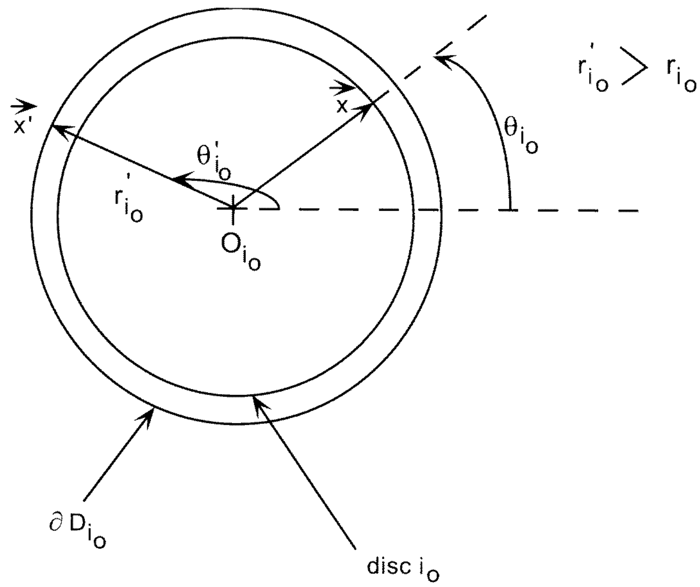

Figure 4. Disc i_0 and its boundary.

We also express $G_k(\boldsymbol{x}, \boldsymbol{x}')$ in the coordinate system $(O_{i_0}xy)$. We have

$$G_k(\boldsymbol{x}, \boldsymbol{x}') = \frac{\mathrm{i}}{4} \sum_{p=-\infty}^{+\infty} J_p(ka) H_p^{(1)}(kr'_{i_0}) \mathrm{e}^{\mathrm{i}p(\theta_{i_0} - \theta'_{i_0})} \tag{25}$$

so that

$$\boldsymbol{n}' \cdot \boldsymbol{\nabla}_{x'} G_k(\boldsymbol{x}, \boldsymbol{x}') = -\frac{\mathrm{i}k}{4} \sum_{p=-\infty}^{+\infty} J_p(ka) H_p^{(1)\prime}(ka) \mathrm{e}^{\mathrm{i}p(\theta_{i_0} - \theta'_{i_0})}. \tag{26}$$

We then obtain

$$I_{i_0}^{(2)}(\boldsymbol{x}) = -\frac{\mathrm{i}\pi a}{2} \sum_{p=-\infty}^{+\infty} k A_{mp}^{(i_0)} J_p(ka) H_p^{(1)\prime}(ka) \mathrm{e}^{\mathrm{i}p\theta_{i_0}}. \tag{27}$$

Thus, the line integral $I_{i_0}(\boldsymbol{x})$ is given by

$$I_{i_0}(\boldsymbol{x}) = \frac{\mathrm{i}\pi a}{2} \sum_{p=-\infty}^{+\infty} J_p(ka) \mathrm{e}^{\mathrm{i}p\theta_{i_0}} [B_{mp}^{(i_0)} H_p^{(1)}(ka) + k A_{mp}^{(i_0)} H_p^{(1)\prime}(ka)]. \tag{28}$$

We finally evaluate the integrals $I_j(\boldsymbol{x})$ for $j \neq i_0$. We have $I_j(\boldsymbol{x}) = I_j^{(1)}(\boldsymbol{x}) - I_j^{(2)}(\boldsymbol{x})$ with

$$I_j^{(1)}(\boldsymbol{x}) = \int_{\partial D_j} \mathrm{d}\boldsymbol{S}_{\boldsymbol{x}'} \cdot [G_k(\boldsymbol{x}, \boldsymbol{x}') \boldsymbol{\nabla}_{\boldsymbol{x}'} \phi_m(\boldsymbol{x}')] \tag{29}$$

and

$$I_j^{(2)}(\boldsymbol{x}) = \int_{\partial D_j} \mathrm{d}\boldsymbol{S}_{\boldsymbol{x}'} \cdot [\phi_m(\boldsymbol{x}') \boldsymbol{\nabla}_{\boldsymbol{x}'} G_k(\boldsymbol{x}, \boldsymbol{x}')]. \tag{30}$$

As far as the calculation of $I_j^{(1)}(\boldsymbol{x})$ is concerned, we directly obtain

$$I_j^{(1)}(\boldsymbol{x}) = \frac{\mathrm{i}\pi a}{2} \sum_{p=-\infty}^{+\infty} B_{mp}^{(j)} J_p(ka) H_p^{(1)}(kr_j) \mathrm{e}^{\mathrm{i}p\theta_j} \tag{31}$$

by expressing $G_k(\boldsymbol{x}, \boldsymbol{x}')$ in the coordinate system $(O_j xy)$. In this case, $\boldsymbol{x}$ still belongs to the boundary of disc i_0, but now $\boldsymbol{x}'$ lies on ∂D_j (see figure 5). $H_p^{(1)}(kr_j)$ can be expressed in the coordinate system (r_{i_0}, θ_{i_0}) by using Graf's theorem

$$H_p^{(1)}(kr_j) \mathrm{e}^{\mathrm{i}p(\phi_{ji_0} - \theta_j)} = \sum_{q=-\infty}^{+\infty} H_{p+q}^{(1)}(kr_{i_0 j}) J_q(ka) \mathrm{e}^{\mathrm{i}q(\pi - \phi_{ji_0} + \theta_{i_0})}. \tag{32}$$

We then obtain

$$I_j^{(1)}(\boldsymbol{x}) = \frac{\mathrm{i}\pi a}{2} \sum_{p=-\infty}^{+\infty} \sum_{q=-\infty}^{+\infty} B_{mq}^{(j)} J_q(ka) J_p(ka) H_{q-p}^{(1)}(kr_{i_0 j}) \mathrm{e}^{\mathrm{i}(q-p)\phi_{ji_0}} \mathrm{e}^{\mathrm{i}p\theta_{i_0}}. \tag{33}$$

The calculation of $I_j^{(2)}(\boldsymbol{x})$ is similar to that of $I_j^{(1)}(\boldsymbol{x})$. From the relation

$$\boldsymbol{n}_j' \cdot \boldsymbol{\nabla}_{\boldsymbol{x}'} G_k(\boldsymbol{x}, \boldsymbol{x}') = -\frac{\mathrm{i}k}{4} \sum_{p=-\infty}^{+\infty} J_p'(ka) H_p^{(1)}(kr_j) \mathrm{e}^{\mathrm{i}p(\theta_j - \theta_j')} \tag{34}$$

we obtain

$$I_j^{(2)}(\boldsymbol{x}) = -\frac{\mathrm{i}\pi a}{2} \sum_{p=-\infty}^{+\infty} \sum_{q=-\infty}^{+\infty} k A_{mq}^{(j)} J_q'(ka) J_p(ka) H_{q-p}^{(1)}(kr_{i_0 j}) \mathrm{e}^{\mathrm{i}(q-p)\phi_{ji_0}} \mathrm{e}^{\mathrm{i}p\theta_{i_0}}. \tag{35}$$

Finally, from equations (33) and (35), we have

$$I_j(\boldsymbol{x}) = \frac{\mathrm{i}\pi a}{2} \sum_{p=-\infty}^{+\infty} \sum_{q=-\infty}^{+\infty} \mathrm{e}^{\mathrm{i}[(q-p)\phi_{ji_0} + p\theta_{i_0}]} J_p(ka) H_{q-p}^{(1)}(kr_{i_0 j}) [B_{mq}^{(j)} J_q(ka) + k A_{mq}^{(j)} J_q'(ka)]. \tag{36}$$

By combining equations (21), (28) and (36), in equation (11), we find

$$C_{mp}^{(i)} = \sum_{j=1}^{N} \sum_{q=-\infty}^{+\infty} \{\tilde{B}_{mq}^{(j)} M_{qp}^{(ij)} + \tilde{A}_{mq}^{(j)} N_{qp}^{(ij)}\} \tag{37}$$

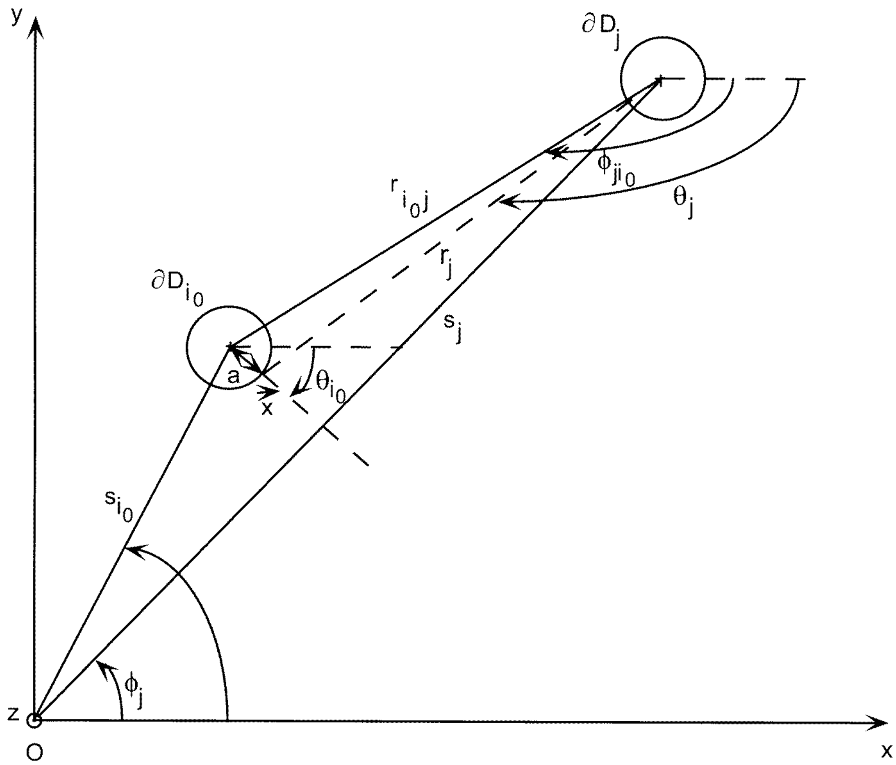

Figure 5. From the coordinate system (r_j, θ_j) to the coordinate system (r_{i_0}, θ_{i_0}).

where

$$\tilde{B}^{(j)}_{mq} = B^{(j)}_{mq} e^{iq\phi_j} \quad \text{and} \quad \tilde{A}^{(j)}_{mq} = kA^{(j)}_{mq} e^{iq\phi_j} \tag{38}$$

and

$$C^{(i)}_{mp} = e^{im\phi_i} \frac{J_{m-p}(ks_i)}{H^{(1)}_p(ka)}. \tag{39}$$

Here the matrices $M^{(ij)}_{qp}$ and $N^{(ij)}_{qp}$ are given by

$$M^{(ij)}_{qp} = \frac{\pi a}{2i} \left\{ \delta_{qp}\delta_{ij} + \frac{J_q(ka)}{H^{(1)}_p(ka)} H^{(1)}_{q-p}(kr_{ij}) \xi_{ij}(p,q) \right\} \tag{40}$$

$$N^{(ij)}_{qp} = \frac{\pi a}{2i} \left\{ \frac{H^{(1)'}_q(ka)}{H^{(1)}_p(ka)} \delta_{qp}\delta_{ij} + \frac{J'_q(ka)}{H^{(1)}_p(ka)} H^{(1)}_{q-p}(kr_{ij}) \xi_{ij}(p,q) \right\} \tag{41}$$

with

$$\xi_{ij}(p,q) = \begin{cases} 0 & \text{if } i = j \\ e^{ip(\phi_i - \phi_{ji})} e^{iq(\phi_{ji} - \phi_j)} & \text{if } i \neq j. \end{cases} \tag{42}$$

2.2.3. Second step: $\boldsymbol{x}$ is at a large distance from the N-disc scatterer inside domain D. Now we choose $\boldsymbol{x}$ at a large distance from the N-disc scatterer and inside domain D, so that $\phi_m(\boldsymbol{x})$ is given by its asymptotic behaviour in equation (4). So, in this case, equation (9) reads

$$J_\infty(\boldsymbol{x}) + \sum_{i=1}^{N} J_i(\boldsymbol{x}) = \frac{1}{\sqrt{2\pi kr}} \sum_{p=-\infty}^{+\infty} [\mathrm{e}^{-\mathrm{i}(kr-p\pi/2-\pi/4)}\delta_{mp} + \mathrm{e}^{\mathrm{i}(kr-p\pi/2-\pi/4)} S_{mp}]\mathrm{e}^{\mathrm{i}p\theta} \tag{43}$$

with

$$J_\infty(\boldsymbol{x}) = \int_{\partial D_\infty} \mathrm{d}\boldsymbol{S}_{\boldsymbol{x}'} \cdot [G_k(\boldsymbol{x},\boldsymbol{x}')\boldsymbol{\nabla}_{\boldsymbol{x}'}\phi_m(\boldsymbol{x}') - \phi_m(\boldsymbol{x}')\boldsymbol{\nabla}_{\boldsymbol{x}'}G_k(\boldsymbol{x},\boldsymbol{x}')] \tag{44}$$

and

$$J_i(\boldsymbol{x}) = \int_{\partial D_i} \mathrm{d}\boldsymbol{S}_{\boldsymbol{x}'} \cdot [G_k(\boldsymbol{x},\boldsymbol{x}')\boldsymbol{\nabla}_{\boldsymbol{x}'}\phi_m(\boldsymbol{x}') - \phi_m(\boldsymbol{x}')\boldsymbol{\nabla}_{\boldsymbol{x}'}G_k(\boldsymbol{x},\boldsymbol{x}')]. \tag{45}$$

We first evaluate the line integral $J_\infty(\boldsymbol{x})$ at large distance. It should be noted that $r < r'$. Indeed r' is on the boundary ∂D_∞ while r, which is far from the diffusors, still remains inside domain D. Consequently, the calculation of $J_\infty(\boldsymbol{x})$ is the same that the calculation of $I_\infty(\boldsymbol{x})$ performed in section 2.2.2. We have

$$J_\infty(\boldsymbol{x}) = J_m(kr)\mathrm{e}^{\mathrm{i}m\theta}. \tag{46}$$

Moreover, since r tends to infinity, $J_\infty(\boldsymbol{x})$ is given by

$$J_\infty(\boldsymbol{x}) \underset{r\to\infty}{\sim} \frac{1}{\sqrt{2\pi kr}} \sum_{p=-\infty}^{+\infty} [\mathrm{e}^{-\mathrm{i}(kr-m\pi/2-\pi/4)}\delta_{mp} + \mathrm{e}^{\mathrm{i}(kr-m\pi/2-\pi/4)}\delta_{mp}]\mathrm{e}^{\mathrm{i}p\theta}. \tag{47}$$

We then evaluate the line integral $J_i(\boldsymbol{x})$. We can write

$$J_i(\boldsymbol{x}) = J_i^{(1)}(\boldsymbol{x}) - J_i^{(2)}(\boldsymbol{x}) \tag{48}$$

with

$$J_i^{(1)}(\boldsymbol{x}) = \int_{\partial D_i} \mathrm{d}\boldsymbol{S}_{\boldsymbol{x}'} \cdot [G_k(\boldsymbol{x},\boldsymbol{x}')\boldsymbol{\nabla}_{\boldsymbol{x}'}\phi_m(\boldsymbol{x}')] \tag{49}$$

and

$$J_i^{(2)}(\boldsymbol{x}) = \int_{\partial D_i} \mathrm{d}\boldsymbol{S}_{\boldsymbol{x}'} \cdot [\phi_m(\boldsymbol{x}')\boldsymbol{\nabla}_{\boldsymbol{x}'}G_k(\boldsymbol{x},\boldsymbol{x}')]. \tag{50}$$

In order to evaluate $J_i^{(1)}(\boldsymbol{x})$, we first express $G_k(\boldsymbol{x},\boldsymbol{x}')$ in the coordinate system (r_i,θ_i). Then, by using Graf's addition theorem (see figure 6), we express $G_k(\boldsymbol{x},\boldsymbol{x}')$ in the coordinate system (r,θ).

As a consequence, we obtain

$$J_i^{(1)}(\boldsymbol{x}) = \frac{\mathrm{i}\pi a}{2} \sum_{p=-\infty}^{+\infty} \sum_{q=-\infty}^{+\infty} B_{mq}^{(i)} \mathrm{e}^{\mathrm{i}q\phi_i} J_q(ka) H_p^{(1)}(kr) J_{p-q}(ks_i) \mathrm{e}^{\mathrm{i}p(\theta-\phi_i)}. \tag{51}$$

In this case, $H_p^{(1)}(kr)$ is still given by its asymptotic expansion for large arguments (equation (16)). In order to calculate $J_i^{(2)}(\boldsymbol{x})$, we still express $G_k(\boldsymbol{x},\boldsymbol{x}')$ in the coordinate system (r_i,θ_i), so that the gradient is still given by equation (34). Thus, we obtain

$$J_i^{(2)}(\boldsymbol{x}) = -\frac{\mathrm{i}\pi a}{2} \sum_{p=-\infty}^{+\infty} \sum_{q=-\infty}^{+\infty} kA_{mq}^{(i)} \mathrm{e}^{\mathrm{i}q\phi_i} J_q'(ka) H_p^{(1)}(kr) J_{p-q}(ks_i) \mathrm{e}^{\mathrm{i}p(\theta-\phi_i)}. \tag{52}$$

Finally, from equations (51) and (52), we find

$$J_i(\boldsymbol{x}) = \frac{\mathrm{i}\pi a}{2} \sum_{p=-\infty}^{+\infty} \sum_{q=-\infty}^{+\infty} H_p^{(1)}(kr) J_{p-q}(ks_i) \mathrm{e}^{\mathrm{i}p(\theta-\phi_i)} \mathrm{e}^{\mathrm{i}q\phi_i} [B_{mq}^{(i)} J_q(ka) + kA_{mq}^{(i)} J_q'(ka)] \tag{53}$$

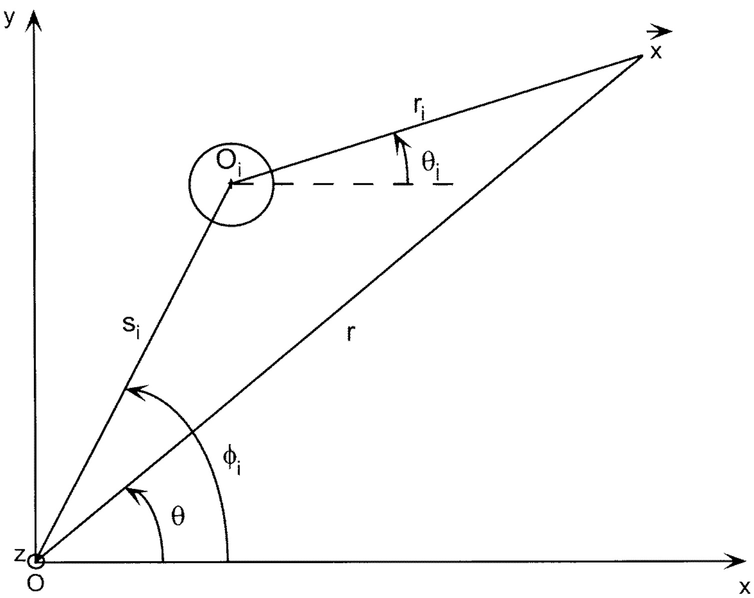

Figure 6. From the coordinate system (r_i, θ_i) to the coordinate system (r, θ).

with $H_p^{(1)}(kr)$ given by its asymptotic expansion for large arguments.

Introducing the results established in equations (47) and (53) in equation (43), we obtain

$$S_{mp} = \delta_{mp} + \mathrm{i} \sum_{j=1}^{N} \sum_{q=-\infty}^{+\infty} [\tilde{B}_{mq}^{(j)} D_{qp}^{(j)} + \tilde{A}_{mq}^{(j)} E_{qp}^{(j)}] \tag{54}$$

where the matrix elements $\tilde{A}_{mq}^{(j)}$ and $\tilde{B}_{mq}^{(j)}$ are given by equation (38) and the matrices $D_{qp}^{(j)}$ and $E_{qp}^{(j)}$ by

$$D_{qp}^{(j)} = \pi a \mathrm{e}^{-\mathrm{i}p\phi_j} J_{p-q}(ks_j) J_q(ka) \tag{55}$$

and

$$E_{qp}^{(j)} = \pi a \mathrm{e}^{-\mathrm{i}p\phi_j} J_{p-q}(ks_j) J_q'(ka). \tag{56}$$

3. Study of some particular boundary conditions

3.1. Dirichlet boundary condition

In quantum mechanics, when we study the particle scattering by hard discs, a Dirichlet boundary condition must be satisfied by the wavefunction [1–12]. In acoustics, it also must be satisfied by the pressure field describing ultrasonic wave scattering by soft discs. Similarly, in electromagnetism and more particularly in the study of microwave scattering by perfect metallic conductors [16], this boundary condition must be satisfied by the transverse component of the electric field. In all those cases, the partial wave $\phi_m(\boldsymbol{x})$ vanishes on the boundaries of the N discs, so

$$\tilde{A}_{mp}^{(i)} = 0 \text{ for } i = 1, \ldots, N. \tag{57}$$

In contrast, the gradient of the partial wave $\phi_m(\boldsymbol{x})$ is defined by the unknown coefficients $\tilde{B}^{(i)}_{mp}$ given by equation (3). Consequently, the S-matrix given by equation (54) reduces to

$$S_{mp} = \delta_{mp} + \mathrm{i} \sum_{j=1}^{N} \sum_{q=-\infty}^{+\infty} \tilde{B}^{(j)}_{mq} D^{(j)}_{qp}. \tag{58}$$

Here $D^{(j)}_{qp}$ is given by equation (55) and the coefficients $\tilde{B}^{(j)}_{mp}$ are determined from equation (37) by

$$C^{(i)}_{mp} = \sum_{j=1}^{N} \sum_{q=-\infty}^{+\infty} \tilde{B}^{(j)}_{mq} M^{(ij)}_{qp} \tag{59}$$

with $C^{(i)}_{mp}$ and $M^{(ij)}_{qp}$ are given by equations (39) and (40).

3.2. Neumann boundary condition

In acoustics, the pressure field describing ultrasonic wave scattering by hard discs satisfies a Neumann boundary condition. In that case, the gradient of the partial wave $\phi_m(\boldsymbol{x})$ vanishes on the boundaries of the N discs, thus

$$\tilde{B}^{(i)}_{mp} = 0 \qquad \text{for } i = 1, \ldots, N. \tag{60}$$

Now, the partial wave $\phi_m(\boldsymbol{x})$ is defined by the unknown coefficients $\tilde{A}^{(i)}_{mp}$ given by equation (2). Consequently, the S-matrix given by equation (54) reduces to

$$S_{mp} = \delta_{mp} + \mathrm{i} \sum_{j=1}^{N} \sum_{q=-\infty}^{+\infty} \tilde{A}{}^{(j)}_{mq} E^{(j)}_{qp}. \tag{61}$$

Here $E^{(j)}_{qp}$ is given by equation (56) and the coefficients $\tilde{A}{}^{(j)}_{mp}$ are determined from equation (37) by

$$C^{(i)}_{mp} = \sum_{j=1}^{N} \sum_{q=-\infty}^{+\infty} \tilde{A}{}^{(j)}_{mq} N^{(ij)}_{qp}$$

with $C^{(i)}_{mp}$ and $N^{(ij)}_{qp}$ are given by equations (39) and (41).

3.3. Impedance boundary conditions

In electromagnetism and more particularly in the study of microwave scattering by metallic conductors with a given constant impedance Z, the impedance boundary condition must be satisfied by the transverse components of the electric and magnetic fields. More precisely, the partial wave $\phi_m(\boldsymbol{x})$ and its gradient are linked on the boundaries of the N discs by (see for example [21])

$$\frac{\partial \phi_m}{\partial r_i} + \mathrm{i}k\zeta \phi_m = 0. \tag{62}$$

For TM-waves, $\zeta = Z$, while for TE-waves, $\zeta = 1/Z$. We then obtain

$$\tilde{B}{}^{(i)}_{mp} = \mathrm{i}\zeta \tilde{A}{}^{(i)}_{mp} \qquad \text{for } i = 1, \ldots, N.$$

Consequently, the S-matrix given by equation (54) reduces to

$$S_{mp} = \delta_{mp} + \mathrm{i} \sum_{j=1}^{N} \sum_{q=-\infty}^{+\infty} \tilde{A}{}^{(j)}_{mq} [\mathrm{i}\zeta D^{(j)}_{qp} + E^{(j)}_{qp}]. \tag{63}$$

Here $D_{qp}^{(j)}$ and $E_{qp}^{(j)}$ are respectively given by equations (55) and (56) and the coefficients $\tilde{A}{}_{mp}^{(j)}$ are determined from the following system

$$C_{mp}^{(i)} = \sum_{j=1}^{N} \sum_{q=-\infty}^{+\infty} \tilde{A}{}_{mq}^{(j)} [\mathrm{i}\zeta M_{qp}^{(ij)} + N_{qp}^{(ij)}] \tag{64}$$

with $C_{mp}^{(i)}$, $M_{qp}^{(ij)}$ and $N_{qp}^{(ij)}$ are respectively given by equations (39)–(41).

3.4. Mixed boundary conditions

Such boundary conditions occur in quantum mechanics for the wavefunction describing particle scattering by a square well and by a square barrier in the 'overdense' and 'underdense' cases. In that case, equation (1) is the time-independent Schrödinger equation and the corresponding potential $V(r)$ vanishes outside the discs and is constant inside each disc where it takes the value V_0. We denote by $E > 0$ the total energy of the incident particle. Then the wavenumbers outside and inside the discs are respectively given by $k = (1/\hbar)\sqrt{2mE}$ and $k' = nk$ with the refraction index $n = \sqrt{1 - V_0/E}$.

The expression of the inner wavefunction in each disc i can be written in the form

$$\phi_{\mathrm{int}}^{(i)} = \sum_{p=-\infty}^{+\infty} c_{mp}^{(i)} J_p(k' r_i) \mathrm{e}^{\mathrm{i}p\theta_i} \tag{65}$$

where the $c_{mp}^{(i)}$ are a set of unknown coefficients which can be linked to the coefficients $A_{mp}^{(i)}$ and $B_{mp}^{(i)}$ by using the continuity of the wavefunction and its normal derivative on the boundaries of the N discs. We obtain

$$A_{mp}^{(i)} = c_{mp}^{(i)} J_p(k'a) \tag{66}$$

$$B_{mp}^{(i)} = -k' c_{mp}^{(i)} J_p'(k'a). \tag{67}$$

We then find that the S-matrix is given by

$$S_{mp} = \delta_{mp} + \mathrm{i} \sum_{j=1}^{N} \sum_{q=-\infty}^{+\infty} \tilde{c}_{mq}^{(j)} F_{qp}^{(j)} \tag{68}$$

with

$$F_{qp}^{(j)} = \pi a \mathrm{e}^{-\mathrm{i}p\phi_j} J_{p-q}(ks_j) D_q^{[1]} \tag{69}$$

and the coefficients $\tilde{c}_{mq}^{(j)} = c_{mq}^{(j)} \mathrm{e}^{\mathrm{i}q\phi_j}$ are the solution of the following system (equation (37))

$$C_{mp}^{(i)} = \sum_{j=1}^{N} \sum_{q=-\infty}^{+\infty} \tilde{c}_{mq}^{(j)} M_{qp}^{(ij)} \tag{70}$$

with

$$C_{mp}^{(i)} = -\mathrm{e}^{\mathrm{i}m\phi_i} \frac{J_{m-p}(ks_i)}{D_p} \tag{71}$$

$$M_{qp}^{(ij)} = \frac{\pi a}{2\mathrm{i}} \left\{ \delta_{qp}\delta_{ij} - \frac{D_q^{[1]}}{D_p} H_{q-p}^{(1)}(kr_{ij}) \xi_{ij}(p,q) \right\}. \tag{72}$$

The coefficients $D_q^{[1]}$ and D_p are 2×2 determinants which take into account the boundary conditions and are given by

$$D_q^{[1]} = \begin{vmatrix} kJ_q'(ka) & k'J_q'(k'a) \\ J_q(ka) & J_q(k'a) \end{vmatrix} \qquad \text{and } D_p = -\begin{vmatrix} kH_p^{(1)'}(ka) & k'J_p'(k'a) \\ H_p^{(1)}(ka) & J_p(k'a) \end{vmatrix}. \tag{73}$$

3.5. Elastic boundary conditions

Elastic boundary conditions occur in acoustics in the study of ultrasonic wave scattering by elastic cylinders immersed in water or in a perfect fluid. In that case, the determination of the coefficients $A_{mp}^{(i)}$ and $B_{mp}^{(i)}$ is more complicated: it involves the scalar and vector potentials associated respectively with compressional and shear waves [22] and it is necessary to write, at the surface of each cylinder, the continuity of the radial component of displacement and of the normal component of the stress tensor. After tedious calculations, one finds [23]

$$S_{mp} = \delta_{mp} + \mathrm{i} \sum_{j=1}^{N} \sum_{q=-\infty}^{+\infty} \tilde{a}_{mq}^{(j)} G_{qp}^{(j)} \tag{74}$$

with

$$G_{qp}^{(j)} = \pi a \mathrm{e}^{-\mathrm{i}p\phi_j} J_{p-q}(ks_j) D_q^{[1]}. \tag{75}$$

The coefficients $\tilde{a}_{mq}^{(j)}$, which define the vector displacement potential of cylinder j, are the solution of

$$C_{mp}^{(i)} = \sum_{j=1}^{N} \sum_{q=-\infty}^{+\infty} \tilde{a}_{mq}^{(j)} M_{qp}^{(ij)} \tag{76}$$

with

$$C_{mp}^{(i)} = -\mathrm{e}^{\mathrm{i}m\phi_i} \frac{J_{m-p}(ks_i)}{D_p} \tag{77}$$

$$M_{qp}^{(ij)} = \frac{\pi a}{2\mathrm{i}} \left\{ \delta_{qp}\delta_{ij} - \frac{D_q^{[1]}}{D_p} H_{q-p}^{(1)}(kr_{ij}) \xi_{ij}(p,q) \right\}. \tag{78}$$

Here $D^{[1]}$ and D are the usual 3×3 determinants defining the scattering wave by only one cylinder and which take into account the boundary conditions [24]. They are given by

$$D_q^{[1]} = \begin{vmatrix} -(k_T a)^2 J_q(ka) & d_{12} & d_{13} \\ (\rho'/\rho) ka J_q^{'}(ka) & d_{22} & d_{23} \\ 0 & d_{32} & d_{33} \end{vmatrix} \tag{79}$$

$$D_q = - \begin{vmatrix} -(k_T a)^2 H_q^{(1)}(ka) & d_{12} & d_{13} \\ (\rho'/\rho) ka H_q^{(1)\prime}(ka) & d_{22} & d_{23} \\ 0 & d_{32} & d_{33} \end{vmatrix} \tag{80}$$

with

$$d_{12} = [(k_T a)^2 - 2q^2] J_q(k_L a) + 2k_L a J_q^{'}(k_L a) \tag{81}$$

$$d_{22} = -k_L a J_q^{'}(k_L a) \tag{82}$$

$$d_{32} = 2q[k_L a J_q^{'}(k_L a) - J_q(k_L a)] \tag{83}$$

$$d_{13} = 2q[x_T J_q^{'}(k_T a) - J_q(k_T a)] \tag{84}$$

$$d_{23} = q J_q(k_T a) \tag{85}$$

$$d_{33} = [(k_T a)^2 - 2q^2] J_q(k_T a) + 2k_T a J_q^{\prime}(k_T a). \tag{86}$$

Here k is the wavenumber in the fluid medium linked to the velocity c of sound by $k = \omega/c$ (ω denotes the angular frequency of the incident wave). k_L and k_T are respectively the wavenumbers associated with compressional and shear waves propagating inside the cylinders. They are linked to the velocities c_L and c_T of compressional and shear waves by $k_L = \omega/c_L$ and $k_T = \omega/c_T$. Furthermore, ρ and ρ' denote respectively the density of the fluid and that of the scatterers.

3.6. Summary

It is easy to show that, for all the boundary conditions studied above, the S-matrix is expressible in the form

$$S_{mp} = \delta_{mp} + \mathrm{i} \sum_{j=1}^{N} \sum_{q=-\infty}^{+\infty} \tilde{X}{}^{(j)}_{mq} E^{(j)}_{qp} \tag{87}$$

where the unknown coefficients $\tilde{X}{}^{(j)}$ are deduced from the following system

$$C^{(i)}_{mp} = \sum_{j=1}^{N} \sum_{q=-\infty}^{+\infty} \tilde{X}{}^{(j)}_{mq} M^{(ij)}_{qp} \tag{88}$$

with the matrices C, M and E given by

$$C^{(i)}_{mp} = -\mathrm{e}^{\mathrm{i}m\phi_i} \frac{J_{m-p}(ks_i)}{D_p} \tag{89}$$

$$M^{(ij)}_{qp} = \frac{\pi a}{2\mathrm{i}} \left\{ \delta_{qp}\delta_{ij} - \frac{D^{[1]}_q}{D_p} H^{(1)}_{q-p}(kr_{ij})\xi_{ij}(p,q) \right\} \tag{90}$$

$$E^{(j)}_{qp} = \pi a \mathrm{e}^{-\mathrm{i}p\phi_j} J_{p-q}(ks_j) D^{[1]}_q . \tag{91}$$

Here $D^{[1]}$ and D are determinants taking into account the boundary conditions. For a Dirichlet boundary condition, one writes

$$D^{[1]}_q = J_q(ka) \tag{92}$$

$$D_q = -H^{(1)}_q(ka). \tag{93}$$

For a Neumann boundary condition, we have

$$D^{[1]}_q = J'_q(ka) \tag{94}$$

$$D_q = -H^{(1)\prime}_q(ka). \tag{95}$$

For impedance boundary conditions, $D^{[1]}$ and D read

$$D^{[1]}_q = J'_q(ka) + \mathrm{i}\zeta J_q(ka)$$

$$D_q = -(H^{(1)\prime}_q(ka) + \mathrm{i}\zeta H^{(1)}_q(ka)).$$

For mixed boundary conditions, the determinants $D^{[1]}_q$ and D_q are expressed in equations (73). And for elastic boundary conditions, they are expressed in equations (79) and (80).

In matrix notation, equations (87) and (88) become

$$S = I + \mathrm{i}\widetilde{X} E \tag{96}$$

and

$$C = \widetilde{X} M. \tag{97}$$

Thus we can write

$$S = I + \mathrm{i} C M^{-1} E. \tag{98}$$

Consequently, the poles of the S-matrix, which are intrinsic to the scatterer, appear through the inversion of the matrix M. The scattering resonances are thus the complex zeros of the characteristic determinant

$$\det M(ka) = 0 \tag{99}$$

in the complex ka-plane.

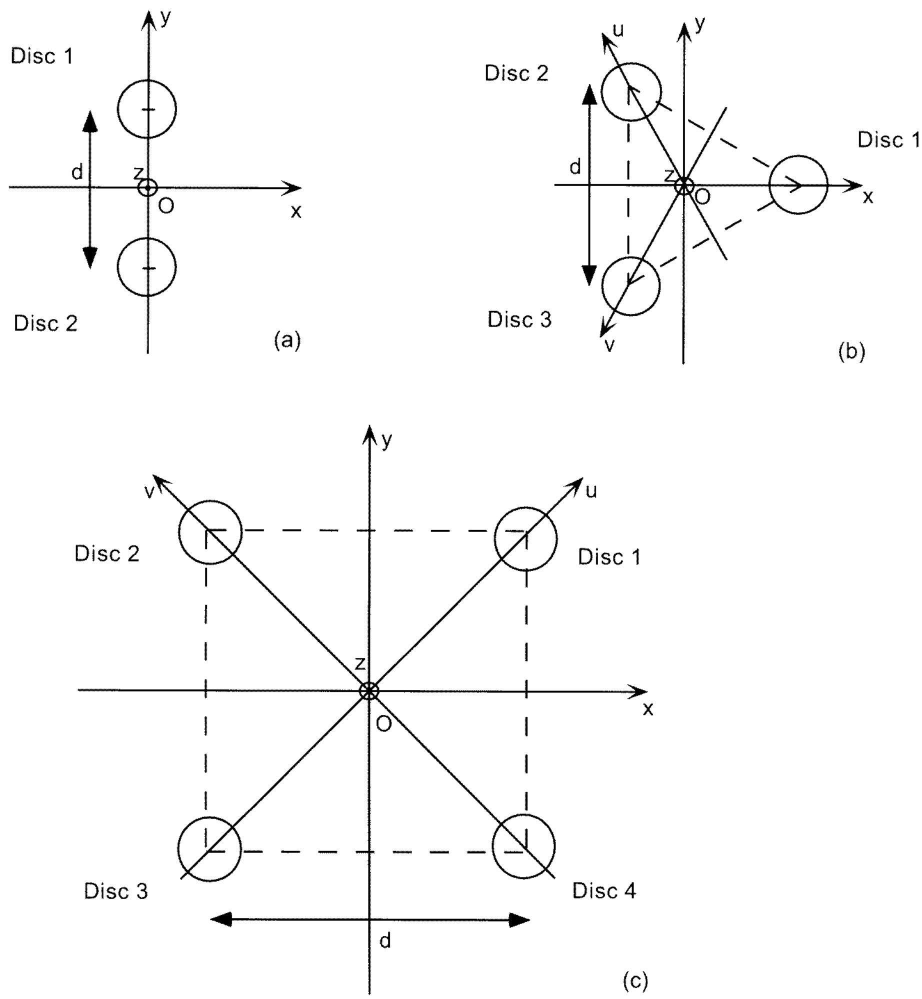

Figure 7. (*a*) Symmetry $\mathcal{C}_{2v}$. (*b*) Symmetry $\mathcal{C}_{3v}$. (*c*) Symmetry $\mathcal{C}_{4v}$.

4. Symmetry considerations

4.1. General aspects

In what follows, we shall study three different configurations presenting symmetry properties (figure 7):

—the two-disc scatterer. This system is invariant under the symmetry group $\mathcal{C}_{2v}$. We denote by d the separation distance between the centres of the scatterers,

—the three-disc scatterer. The centres of the discs are located at the vertices of an equilateral triangle of side d. The three-disc system is invariant under the symmetry group $\mathcal{C}_{3v}$,

—the four-disc scatterer. The centres of the discs are located at the vertices of a square of side d. This system is invariant under the symmetry group $\mathcal{C}_{4v}$.

In these three cases, symmetry properties of the scatterers permit us to simplify the formalism of sections 2 and 3. Indeed it is possible to expand the partial wave ϕ_m in terms

Table 1. Character table of $\mathcal{C}_{2v}$.

$\mathcal{C}_{2v}$:	E	C_2	σ_x	σ_y
A_1	1	1	1	1
A_2	1	1	−1	−1
B_1	1	−1	1	−1
B_2	1	−1	−1	1

of the irreducible representations of the symmetry groups. Let us consider a finite symmetry group G of order g. This group is made up of the geometric transformations R leaving the system invariant. We denote by Γ the set of the n_γ-dimensional irreducible representations γ associated with G. We can write [17]

$$\phi_m = \sum_{\gamma\in\Gamma} \sum_{i=1}^{n_\gamma} (\phi_m)_i^{(\gamma)} \tag{100}$$

with

$$(\phi_m)_i^{(\gamma)} = \frac{n_\gamma}{g} \sum_{R\in G} D_{ii}^{(\gamma)*}(R)(O_R\phi_m) \tag{101}$$

where O_R denotes the linear operators associated with the transformations R of the group G. $D_{ii}^{(\gamma)}(R)$ represent the diagonal elements (or characters) of the representative matrix D of the symmetry group in the representation γ.

In the following, we shall split equations (96) and (97) over the different representations of the symmetry group considered. Thus, we solve the problem described by equations (1)–(4) for the component $(\phi_m)^{(\gamma)}$ of the partial wave.

4.2. Symmetry $\mathcal{C}_{2v}$

The transformations of the symmetry group $\mathcal{C}_{2v}$ of order $g = 4$ are E, C_2, σ_x and σ_y. E denotes the identity transformation, C_2 the rotation through π about the main axis Oz of figure 7(a), σ_x and σ_y the mirror reflections in the two planes Oxz and Oyz. Four one-dimensional irreducible representations labelled by A_1, A_2, B_1, B_2 are associated with this symmetry group. Table 1 is the corresponding character table.

The character table permits us to split up any function f given by

$$f = \sum_{p=-\infty}^{+\infty} f_p \mathrm{e}^{\mathrm{i}p\theta} \tag{102}$$

as a sum of functions belonging to the four irreducible representations of $\mathcal{C}_{2v}$

$$f = f^{A_1} + f^{A_2} + f^{B_1} + f^{B_2}. \tag{103}$$

We have

$$f^{A_1} = \tfrac{1}{4} \sum_{p=-\infty}^{+\infty} [1 + (-1)^p](f_p + f_{-p})\mathrm{e}^{\mathrm{i}p\theta} \tag{104}$$

$$f^{A_2} = \tfrac{1}{4} \sum_{p=-\infty}^{+\infty} [1 + (-1)^p](f_p - f_{-p})\mathrm{e}^{\mathrm{i}p\theta} \tag{105}$$

$$f^{B_1} = \tfrac{1}{4} \sum_{p=-\infty}^{+\infty} [1 - (-1)^p](f_p + f_{-p})\mathrm{e}^{\mathrm{i}p\theta} \tag{106}$$

$$f^{B_2} = \tfrac{1}{4} \sum_{p=-\infty}^{+\infty} [1 - (-1)^p](f_p - f_{-p}) \mathrm{e}^{\mathrm{i}p\theta}. \tag{107}$$

We deduce from the previous equations the asymptotic behaviour of ϕ_m in the different representations and, as a consequence, the expression of $C^{(1)}_{mp}$ given in equation (89) in each representation. So, we obtain

$$C^{(1)A_1}_{mp} = -\frac{\mathrm{i}^m + \mathrm{i}^{-m}}{4} \left[\frac{J_{m-p}(kd/2)}{D_p} + (-1)^p \frac{J_{m+p}(kd/2)}{D_p} \right] \tag{108}$$

$$C^{(1)A_2}_{mp} = -\frac{\mathrm{i}^m + \mathrm{i}^{-m}}{4} \left[\frac{J_{m-p}(kd/2)}{D_p} - (-1)^p \frac{J_{m+p}(kd/2)}{D_p} \right] \tag{109}$$

$$C^{(1)B_1}_{mp} = -\frac{\mathrm{i}^m - \mathrm{i}^{-m}}{4} \left[\frac{J_{m-p}(kd/2)}{D_p} - (-1)^p \frac{J_{m+p}(kd/2)}{D_p} \right] \tag{110}$$

$$C^{(1)B_2}_{mp} = -\frac{\mathrm{i}^m - \mathrm{i}^{-m}}{4} \left[\frac{J_{m-p}(kd/2)}{D_p} + (-1)^p \frac{J_{m+p}(kd/2)}{D_p} \right]. \tag{111}$$

Now, we would like to split equation (97) in the four representations A_1, A_2, B_1, B_2. In each representation, the unknown coefficients $\widetilde{X}^{(j)}$ respectively satisfy

$$\tilde{X}{}^{(1)A_1}_{mp} = \tilde{X}{}^{(2)A_1}_{mp} \qquad \text{and} \qquad \tilde{X}{}^{(i)A_1}_{m-p} = \tilde{X}{}^{(i)A_1}_{mp} \tag{112}$$

$$\tilde{X}{}^{(1)A_2}_{mp} = \tilde{X}{}^{(2)A_2}_{mp} \qquad \text{and} \qquad \tilde{X}{}^{(i)A_2}_{m-p} = -\tilde{X}{}^{(i)A_2}_{mp} \tag{113}$$

$$\tilde{X}{}^{(1)B_1}_{mp} = -\tilde{X}{}^{(2)B_1}_{mp} \qquad \text{and} \qquad \tilde{X}{}^{(i)B_1}_{m-p} = -\tilde{X}{}^{(i)B_1}_{mp} \tag{114}$$

$$\tilde{X}{}^{(1)B_2}_{mp} = -\tilde{X}{}^{(2)B_2}_{mp} \qquad \text{and} \qquad \tilde{X}{}^{(i)B_2}_{m-p} = \tilde{X}{}^{(i)B_2}_{mp}. \tag{115}$$

We finally deduce

$$C^{(1)A_1}_{mp} = \frac{\pi a}{2\mathrm{i}} \sum_{q=0}^{+\infty} \tilde{X}{}^{(1)A_1}_{mq} \left\{ \delta_{qp} - (-1)^q \frac{\gamma_q}{2} \frac{D^{[1]}_q}{D_p} [H^{(1)}_{q-p}(kd) + (-1)^p H^{(1)}_{q+p}(kd)] \right\} \tag{116}$$

$$C^{(1)A_2}_{mp} = \frac{\pi a}{2\mathrm{i}} \sum_{q=1}^{+\infty} \tilde{X}{}^{(1)A_2}_{mq} \left\{ \delta_{qp} - (-1)^q \frac{D^{[1]}_q}{D_p} [H^{(1)}_{q-p}(kd) - (-1)^p H^{(1)}_{q+p}(kd)] \right\} \tag{117}$$

$$C^{(1)B_1}_{mp} = \frac{\pi a}{2\mathrm{i}} \sum_{q=1}^{+\infty} \tilde{X}{}^{(1)B_1}_{mq} \left\{ \delta_{qp} + (-1)^q \frac{D^{[1]}_q}{D_p} [H^{(1)}_{q-p}(kd) - (-1)^p H^{(1)}_{q+p}(kd)] \right\} \tag{118}$$

$$C^{(1)B_2}_{mp} = \frac{\pi a}{2\mathrm{i}} \sum_{q=0}^{+\infty} \tilde{X}{}^{(1)B_2}_{mq} \left\{ \delta_{qp} + (-1)^q \frac{\gamma_q}{2} \frac{D^{[1]}_q}{D_p} [H^{(1)}_{q-p}(kd) + (-1)^p H^{(1)}_{q+p}(kd)] \right\}. \tag{119}$$

Similarly, from the asymptotic behaviour of ϕ_m in the different representations and from the properties (112)–(115) of the unknown coefficients $\widetilde{X}^{(j)}$, we determine the expression of the S-matrix in each representation. By combining all those results, we obtain

$$S_{mp} = \delta_{mp} + \mathrm{i}\pi a(\mathrm{i}^p + \mathrm{i}^{-p}) \sum_{q=0}^{+\infty} \frac{\gamma_q}{2} \tilde{X}{}^{(1)A_1}_{mq} D^{[1]}_q \left[J_{p-q}\left(\frac{kd}{2}\right) + (-1)^q J_{p+q}\left(\frac{kd}{2}\right) \right]$$
$$+\mathrm{i}\pi a(\mathrm{i}^p + \mathrm{i}^{-p}) \sum_{q=1}^{+\infty} \tilde{X}{}^{(1)A_2}_{mq} D^{[1]}_q \left[J_{p-q}\left(\frac{k\mathrm{d}}{2}\right) - (-1)^q J_{p+q}\left(\frac{kd}{2}\right) \right]$$

Table 2. Character table of $\mathcal{C}_{3v}$.

$\mathcal{C}_{3v}$:	$E(1)$	$C_3, C_3^2(2)$	$\sigma_x, \sigma_u, \sigma_v(3)$
A_1	1	1	1
A_2	1	1	−1
E	2	−1	0

$$+\mathrm{i}\pi a(\mathrm{i}^p - \mathrm{i}^{-p}) \sum_{q=1}^{+\infty} \tilde{X}{}_{mq}^{(1)B_1} D_q^{[1]} \left[J_{p-q}\left(\frac{kd}{2}\right) - (-1)^q J_{p+q}\left(\frac{kd}{2}\right) \right]$$
$$+\mathrm{i}\pi a(\mathrm{i}^p - \mathrm{i}^{-p}) \sum_{q=0}^{+\infty} \frac{\gamma_q}{2} \tilde{X}{}_{mq}^{(1)B_2} D_q^{[1]} \left[J_{p-q}\left(\frac{kd}{2}\right) + (-1)^q J_{p+q}\left(\frac{kd}{2}\right) \right]. \quad (120)$$

4.3. Symmetry $\mathcal{C}_{3v}$

The symmetry group $\mathcal{C}_{3v}$ is a non-Abelian group of order $g = 6$. Its elements are E, C_3, C_3^2, σ_x, σ_u and σ_v. E denotes the identity transformation, C_3 the rotation through $2\pi/3$ about the main axis Oz of figure 7(b), C_3^2 the rotation through $4\pi/3$ about the same axis, σ_x, σ_u and σ_v the mirror reflections respectively in the planes Oxz, Ouz and Ovz. Three irreducible representations labelled by A_1, A_2, E are associated with this symmetry group. A_1 and A_2 are one-dimensional, while E is two-dimensional. Table 2 is the corresponding character table.

Table 2 permits us to split up any function f given by

$$f = \sum_{p=-\infty}^{+\infty} f_p \mathrm{e}^{\mathrm{i}p\theta} \quad (121)$$

as a sum of functions belonging to the three irreducible representations of $\mathcal{C}_{3v}$

$$f = f^{A_1} + f^{A_2} + f^{E}. \quad (122)$$

We have

$$f^{A_1} = \tfrac{1}{6} \sum_{p=-\infty}^{+\infty} [1 + \epsilon^p + \epsilon^{2p}](f_p + f_{-p})\mathrm{e}^{\mathrm{i}p\theta} \quad (123)$$

$$f^{A_2} = \tfrac{1}{6} \sum_{p=-\infty}^{+\infty} [1 + \epsilon^p + \epsilon^{2p}](f_p - f_{-p})\mathrm{e}^{\mathrm{i}p\theta} \quad (124)$$

$$f^{E_{(1)}} = \tfrac{1}{3} \sum_{p=-\infty}^{+\infty} [1 + \epsilon^{p+1} + \epsilon^{2(p+1)}] f_p \mathrm{e}^{\mathrm{i}p\theta} \quad (125)$$

$$f^{E_{(2)}} = \tfrac{1}{3} \sum_{p=-\infty}^{+\infty} [1 + \epsilon^{p-1} + \epsilon^{2(p-1)}] f_p \mathrm{e}^{\mathrm{i}p\theta} \quad (126)$$

where $\epsilon = \mathrm{e}^{\mathrm{i}2\pi/3}$. Here $f^{E_{(1)}}$ and $f^{E_{(2)}}$ denote the two components of f^E.

After calculations similar to those performed for the symmetry group $\mathcal{C}_{2v}$, we obtain the S-matrix in the form

$$S_{mp} = \delta_{mp} + \mathrm{i}\pi a(1 + \epsilon^p + \epsilon^{2p}) \sum_{q=0}^{+\infty} \frac{\gamma_q}{2} \tilde{X}{}_{mq}^{(1)A_1} D_q^{[1]} \left[J_{p-q}\left(\frac{kd}{\sqrt{3}}\right) + (-1)^q J_{p+q}\left(\frac{kd}{\sqrt{3}}\right) \right]$$

$$+\mathrm{i}\pi a(1+\epsilon^{p}+\epsilon^{2p})\sum_{q=1}^{+\infty}\overset{\sim(1)A_2}{X}_{mq}D_q^{[1]}\left[J_{p-q}\left(\frac{kd}{\sqrt{3}}\right)-(-1)^{q}J_{p+q}\left(\frac{kd}{\sqrt{3}}\right)\right]$$
$$+\mathrm{i}\pi a\sum_{q=-\infty}^{+\infty}\{(1+\epsilon^{p-1}+\epsilon^{2(p-1)})\overset{\sim(1)E_{(1)}}{X}_{mq}$$
$$+(1+\epsilon^{p+1}+\epsilon^{2(p+1)})\overset{\sim(1)E_{(2)}}{X}_{mq}\}D_q^{[1]}J_{p-q}\left(\frac{kd}{\sqrt{3}}\right) \tag{127}$$

with the coefficients $\widetilde{X}$ satisfying the following properties

$$\overset{\sim(1)A_1}{X}_{mp}=\overset{\sim(2)A_1}{X}_{mp}=\overset{\sim(3)A_1}{X}_{mp}\qquad\text{and}\qquad\overset{\sim(i)A_1}{X}_{m-p}=\overset{\sim(i)A_1}{X}_{mp} \tag{128}$$
$$\overset{\sim(1)A_2}{X}_{mp}=\overset{\sim(2)A_2}{X}_{mp}=\overset{\sim(3)A_2}{X}_{mp}\qquad\text{and}\qquad\overset{\sim(i)A_2}{X}_{m-p}=-\overset{\sim(i)A_2}{X}_{mp} \tag{129}$$
$$\overset{\sim(2)E_{(1)}}{X}_{mp}=\epsilon\overset{\sim(1)E_{(1)}}{X}_{mp}\qquad\text{and}\qquad\overset{\sim(3)E_{(1)}}{X}_{mp}=\epsilon^{2}\overset{\sim(1)E_{(1)}}{X}_{mp} \tag{130}$$
$$\overset{\sim(2)E_{(2)}}{X}_{mp}=\epsilon^{2}\overset{\sim(1)E_{(2)}}{X}_{mp}\qquad\text{and}\qquad\overset{\sim(3)E_{(2)}}{X}_{mp}=\epsilon\overset{\sim(1)E_{(2)}}{X}_{mp} \tag{131}$$

and solving the following system

$$C_{mp}^{(1)A_1}=\frac{\pi a}{2\mathrm{i}}\sum_{q=0}^{+\infty}\overset{\sim(1)A_1}{X}_{mq}\left\{\delta_{qp}-\gamma_q\frac{D_q^{[1]}}{D_p}\left[H_{q-p}^{(1)}(kd)\cos\frac{\pi}{6}(p-5q)\right.\right.$$
$$\left.\left.+(-1)^{p}H_{q+p}^{(1)}(kd)\cos\frac{\pi}{6}(p+5q)\right]\right\} \tag{132}$$
$$C_{mp}^{(1)A_2}=\frac{\pi a}{2\mathrm{i}}\sum_{q=1}^{+\infty}\overset{\sim(1)A_2}{X}_{mq}\left\{\delta_{qp}-2\frac{D_q^{[1]}}{D_p}\left[H_{q-p}^{(1)}(kd)\cos\frac{\pi}{6}(p-5q)\right.\right.$$
$$\left.\left.-(-1)^{p}H_{q+p}^{(1)}(kd)\cos\frac{\pi}{6}(p+5q)\right]\right\} \tag{133}$$
$$C_{mp}^{(1)E_{(1)}}=\frac{\pi a}{2\mathrm{i}}\sum_{q=-\infty}^{+\infty}\overset{\sim(1)E_{(1)}}{X}_{mq}\left\{\delta_{qp}-2\frac{D_q^{[1]}}{D_p}H_{q-p}^{(1)}(kd)\cos\frac{\pi}{6}(p-5q+4)\right\} \tag{134}$$
$$C_{mp}^{(1)E_{(2)}}=\frac{\pi a}{2\mathrm{i}}\sum_{q=-\infty}^{+\infty}\overset{\sim(1)E_{(2)}}{X}_{mq}\left\{\delta_{qp}-2\frac{D_q^{[1]}}{D_p}H_{q-p}^{(1)}(kd)\cos\frac{\pi}{6}(p-5q-4)\right\} \tag{135}$$

where

$$C_{mp}^{(1)A_1}=-\frac{1+\epsilon^{m}+\epsilon^{2m}}{6}\left[\frac{J_{m-p}(kd/\sqrt{3})}{D_p}+(-1)^{p}\frac{J_{m+p}(kd/\sqrt{3})}{D_p}\right] \tag{136}$$
$$C_{mp}^{(1)A_2}=-\frac{1+\epsilon^{m}+\epsilon^{2m}}{6}\left[\frac{J_{m-p}(kd/\sqrt{3})}{D_p}-(-1)^{p}\frac{J_{m+p}(kd/\sqrt{3})}{D_p}\right] \tag{137}$$
$$C_{mp}^{(1)E_{(1)}}=-\frac{1+\epsilon^{m+1}+\epsilon^{2(m+1)}}{3}\left[\frac{J_{m-p}(kd/\sqrt{3})}{D_p}\right] \tag{138}$$
$$C_{mp}^{(1)E_{(2)}}=-\frac{1+\epsilon^{m-1}+\epsilon^{2(m-1)}}{3}\left[\frac{J_{m-p}(kd/\sqrt{3})}{D_p}\right]. \tag{139}$$

Table 3. Character table of $\mathcal{C}_{4v}$.

$\mathcal{C}_{4v}$:	$E(1)$	$C_4^2(1)$	$C_4, C_4^3(2)$	$\sigma_x, \sigma_y(2)$	$\sigma_u, \sigma_v(2)$
A_1	1	1	1	1	1
A_2	1	1	1	−1	−1
B_1	1	1	−1	1	−1
B_2	1	1	−1	−1	1
E	2	−2	0	0	0

4.4. Symmetry $\mathcal{C}_{4v}$

The symmetry group $\mathcal{C}_{4v}$ is a non-Abelian group of order $g = 8$. Its elements are E, C_4, C_2, C_4^3, σ_x, σ_y, σ_u and σ_v. E denotes the identity transformation, C_4 denotes the operation of rotation through $\pi/2$ about the main axis Oz of the figure 7(c), C_4^3 the rotation through $3\pi/2$ about the same axis, σ_x, σ_y, σ_u and σ_v the mirror reflections respectively in the planes Oxz, Oyz, Ouz, and Ovz. Five irreducible representations labelled by A_1, A_2, B_1, B_2 and E are associated with this symmetry group. A_1, A_2, B_1 and B_2 are one-dimensional, while E is two-dimensional. Table 3 is the corresponding character table.

Table 3 permits us to split up any function f given by

$$f = \sum_{p=-\infty}^{+\infty} f_p \mathrm{e}^{\mathrm{i}p\theta} \tag{140}$$

as a sum of functions belonging to the five irreducible representations of $\mathcal{C}_{4v}$

$$f = f^{A_1} + f^{A_2} + f^{B_1} + f^{B_2} + f^{E}. \tag{141}$$

We have

$$f^{A_1} = \tfrac{1}{8} \sum_{p=-\infty}^{+\infty} [1 + (-1)^p + \mathrm{i}^p + \mathrm{i}^{-p}](f_p + f_{-p})\mathrm{e}^{\mathrm{i}p\theta} \tag{142}$$

$$f^{A_2} = \tfrac{1}{8} \sum_{p=-\infty}^{+\infty} [1 + (-1)^p + \mathrm{i}^p + \mathrm{i}^{-p}](f_p - f_{-p})\mathrm{e}^{\mathrm{i}p\theta} \tag{143}$$

$$f^{B_1} = \tfrac{1}{8} \sum_{p=-\infty+}^{+\infty} [1 - (-1)^p - \mathrm{i}^p - \mathrm{i}^{-p}](f_p + f_{-p})\mathrm{e}^{\mathrm{i}p\theta} \tag{144}$$

$$f^{B_2} = \tfrac{1}{8} \sum_{p=-\infty}^{+\infty} [1 - (-1)^p - \mathrm{i}^p - \mathrm{i}^{-p}](f_p - f_{-p})\mathrm{e}^{\mathrm{i}p\theta} \tag{145}$$

$$f^{E_{(1)}} = \tfrac{1}{4} \sum_{p=-\infty}^{+\infty} [1 - (-1)^p + \mathrm{i}^{p+1} - \mathrm{i}^{-p+1}] f_p \mathrm{e}^{\mathrm{i}p\theta} \tag{146}$$

$$f^{E_{(2)}} = \tfrac{1}{4} \sum_{p=-\infty}^{+\infty} [1 - (-1)^p - \mathrm{i}^{p+1} + \mathrm{i}^{-p+1}] f_p \mathrm{e}^{\mathrm{i}p\theta}. \tag{147}$$

Here $f^{E_{(1)}}$ and $f^{E_{(2)}}$ denote the two components of f^E.

After tedious calculations similar to those done for the symmetries $\mathcal{C}_{2v}$ and $\mathcal{C}_{3v}$, we obtain the S-matrix in the form

$$S_{mp} = \delta_{mp} + \mathrm{i}\pi a(\eta^p + \eta^{3p} + \eta^{5p} + \eta^{7p}) \sum_{q=0}^{+\infty} \frac{\gamma_q}{2} \tilde{X}_{mq}^{(1)A_1} D_q^{[1]}$$

$$
\begin{aligned}
&\times\left[J_{p-q}\left(\frac{kd}{\sqrt{2}}\right)+(-1)^q J_{p+q}\left(\frac{kd}{\sqrt{2}}\right)\right]+\mathrm{i}\pi a(\eta^p+\eta^{3p}+\eta^{5p}+\eta^{7p})\\
&\times\sum_{q=1}^{+\infty}\tilde{X}{}^{(1)A_2}_{mq} D_q^{[1]}\left[J_{p-q}\left(\frac{kd}{\sqrt{2}}\right)-(-1)^q J_{p+q}\left(\frac{kd}{\sqrt{2}}\right)\right]\\
&+\mathrm{i}\pi a(-\eta^p+\eta^{3p}-\eta^{5p}+\eta^{7p})\\
&\times\sum_{q=1}^{+\infty}\tilde{X}{}^{(1)B_1}_{mq} D_q^{[1]}\left[J_{p-q}\left(\frac{kd}{\sqrt{2}}\right)-(-1)^q J_{p+q}\left(\frac{kd}{\sqrt{2}}\right)\right]\\
&+\mathrm{i}\pi a(-\eta^p+\eta^{3p}-\eta^{5p}+\eta^{7p})\\
&\times\sum_{q=0}^{+\infty}\frac{\gamma_q}{2}\tilde{X}{}^{(1)B_2}_{mq} D_q^{[1]}\left[J_{p-q}\left(\frac{kd}{\sqrt{2}}\right)+(-1)^q J_{p+q}\left(\frac{kd}{\sqrt{2}}\right)\right]\\
&+\mathrm{i}\pi a(-\eta^p+\eta^{3p+2}+\eta^{5p}-\eta^{7p+2})\sum_{q=-\infty}^{+\infty}\tilde{X}{}^{(1)E_{(1)}}_{mq} D_q^{[1]} J_{p-q}\left(\frac{kd}{\sqrt{2}}\right)\\
&+\mathrm{i}\pi a(-\eta^p-\eta^{3p+2}+\eta^{5p}+\eta^{7p+2})\sum_{q=-\infty}^{+\infty}\tilde{X}{}^{(1)E_{(2)}}_{mq} D_q^{[1]} J_{p-q}\left(\frac{kd}{\sqrt{2}}\right)
\end{aligned}
\tag{148}
$$

where $\eta=\mathrm{e}^{\mathrm{i}\pi/4}$. The coefficients $\widetilde{X}$ satisfy the following properties

$$\tilde{X}{}^{(1)A_1}_{mp}=\tilde{X}{}^{(2)A_1}_{mp}=\tilde{X}{}^{(3)A_1}_{mp}=\tilde{X}{}^{(4)A_1}_{mp}\quad\text{and}\quad\tilde{X}{}^{(i)A_1}_{m-p}=\tilde{X}{}^{(i)A_1}_{mp}\tag{149}$$

$$\tilde{X}{}^{(1)A_2}_{mp}=\tilde{X}{}^{(2)A_2}_{mp}=\tilde{X}{}^{(3)A_2}_{mp}=\tilde{X}{}^{(4)A_2}_{mp}\quad\text{and}\quad\tilde{X}{}^{(i)A_2}_{m-p}=-\tilde{X}{}^{(i)A_2}_{mp}\tag{150}$$

$$\tilde{X}{}^{(1)B_1}_{mp}=-\tilde{X}{}^{(2)B_1}_{mp}=\tilde{X}{}^{(3)B_1}_{mp}=-\tilde{X}{}^{(4)B_1}_{mp}\quad\text{and}\quad\tilde{X}{}^{(i)B_1}_{m-p}=-\tilde{X}{}^{(i)B_1}_{mp}\tag{151}$$

$$\tilde{X}{}^{(1)B_2}_{mp}=-\tilde{X}{}^{(2)B_2}_{mp}=\tilde{X}{}^{(3)B_2}_{mp}=-\tilde{X}{}^{(4)B_2}_{mp}\quad\text{and}\quad\tilde{X}{}^{(i)B_2}_{m-p}=\tilde{X}{}^{(i)B_2}_{mp}\tag{152}$$

$$\tilde{X}{}^{(2)E_{(1)}}_{mp}=\eta^2\tilde{X}{}^{(1)E_{(1)}}_{mp}\qquad\tilde{X}{}^{(3)E_{(1)}}_{mp}=\eta^4\tilde{X}{}^{(1)E_{(1)}}_{mp}\quad\text{and}\quad\tilde{X}{}^{(4)E_{(1)}}_{mp}=\eta^6\tilde{X}{}^{(1)E_{(1)}}_{mp}\tag{153}$$

$$\tilde{X}{}^{(2)E_{(2)}}_{mp}=\eta^6\tilde{X}{}^{(1)E_{(2)}}_{mp}\qquad\tilde{X}{}^{(3)E_{(2)}}_{mp}=\eta^4\tilde{X}{}^{(1)E_{(2)}}_{mp}\quad\text{and}\quad\tilde{X}{}^{(4)E_{(2)}}_{mp}=\eta^2\tilde{X}{}^{(1)E_{(2)}}_{mp}\tag{154}$$

and solve the following system

$$
\begin{aligned}
C^{(1)A_1}_{mp}=\frac{\pi a}{2\mathrm{i}}\sum_{q=0}^{+\infty}\tilde{X}{}^{(1)A_1}_{mq}\Bigg\{&\delta_{qp}-\frac{\gamma_q}{2}\frac{D_q^{[1]}}{D_p}\Bigg[(-1)^q[H^{(1)}_{q-p}(\sqrt{2}kd)+(-1)^p H^{(1)}_{q+p}(\sqrt{2}kd)]\\
&+2\left(H^{(1)}_{q-p}(kd)\cos\frac{\pi}{4}(3q-p)+(-1)^p H^{(1)}_{q+p}(kd)\cos\frac{\pi}{4}(3q+p)\right)\Bigg]\Bigg\}
\end{aligned}
\tag{155}
$$

$$
\begin{aligned}
C^{(1)A_2}_{mp}=\frac{\pi a}{2\mathrm{i}}\sum_{q=1}^{+\infty}\tilde{X}{}^{(1)A_2}_{mq}\Bigg\{&\delta_{qp}-\frac{D_q^{[1]}}{D_p}\Bigg[(-1)^q\left[H^{(1)}_{q-p}(\sqrt{2}kd)-(-1)^p H^{(1)}_{q+p}(\sqrt{2}kd)\right]\\
&+2\left(H^{(1)}_{q-p}(kd)\cos\frac{\pi}{4}(3q-p)-(-1)^p H^{(1)}_{q+p}(kd)\cos\frac{\pi}{4}(3q+p)\right)\Bigg]\Bigg\}
\end{aligned}
\tag{156}
$$

$$
\begin{aligned}
C^{(1)B_1}_{mp}=\frac{\pi a}{2\mathrm{i}}\sum_{q=1}^{+\infty}\tilde{X}{}^{(1)B_1}_{mq}\Bigg\{&\delta_{qp}+\frac{D_q^{[1]}}{D_p}\Bigg[-(-1)^q\left[H^{(1)}_{q-p}(\sqrt{2}kd)-(-1)^p H^{(1)}_{q+p}(\sqrt{2}kd)\right]\\
&+2\left(H^{(1)}_{q-p}(kd)\cos\frac{\pi}{4}(3q-p)-(-1)^p H^{(1)}_{q+p}(kd)\cos\frac{\pi}{4}(3q+p)\right)\Bigg]\Bigg\}
\end{aligned}
\tag{157}
$$

$$C_{mp}^{(1)B_2} = \frac{\pi a}{2\mathrm{i}} \sum_{q=0}^{+\infty} \tilde{X}{}_{mq}^{(1)B_2} \left\{ \delta_{qp} + \frac{\gamma_q}{2} \frac{D_q^{[1]}}{D_p} \left[-(-1)^q \left[H_{q-p}^{(1)}(\sqrt{2}kd) + (-1)^p H_{q+p}^{(1)}(\sqrt{2}kd) \right] \right.\right.$$
$$\left.\left. +2\left(H_{q-p}^{(1)}(kd)\cos\frac{\pi}{4}(3q-p) + (-1)^p H_{q+p}^{(1)}(kd)\cos\frac{\pi}{4}(3q+p)\right)\right]\right\} \tag{158}$$

$$C_{mp}^{(1)E_{(1)}} = \frac{\pi a}{2\mathrm{i}} \sum_{q=-\infty}^{+\infty} \tilde{X}{}_{mq}^{(1)E_{(1)}}$$
$$\times \left\{ \delta_{qp} + \frac{D_q^{[1]}}{D_p} \left[(-1)^q H_{q-p}^{(1)}(\sqrt{2}kd) - 2\sin\frac{\pi}{4}(3q-p) H_{q-p}^{(1)}(kd) \right] \right\} \tag{159}$$

$$C_{mp}^{(1)E_{(2)}} = \frac{\pi a}{2\mathrm{i}} \sum_{q=-\infty}^{+\infty} \tilde{X}{}_{mq}^{(1)E_{(2)}}$$
$$\times \left\{ \delta_{qp} - \frac{D_q^{[1]}}{D_p} \left[(-1)^q H_{q-p}^{(1)}(\sqrt{2}kd) - 2\sin\frac{\pi}{4}(3q-p) H_{q-p}^{(1)}(kd) \right] \right\} \tag{160}$$

where

$$C_{mp}^{(1)A_1} = -\frac{\eta^m + \eta^{3m} + \eta^{5m} + \eta^{7m}}{8} \left[\frac{J_{m-p}(kd/\sqrt{2})}{D_p} + (-1)^p \frac{J_{m+p}(kd/\sqrt{2})}{D_p} \right] \tag{161}$$

$$C_{mp}^{(1)A_2} = -\frac{\eta^m + \eta^{3m} + \eta^{5m} + \eta^{7m}}{8} \left[\frac{J_{m-p}(kd/\sqrt{2})}{D_p} - (-1)^p \frac{J_{m+p}(kd/\sqrt{2})}{D_p} \right] \tag{162}$$

$$C_{mp}^{(1)B_1} = -\frac{\eta^m - \eta^{3m} + \eta^{5m} - \eta^{7m}}{8} \left[\frac{J_{m-p}(kd/\sqrt{2})}{D_p} - (-1)^p \frac{J_{m+p}(kd/\sqrt{2})}{D_p} \right] \tag{163}$$

$$C_{mp}^{(1)B_2} = -\frac{\eta^m - \eta^{3m} + \eta^{5m} - \eta^{7m}}{8} \left[\frac{J_{m-p}(kd/2)}{D_p} + (-1)^p \frac{J_{m+p}(kd/2)}{D_p} \right] \tag{164}$$

$$C_{mp}^{(1)E_{(1)}} = -\frac{\eta^m + \eta^{3m+2} - \eta^{5m} - \eta^{7m+2}}{4} \left[\frac{J_{m-p}(kd/\sqrt{2})}{D_p} \right] \tag{165}$$

$$C_{mp}^{(1)E_{(2)}} = -\frac{\eta^m - \eta^{3m+2} - \eta^{5m} + \eta^{7m+2}}{4} \left[\frac{J_{m-p}(kd/\sqrt{2})}{D_p} \right]. \tag{166}$$

5. Conclusion and perspectives

In this paper, we have developed an exact formalism to calculate the S-matrix valid for various realistic problems of physics. Since the N-disc system is one of the paradigmatic models in the field of chaotic scattering, we hope that the present work will be useful in this context. In the second part of this work [25], we shall complete our study by emphasizing the physical aspects linked to the scattering resonances of the two- and three-disc systems.

6. Appendix. Unitarity and reciprocity of the S-matrix

In this short appendix, the properties of the S-matrix (unitarity and reciprocity [26]) are linked to the properties of the coefficients defining the partial waves and their gradients on the boundaries of the discs. Unitarity is associated with energy conservation in acoustics and electromagnetism, and with particle number conservation in quantum mechanics.

Reciprocity is associated with time-reversal invariance in acoustics, electromagnetism, as well as in quantum mechanics.

Green's theorem (equation (7)) considered for $g = \phi_{m_1}$ and $f = \phi^*_{m_2}$ reads

$$0 = \int_{\partial D_\infty} \mathrm{d}\boldsymbol{S}_{\boldsymbol{x}} \cdot [\phi_{m_1}(\boldsymbol{x})\boldsymbol{\nabla}_{\boldsymbol{x}}\phi^*_{m_2}(\boldsymbol{x}) - \phi^*_{m_2}(\boldsymbol{x})\boldsymbol{\nabla}_{\boldsymbol{x}}\phi_{m_1}(\boldsymbol{x})] + \sum_{i=1}^{N}\int_{\partial D_i} \mathrm{d}\boldsymbol{S}_{\boldsymbol{x}} \cdot [\phi_{m_1}(\boldsymbol{x})\boldsymbol{\nabla}_{\boldsymbol{x}}\phi^*_{m_2}(\boldsymbol{x}) - \phi^*_{m_2}(\boldsymbol{x})\boldsymbol{\nabla}_{\boldsymbol{x}}\phi_{m_1}(\boldsymbol{x})] \tag{A.1}$$

since ϕ_{m_1} and $\phi^*_{m_2}$ are solutions of the Helmholtz equation. From the asymptotic behaviour of the partial waves (equation (4)), we easily find the integral over ∂D_∞

$$\int_{\partial D_\infty} \mathrm{d}\boldsymbol{S}_{\boldsymbol{x}} \cdot [\phi_{m_1}(\boldsymbol{x})\boldsymbol{\nabla}_{\boldsymbol{x}}\phi^*_{m_2}(\boldsymbol{x}) - \phi^*_{m_2}(\boldsymbol{x})\boldsymbol{\nabla}_{\boldsymbol{x}}\phi_{m_1}(\boldsymbol{x})] = 2\mathrm{i}\left[\delta_{m_1m_2} - \sum_{p=-\infty}^{+\infty} S_{m_1p}S^*_{m_2p}\right]. \tag{A.2}$$

From the general boundary conditions given by equations (2) and (3), we obtain for the integral over ∂D_i

$$\int_{\partial D_i} \mathrm{d}\boldsymbol{S}_{\boldsymbol{x}} \cdot [\phi_{m_1}(\boldsymbol{x})\boldsymbol{\nabla}_{\boldsymbol{x}}\phi^*_{m_2}(\boldsymbol{x}) - \phi^*_{m_2}(\boldsymbol{x})\boldsymbol{\nabla}_{\boldsymbol{x}}\phi_{m_1}(\boldsymbol{x})] = 2\pi a \sum_{p=-\infty}^{+\infty} [A^{(i)}_{m_1p}B^{(i)*}_{m_2p} - A^{(i)*}_{m_2p}B^{(i)}_{m_1p}]. \tag{A.3}$$

Therefore, we finally find that

$$\sum_{p=-\infty}^{+\infty} S_{m_1p}S^*_{m_2p} = \delta_{m_1m_2} - \mathrm{i}\pi a \sum_{i=1}^{N}\sum_{p=-\infty}^{+\infty} [A^{(i)}_{m_1p}B^{(i)*}_{m_2p} - A^{(i)*}_{m_2p}B^{(i)}_{m_1p}] \tag{A.4}$$

which can be written in matrix notation

$$SS^\dagger = I - \mathrm{i}\pi a \sum_{i=1}^{N}[A^{(i)}B^{\dagger(i)} - B^{(i)}A^{\dagger(i)}]. \tag{A.5}$$

So, under the condition

$$\sum_{i=1}^{N}[A^{(i)}B^{\dagger(i)} - B^{(i)}A^{\dagger(i)}] = 0 \tag{A.6}$$

the S-matrix is unitary. It should be noted that such a condition is not always satisfied for the boundary conditions examined in section 3. For example in electromagnetism, for metallic conductors with a given constant impedance Z, energy conservation is not satisfied because of the Joule effect, so that S is not unitary.

Green's theorem (equation (7)) considered for $g = \phi_{m_1}$ and $f = \phi_{m_2}$ reads

$$0 = \int_{\partial D_\infty} \mathrm{d}\boldsymbol{S}_{\boldsymbol{x}} \cdot [\phi_{m_1}(\boldsymbol{x})\boldsymbol{\nabla}_{\boldsymbol{x}}\phi_{m_2}(\boldsymbol{x}) - \phi_{m_2}(\boldsymbol{x})\boldsymbol{\nabla}_{\boldsymbol{x}}\phi_{m_1}(\boldsymbol{x})] + \sum_{i=1}^{N}\int_{\partial D_i} \mathrm{d}\boldsymbol{S}_{\boldsymbol{x}} \cdot [\phi_{m_1}(\boldsymbol{x})\boldsymbol{\nabla}_{\boldsymbol{x}}\phi_{m_2}(\boldsymbol{x}) - \phi_{m_2}(\boldsymbol{x})\boldsymbol{\nabla}_{\boldsymbol{x}}\phi_{m_1}(\boldsymbol{x})]. \tag{A.7}$$

From the asymptotic behaviour of the partial waves (equation (4)), we easily find the integral over ∂D_∞

$$\int_{\partial D_\infty} \mathrm{d}\boldsymbol{S}_{\boldsymbol{x}} \cdot \left[\phi_{m_1}(\boldsymbol{x})\boldsymbol{\nabla}_{\boldsymbol{x}}\phi_{m_2}(\boldsymbol{x}') - \phi_{m_2}(\boldsymbol{x})\boldsymbol{\nabla}_{\boldsymbol{x}}\phi_{m_1}(\boldsymbol{x})\right] = 2\mathrm{i}\left[(-1)^{m_1}S_{m_2-m_1} - (-1)^{m_2}S_{m_1-m_2}\right]. \tag{A.8}$$

From the general boundary conditions given by equations (2) and (3), we obtain for the integral over ∂D_i

$$\int_{\partial D_i} \mathrm{d}\boldsymbol{S_x} \cdot [\phi_{m_1}(\boldsymbol{x})\boldsymbol{\nabla_x}\phi^*_{m_2}(\boldsymbol{x}') - \phi^*_{m_2}(\boldsymbol{x})\boldsymbol{\nabla_x}\phi_{m_1}(\boldsymbol{x})]$$
$$= 2\pi a \sum_{p=-\infty}^{+\infty} [A^{(i)}_{m_1 p} B^{(i)}_{m_2-p} - A^{(i)}_{m_2 p} B^{(i)}_{m_1-p}]. \qquad \text{(A.9)}$$

We finally find that

$$S_{m_1-m_2} = (-1)^{m_1+m_2} S_{m_2-m_1} - \mathrm{i}\pi a \sum_{i=1}^{N} \sum_{p=-\infty}^{+\infty} (-1)^{m_2} [A^{(i)}_{m_1 p} B^{(i)}_{m_2-p} - A^{(i)}_{m_2 p} B^{(i)}_{m_1-p}]. \qquad \text{(A.10)}$$

So, under the condition

$$\sum_{i=1}^{N} \sum_{p=-\infty}^{+\infty} (-1)^{m_2} [A^{(i)}_{m_1 p} B^{(i)}_{m_2-p} - A^{(i)}_{m_2 p} B^{(i)}_{m_1-p}] = 0 \qquad \text{(A.11)}$$

the S-matrix satisfies the reciprocity property

$$S_{m_1-m_2} = (-1)^{m_1+m_2} S_{m_2-m_1}. \qquad \text{(A.12)}$$

It should be noted that such a property is not always satisfied for the boundary conditions examined in section 3. Indeed, if the scatterer is absorptive, there is no time-reversal invariance.

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