# The Invariant Imbedding T Matrix Approach

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**Abstract** The theoretical foundation of the invariant imbedding **T**-matrix method is revised. We present a consistent analysis of the method, show the connection with the superposition **T**-matrix method, and derive new recurrence relations for **T**-matrix calculation. The first recurrence is a numerical method for integrating the Riccati equations by using the Pade approximation to the matrix exponential, while the second one relies on an integral-matrix approach.

## 2.1 Introduction

At the present time, the invariant imbedding **T**-matrix method seems to be the most efficient tool for analyzing the electromagnetic scattering by large and highly aspherical particles. The method initially proposed by Johnson [4], is based on an electromagnetic volume integral equation in spherical coordinates and iteratively computes the **T** matrix along the radial coordinate. To initialize the iterative procedure, the separation of variables method [1] or the null-field method [2] are used. In the first case, the initial **T** matrix corresponds to a sphere enclosed in the particle, while in the second case, the initial **T** matrix corresponds to a partial volume of the particle generated by the intersection between a sphere and the particle. Because the size parameter of the partial volume of the particle is larger than the size parameter of the sphere enclosed in the particle, the second combined approach is more efficient than the first one. As the volume integral equation is a Fredholm integral equation of the second kind, the method does not suffer from ill-posedness, and its performances are really remarkable. Excellent numerical results have been obtained

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variant imbedding **T**-matrix method is not very efficient because a fine discretization along the radial coordinate has to be considered. To increase the numerical efficiency of the method and to reduce the computational burden, (I) the symmetry relations of the **T** matrix, such as, mirror and point-group symmetries have been exploited, and (II) parallelizations of the code based on the Message Passing Interface (MPI) technology and OPENMP have been used [1, 2].

This chapter which is merely of theoretical nature revised the fundamentals of the invariant imbedding **T**-matrix method. Our goal is to present a consistent analysis of the method, and to derive new recurrence relations for **T**-matrix calculation.

## 2.2 Mathematical Foundations

Consider a particle which is entirely contained within a sphere of radius $R$ and interior $D$. Assume that for $\mathbf{r} \in D$, the particle is completely described through the relative refractive index $m_r(\mathbf{r})$, while for $\mathbf{r} \notin D$, we have $m_r(\mathbf{r}) = 1$. The invariant imbedding **T** matrix approach involves the following steps:

1. Derive an ordinary Fredholm integral equation for the radial amplitude vector by making use on a volume integral equation for the electric field and a spherical wave expansion of the free-space dyadic Green's function.
2. Derive a two-terms recurrence relation for the **T** matrix by discretizing the Fredholm integral equation with respect to the radial coordinate and by applying the invariant imbedding procedure to the discretized equation.
3. Derive a matrix Riccati equation for the **T** matrix by passing to the limit $\Delta R \to 0$ in the **T**-matrix recurrence relation, where $\Delta R$ is the radial grid spacing.

In the following we will derive the matrix Riccati equation for the **T** matrix by applying the invariant imbedding procedure on the continuous form of the Fredholm integral equation rather than on its discrete form. We will then derive two new recurrence relations for the **T** matrix, by using a numerical scheme for integrating the matrix Riccati equation and an integral-matrix approach.

### 2.2.1 *The Volume Integral Equation in Spherical Coordinates*

For the assumed geometry, the total field electric field **E** solves the volume integral equation

$$\mathbf{E}(\mathbf{r}) = \mathbf{E}_0(\mathbf{r}) + \int_D \chi(\mathbf{r}')\overline{\mathbf{G}}(\mathbf{r},\mathbf{r}') \cdot \mathbf{E}(\mathbf{r}')\,\mathrm{d}V', \tag{2.1}$$

$$\overline{\mathbf{G}}(\mathbf{r},\mathbf{r}') = \overline{\mathbf{G}}_0(\mathbf{r},\mathbf{r}') - \frac{1}{k_s^2}\delta(\mathbf{r}-\mathbf{r}')\mathbf{e}_r \otimes \mathbf{e}_r, \tag{2.2}$$

where

$$\overline{\mathbf{G}}_0(\mathbf{r},\mathbf{r}') = \frac{\mathrm{j}k_s}{\pi}\sum_\alpha \begin{cases} \mathbf{M}^3_\alpha(k_s\mathbf{r}) \otimes \mathbf{M}^1_{\overline{\alpha}}(k_s\mathbf{r}') \\ +\mathbf{N}^3_\alpha(k_s\mathbf{r}) \otimes \mathbf{N}^1_{\overline{\alpha}}(k_s\mathbf{r}'), & r > r' \\ \mathbf{M}^1_\alpha(k_s\mathbf{r}) \otimes \mathbf{M}^3_{\overline{\alpha}}(k_s\mathbf{r}') \\ +\mathbf{N}^1_\alpha(k_s\mathbf{r}) \otimes \mathbf{N}^3_{\overline{\alpha}}(k_s\mathbf{r}'), & r < r' \end{cases}. \tag{2.3}$$

Here, $\alpha$ is a multiindex incorporating the azimuthal-mode index $m$ and the expansion-order index $n$, i.e., $\alpha = (m, n)$, while $\overline{\alpha} = (-m, n)$. In the following it is convenient to represent the vector $\mathbf{X} = X_r\mathbf{e}_r + X_\theta\mathbf{e}_\theta + X_\varphi\mathbf{e}_\varphi$ by the column vector $\mathscr{X} = [X_r, X_\theta, X_\varphi]^T$. In this context, the column vector representation of the electric field expansion $\mathbf{E}(\mathbf{r}) = \sum_\alpha a_\alpha\mathbf{M}^{1,3}_\alpha(k\mathbf{r}) + b_\alpha\mathbf{N}^{1,3}_\alpha(k\mathbf{r})$ is $\mathscr{E}(\mathbf{r}) = \sum_\alpha \mathbf{Y}_\alpha(\boldsymbol{\Omega})\mathbf{X}^{1,3}_\alpha(r)\mathbf{c}_\alpha$, where $\boldsymbol{\Omega} = (\theta, \varphi)$, $\mathbf{Y}_\alpha$ is a $3 \times 3$ matrix depending on the angular functions, $\mathbf{X}^{1,3}_\alpha$ are $3 \times 2$ matrices depending on the spherical Bessel and Hankel functions, and $\mathbf{c}_\alpha = [a_\alpha, b_\alpha]^T$ is a $2 \times 1$ matrix depending on the expansion coefficients of the electric field. For regular and radiating spherical vector wave functions, we will write $\mathbf{X}^1_\alpha(r) = \mathbf{J}_\alpha(r)$ and $\mathbf{X}^3_\alpha(r) = \mathbf{H}_\alpha(r)$, respectively, where the expressions of $\mathbf{J}_\alpha$, $\mathbf{H}_\alpha$ and $\mathbf{Y}_\alpha$ can be found in [4]. Inserting (2.2) into (2.1) yields the matrix form representation of the volume integral equation

$$\begin{aligned} \overline{\mathscr{E}}(\mathbf{r}) &= \mathscr{E}_0(\mathbf{r}) \\ &+ \sum_\alpha \mathbf{Y}_\alpha(\boldsymbol{\Omega}) \int_V \chi(\mathbf{r}')\mathbf{g}_\alpha(r,r')\mathbf{Y}^T_{\overline{\alpha}}(\boldsymbol{\Omega}')\mathbf{Z}(\mathbf{r}')\overline{\mathscr{E}}(\mathbf{r}')\,\mathrm{d}V', \end{aligned} \tag{2.4}$$

where $\overline{\mathscr{E}}$ is defined by $\mathscr{E}(\mathbf{r}) = \mathbf{Z}(\mathbf{r})\overline{\mathscr{E}}(\mathbf{r})$ with $\mathbf{Z}(\mathbf{r}) = \mathrm{diag}[1/m_r^2(\mathbf{r}), 1, 1]$, $\mathscr{E}_0$ and $\mathscr{E}$ are the column vector representation of $\mathbf{E}_0$ and $\mathbf{E}$, respectively, and $\mathbf{g}_\alpha$ is the $3 \times 3$ radial Green's function matrix given by [4]

$$\mathbf{g}_\alpha(r,r') = \frac{\mathrm{j}k_s}{\pi}\begin{cases} \mathbf{H}_\alpha(r)\mathbf{J}^T_{\overline{\alpha}}(r'), & r > r' \\ \mathbf{J}_\alpha(r)\mathbf{H}^T_{\overline{\alpha}}(r'), & r < r' \end{cases}. \tag{2.5}$$

The column vector representation of the scattered field

$$\mathbf{E}_s(\mathbf{r}) = \int_D \chi(\mathbf{r}')\overline{\mathbf{G}}_0(\mathbf{r},\mathbf{r}') \cdot \mathbf{E}(\mathbf{r}')\,\mathrm{d}V' \tag{2.6}$$

$$\alpha$$

where, for $\mathscr{E}_0(\mathbf{r}) = \sum_\alpha \mathbf{Y}_\alpha(\boldsymbol{\Omega})\mathbf{J}_\alpha(r)\mathbf{c}_{0\alpha}$, the expansion coefficients of the scattered field

$$\mathbf{c}_{s\alpha} = \frac{jk_s}{\pi}\int_D \chi(\mathbf{r})\mathbf{J}_{\bar{\alpha}}^T(r)\mathbf{Y}_{\bar{\alpha}}^T(\boldsymbol{\Omega})\mathbf{Z}(\mathbf{r})\overline{\mathscr{E}}(\mathbf{r})\,dV \tag{2.8}$$

are related to the expansion coefficients of the incident field by the **T**-matrix equation

$$\mathbf{c}_{s\alpha} = \sum_\beta \mathbf{T}_{\alpha\beta}\mathbf{c}_{0\beta}. \tag{2.9}$$

### 2.2.2 *An Ordinary Integral Equation*

The volume integral equation (2.4) can be transformed into an ordinary integral equation for the radial amplitude vector

$$\mathbf{F}_\alpha(r) = r^2\int_\Omega \chi(\mathbf{r})\mathbf{Y}_{\bar{\alpha}}^T(\boldsymbol{\Omega})\mathbf{Z}(\mathbf{r})\overline{\mathscr{E}}(\mathbf{r})\,d\Omega, \tag{2.10}$$

which is the analog of the scalar amplitude density function in the quantum mechanical scattering theory [4]. Inserting (2.4) into (2.10) gives the desired equation

$$\mathbf{F}_\alpha(r) = \sum_\beta \mathbf{U}_{\alpha\beta}(r)\mathbf{J}_\beta(r)\mathbf{c}_{0\beta} + \int_0^R \sum_\beta \mathbf{U}_{\alpha\beta}(r)\mathbf{g}_\beta(r,r')\mathbf{F}_\beta(r')\,dr', \tag{2.11}$$

where the $3\times 3$ matrix $\mathbf{U}_{\alpha\beta}$ is defined by

$$\mathbf{U}_{\alpha\beta}(r) = r^2\int_\Omega \chi(\mathbf{r})\mathbf{Y}_{\bar{\alpha}}^T(\boldsymbol{\Omega})\mathbf{Z}(\mathbf{r})\mathbf{Y}_\beta(\boldsymbol{\Omega})\,d\Omega. \tag{2.12}$$

The scattered field coefficients (2.8) can be also expressed in terms of $\mathbf{F}_\alpha$, and the result is

$$\mathbf{c}_{s\alpha} = \frac{jk_s}{\pi}\int_0^R \mathbf{J}_{\bar{\alpha}}^T(r)\mathbf{F}_\alpha(r)\,dr. \tag{2.13}$$

Now, let the $3\times 2$ matrix $\mathbf{F}_{\alpha\beta}$ be the solution of the integral equation

$$+\int_0^R \sum_\gamma \mathbf{U}_{\alpha\gamma}(r)\mathbf{g}_\gamma(r,r')\mathbf{F}_{\gamma\beta}(r')\,dr'. \tag{2.14}$$

Obviously, $\mathbf{F}_\alpha$ and $\mathbf{F}_{\alpha\beta}$ solve a Fredholm integral equation with the same kernel but with different forcing (matrix) functions. The forcing function of (2.14) is $\mathbf{A}_{\alpha\beta} = \mathbf{U}_{\alpha\beta}\mathbf{J}_\beta$, while the forcing function of (2.11) is $\mathbf{A}_\alpha = \sum_\beta \mathbf{A}_{\alpha\beta}\mathbf{c}_{0\beta}$. Consequently, we have $\mathbf{F}_\alpha(r) = \sum_\beta \mathbf{F}_{\alpha\beta}(r)\mathbf{c}_{0\beta}$, and from (2.13) we obtain

$$\mathbf{c}_{s\alpha} = \frac{jk_s}{\pi}\sum_\beta\left[\int_0^R \mathbf{J}_{\bar{\alpha}}^T(r)\mathbf{F}_{\alpha\beta}(r)\,dr\right]\mathbf{c}_{0\beta}. \tag{2.15}$$

Finally, in view of (2.9) and (2.15), we infer that

$$\mathbf{T}_{\alpha\beta} = \frac{jk_s}{\pi}\int_0^R \mathbf{J}_{\bar{\alpha}}^T(r)\mathbf{F}_{\alpha\beta}(r)\,dr. \tag{2.16}$$

Thus, the computation of the $2\times 2$ block matrix elements of the transition matrix requires first, the solution of the Fredholm integral equation (2.14) for $\mathbf{F}_{\alpha\beta}$, and second, the integration of $\mathbf{F}_{\alpha\beta}$ by using (2.16).

Defining the global matrices (or supermatrices) $\mathbf{U} = [\mathbf{U}_{\alpha\beta}]$, $\mathbf{F} = [\mathbf{F}_{\alpha\beta}]$, $\mathbf{J} = [\mathbf{J}_\alpha\delta_{\alpha\beta}]$, $\mathbf{H} = [\mathbf{H}_\alpha\delta_{\alpha\beta}]$, $\mathbf{g} = [\mathbf{g}_\alpha\delta_{\alpha\beta}]$, and $\mathbf{T} = [\mathbf{T}_{\alpha\beta}]$, we express (2.14), (2.16) and (2.5) as

$$\mathbf{F}(r,R) = \mathbf{U}(r)\mathbf{J}(r) + \int_0^R \mathbf{U}(r)\mathbf{g}(r,r')\mathbf{F}(r')\,dr', \tag{2.17}$$

$$\mathbf{T}(R) = \frac{jk_s}{\pi}\int_0^R \mathbf{J}^T(r)\mathbf{F}(r,R)\,dr, \tag{2.18}$$

and

$$\mathbf{g}(r,r') = \frac{jk_s}{\pi}\begin{cases}\mathbf{H}(r)\mathbf{J}^T(r'), & r > r'\\ \mathbf{J}(r)\mathbf{H}^T(r'), & r < r'\end{cases}, \tag{2.19}$$

respectively, where the transposed matrices $\mathbf{J}^T$ and $\mathbf{H}^T$ should be understood as $\mathbf{J}^T = [\mathbf{J}_{\bar{\alpha}}^T\delta_{\alpha\beta}]$ and $\mathbf{H}^T = [\mathbf{H}_{\bar{\alpha}}^T\delta_{\alpha\beta}]$, respectively.

### 2.2.3 *The Matrix Riccati Equation*

In (2.17) and (2.18) we indicated the dependency of **F** and **T** on the length of the integration interval $R$. The reason is that the Fredholm integral equation (2.17) will

Taking the derivative of (2.17) with respect to $R$, and using $\mathbf{g}(r, R) = (\mathrm{j}k_s/\pi)\mathbf{J}(r)\mathbf{H}^T(R)$ gives

$$\frac{\partial \mathbf{F}}{\partial R}(r, R) = \frac{\mathrm{j}k_s}{\pi}\mathbf{U}(r)\mathbf{J}(r)\mathbf{H}^T(R)\mathbf{F}(R, R) + \int_0^R \mathbf{U}(r)\mathbf{g}(r, r')\frac{\partial \mathbf{F}}{\partial R}(r', R)\,\mathrm{d}r'. \tag{2.20}$$

Because the Fredholm integral equations (2.17) and (2.20) have the same kernel but different forcing functions, we deduce that

$$\frac{\partial \mathbf{F}}{\partial R}(r, R) = \frac{\mathrm{j}k_s}{\pi}\mathbf{F}(r, R)\mathbf{H}^T(R)\mathbf{F}(R, R). \tag{2.21}$$

Taking the derivative of (2.18) with respect to $R$, and using (2.21) yields

$$\frac{\mathrm{d}\mathbf{T}}{\mathrm{d}R}(R) = \frac{\mathrm{j}k_s}{\pi}\mathbf{J}^T(R)\mathbf{F}(R, R) + \frac{\mathrm{j}k_s}{\pi}\mathbf{T}(R)\mathbf{H}^T(R)\mathbf{F}(R, R). \tag{2.22}$$

To find a representation for $\mathbf{F}(R, R)$ we set $r = R$ in (2.17) and use $\mathbf{g}(R, r') = (\mathrm{j}k_s/\pi)\mathbf{H}(R)\mathbf{J}^T(r')$; the result is

$$\mathbf{F}(R, R) = \mathbf{U}(R)\mathbf{J}(R) + \mathbf{U}(R)\mathbf{H}(R)\mathbf{T}(R). \tag{2.23}$$

Combining (2.22) and (2.23) we are led to the following matrix Riccati equation for the $\mathbf{T}$ matrix

$$\frac{\mathrm{d}\mathbf{T}}{\mathrm{d}R}(R) = \mathbf{Q}_{11}(R) + \mathbf{Q}_{12}(R)\mathbf{T}(R) + \mathbf{T}(R)\mathbf{Q}_{21}(R) + \mathbf{T}(R)\mathbf{Q}_{21}(R)\mathbf{T}(R), \tag{2.24}$$

where

$$\begin{aligned}
\mathbf{Q}_{11}(R) &= \frac{\mathrm{j}k_s}{\pi}\mathbf{J}^T(R)\mathbf{U}(R)\mathbf{J}(R),\\
\mathbf{Q}_{12}(R) &= \frac{\mathrm{j}k_s}{\pi}\mathbf{J}^T(R)\mathbf{U}(R)\mathbf{H}(R),\\
\mathbf{Q}_{21}(R) &= \frac{\mathrm{j}k_s}{\pi}\mathbf{H}^T(R)\mathbf{U}(R)\mathbf{J}(R),\\
\mathbf{Q}_{22}(R) &= \frac{\mathrm{j}k_s}{\pi}\mathbf{H}^T(R)\mathbf{U}(R)\mathbf{H}(R).
\end{aligned} \tag{2.25}$$

Substantial attention has been paid in the literature to the numerical integration of Riccati equations. Most of the numerical methods are based on the transformation of by using Bernoulli substitution [5–7]. A stable numerical algorithm for this linear differential system is the modified Davison-Maki method of Kenney and Leipnik [6] also known as the Möbius scheme [8]. The algorithm is based on the following two-term recurrence relation with the radial step $\Delta R$:

$$\mathbf{T}(R) = [(\mathbf{I} + \Delta R\mathbf{Q}_{12})\mathbf{T}(R - \Delta R) + \Delta R\mathbf{Q}_{11}] \times [(\mathbf{I} - \Delta R\mathbf{Q}_{21}) - \Delta R\mathbf{Q}_{22}\mathbf{T}(R - \Delta R)]^{-1}, \tag{2.26}$$

where the matrices $\mathbf{Q}_{11}$, $\mathbf{Q}_{12}$, $\mathbf{Q}_{21}$ and $\mathbf{Q}_{22}$ are evaluated at $R - \Delta R$.

### 2.2.4 *A Recurrence Relation for the* T *matrix*

A two-term recurrence relation for the $\mathbf{T}$ matrix, which can be regarded as an efficient algorithm for generating numerical solutions to the matrix Riccati equation (2.24), has been proposed by Johnson [4]. In this section we establish this recurrence relation by employing slightly different arguments as in [4]. We choose $\Delta R$ sufficiently small and approximate the integral of a function $f$ over the interval $[R - \Delta R, R]$ by the right-endpoint quadrature formula $\int_{R-\Delta R}^{R} f(r)\,\mathrm{d}r \approx \Delta R f(R)$. For $\mathbf{F}(R, R)$, we have

$$\mathbf{F}(R, R) = \mathbf{U}(R)\mathbf{J}(R) + \frac{\mathrm{j}k_s}{\pi}\mathbf{U}(R)\mathbf{H}(R)\int_0^{R-\Delta R}\mathbf{J}^T(r)\mathbf{F}(r, R)\,\mathrm{d}r + \Delta R\mathbf{U}(R)\mathbf{g}(R, R)\mathbf{F}(R, R), \tag{2.27}$$

and further

$$\mathbf{F}(R, R) = \frac{1}{\Delta R}\mathbf{Q}(R)\left[\mathbf{J}(R) + \mathbf{H}(R)\mathbf{q}(R)\right], \tag{2.28}$$

where the matrices $\mathbf{Q}$ and $\mathbf{q}$ are given by

$$\mathbf{Q}(R) = \Delta R\left[\mathbf{I} - \Delta R\mathbf{U}(R)\mathbf{g}(R, R)\right]^{-1}\mathbf{U}(R) \tag{2.29}$$

and

$$\mathbf{q}(R) = \frac{\mathrm{j}k_s}{\pi}\int_0^{R-\Delta R}\mathbf{J}^T(r)\mathbf{F}(r, R)\,\mathrm{d}r, \tag{2.30}$$

respectively. For $\mathbf{T}(R)$, we proceed similarly and obtain

$$\mathbf{T}(R) = \overline{\mathbf{Q}}_{11}(R) + \left[\mathbf{I} + \overline{\mathbf{Q}}_{12}(R)\right]\mathbf{q}(R), \tag{2.31}$$

Let us define the matrix $\mathbf{p}$ by the relation

$$\mathbf{p}(R) = \frac{jk_s}{\pi}\Delta R \mathbf{H}^T(R)\mathbf{F}(R, R), \tag{2.32}$$

which in view of (2.28), can be expressed as

$$\mathbf{p}(R) = \overline{\mathbf{Q}}_{21}(R) + \overline{\mathbf{Q}}_{22}(R)\mathbf{q}(R). \tag{2.33}$$

As $\mathbf{F}(r, R)$ and $\mathbf{F}(r, R - \Delta R)$ solve the same Fredholm integral equation but with different forcing functions, i.e.,

$$\mathbf{F}(r, R) = \mathbf{U}(r)\mathbf{J}(r)\left[\mathbf{I} + \frac{jk_s}{\pi}\Delta R \mathbf{H}^T(R)\mathbf{F}(R, R)\right] + \int_0^{R-\Delta R} \mathbf{U}(r)\mathbf{g}(r, r')\mathbf{F}(r', R)\,dr' \tag{2.34}$$

and

$$\mathbf{F}(r, R - \Delta R) = \mathbf{U}(r)\mathbf{J}(r) + \int_0^{R-\Delta R} \mathbf{U}(r)\mathbf{g}(r, r')\mathbf{F}(r' - \Delta R)\,dr' \tag{2.35}$$

respectively, we infer that

$$\mathbf{F}(r, R) = \mathbf{F}(r, R - \Delta R)\left[\mathbf{I} + \mathbf{p}(R)\right]. \tag{2.36}$$

Multiplying the equation for $\mathbf{T}(R - \Delta R)$,

$$\mathbf{T}(R - \Delta R) = \frac{jk_s}{\pi}\int_0^{R-\Delta R} \mathbf{J}^T(r)\mathbf{F}(r, R - \Delta R)\,dr \tag{2.37}$$

from the right by $\mathbf{I} + \mathbf{p}(R)$, and using (2.30) and (2.36) yield

$$\mathbf{T}(R - \Delta R)\left[\mathbf{I} + \mathbf{p}(R)\right] = \mathbf{q}(R). \tag{2.38}$$

Solving (2.33) and (2.38) with respect to $\mathbf{q}$ gives

$$\mathbf{q}(R) = \left[\mathbf{I} - \mathbf{T}(R - \Delta R)\overline{\mathbf{Q}}_{22}(R)\right]^{-1} \times \mathbf{T}(R - \Delta R)\left[\mathbf{I} + \overline{\mathbf{Q}}_{21}(R)\right], \tag{2.39}$$

whence from (2.31), the desired recurrence relation

$$\mathbf{T}(R) = \overline{\mathbf{Q}}_{11} + \left(\mathbf{I} + \overline{\mathbf{Q}}_{12}\right)\left[\mathbf{I} - \mathbf{T}(R - \Delta R)\overline{\mathbf{Q}}_{22}\right]^{-1} \times \mathbf{T}(R - \Delta R)\left(\mathbf{I} + \overline{\mathbf{Q}}_{21}\right) \tag{2.40}$$

readily follows. It should be pointed out that in contrast to (2.26), the matrices $\overline{\mathbf{Q}}_{11}$, $\overline{\mathbf{Q}}_{12}$, $\overline{\mathbf{Q}}_{21}$ and $\overline{\mathbf{Q}}_{22}$ are evaluated at $R$.

### 2.2.5 *An Integral-Matrix Approach*

In this section we describe a combined integral and matrix approach to analyze the scattering by two concentric inhomogeneous spheres. This method, which is similar to the superposition **T**-matrix method, will enable us to derive a recurrence relation for the **T** matrix, without invoking the invariant imbedding procedure. Let us consider two concentric spheres of radii $R_1$ and $R_2 > R_1$, enclosing an inhomogeneous region. The interior of the sphere of radius $R_1$ is denoted by $D_1$, while the domain corresponding to the spherical shell is denoted by $D_2$. For $D = D_1 \cup D_2$, the matrix form representation of the volume integral equation read as

$$\begin{aligned}\overline{\mathscr{E}}(\mathbf{r}) &= \mathscr{E}_0(\mathbf{r}) \\ &+ \sum_\alpha \mathbf{Y}_\alpha(\boldsymbol{\Omega})\int_{D_1} \chi(\mathbf{r}')\mathbf{g}_\alpha(r, r')\mathbf{Y}_{\bar\alpha}^T(\boldsymbol{\Omega}')\mathbf{Z}(\mathbf{r}')\overline{\mathscr{E}}(\mathbf{r}')\,dV' \\ &+ \sum_\alpha \mathbf{Y}_\alpha(\boldsymbol{\Omega})\int_{D_2} \chi(\mathbf{r}')\mathbf{g}_\alpha(r, r')\mathbf{Y}_{\bar\alpha}^T(\boldsymbol{\Omega}')\mathbf{Z}(\mathbf{r}')\overline{\mathscr{E}}(\mathbf{r}')\,dV'.\end{aligned} \tag{2.41}$$

The field scattered by the inhomogeneous spherical shell in $D_1$ is given by ($\mathbf{r} \in D_1$)

$$\begin{aligned}\mathscr{E}_{s2}(\mathbf{r}) &= \sum_\alpha \mathbf{Y}_\alpha(\boldsymbol{\Omega})\int_{D_2} \chi(\mathbf{r}')\mathbf{g}_\alpha(r, r')\mathbf{Y}_{\bar\alpha}^T(\boldsymbol{\Omega}')\mathbf{Z}(\mathbf{r}')\overline{\mathscr{E}}(\mathbf{r}')\,dV' \\ &= \sum_\alpha \mathbf{Y}_\alpha(\boldsymbol{\Omega})\mathbf{J}_\alpha(r)\mathbf{c}_{02\alpha},\end{aligned} \tag{2.42}$$

where

$$\mathbf{c}_{02\alpha} = \frac{jk_s}{\pi}\int_{R_1}^{R_2} \mathbf{H}_\alpha^T(r)\mathbf{F}_\alpha(r)\,dr, \tag{2.43}$$

while, the field scattered by the inhomogeneous sphere of radius $R_1$ in $D_2$ is given by ($\mathbf{r} \in D_2$)

$$= \sum_{\alpha} \mathbf{Y}_{\alpha}(\boldsymbol{\Omega}) \mathbf{H}_{\alpha}(r) \mathbf{c}_{\mathrm{s}1\alpha}, \tag{2.44}$$

where

$$\mathbf{c}_{\mathrm{s}1\alpha} = \frac{\mathrm{j}k_{\mathrm{s}}}{\pi} \int_0^{R_1} \mathbf{J}_{\alpha}^T(r) \mathbf{F}_{\alpha}(r)\, \mathrm{d}r. \tag{2.45}$$

By virtue of (2.44), the integral equation (2.41) inside the spherical shell can be written as ($\mathbf{r} \in D_2$)

$$\begin{aligned} \overline{\mathscr{E}}(\mathbf{r}) &= \sum_{\alpha} \mathbf{Y}_{\alpha}(\boldsymbol{\Omega}) \left[ \mathbf{J}_{\alpha}(r) \mathbf{c}_{0\alpha} + \mathbf{H}_{\alpha}(r) \mathbf{c}_{\mathrm{s}1\alpha} \right] \\ &+ \sum_{\alpha} \mathbf{Y}_{\alpha}(\boldsymbol{\Omega}) \int_{D_2} \chi(\mathbf{r}') \mathbf{g}_{\alpha}(r, r') \mathbf{Y}_{\bar{\alpha}}^T(\boldsymbol{\Omega}') \mathbf{Z}(\mathbf{r}') \overline{\mathscr{E}}(\mathbf{r}')\, \mathrm{d}V'. \end{aligned} \tag{2.46}$$

It is easy to see that the scattering problem requires the solution of the following integral and matrix equations:

$$\begin{aligned} \mathbf{F}_{\alpha}(r) &= \sum_{\beta} \mathbf{U}_{\alpha\beta}(r) \left[ \mathbf{J}_{\beta}(r) \mathbf{c}_{0\beta} + \mathbf{H}_{\beta}(r) \mathbf{c}_{\mathrm{s}1\beta} \right] \\ &+ \int_{R_1}^{R_2} \sum_{\beta} \mathbf{U}_{\alpha\beta}(r) \mathbf{g}_{\beta}(r, r') \mathbf{F}_{\beta}(r')\, \mathrm{d}r', \\ \mathbf{c}_{\mathrm{s}1\alpha} &= \sum_{\beta} \mathbf{T}_{\alpha\beta}^1 \left( \mathbf{c}_{0\beta} + \mathbf{c}_{02\beta} \right), \\ \mathbf{c}_{02\alpha} &= \frac{\mathrm{j}k_{\mathrm{s}}}{\pi} \int_{R_1}^{R_2} \mathbf{H}_{\alpha}^T(r) \mathbf{F}_{\alpha}(r)\, \mathrm{d}r, \end{aligned} \tag{2.47}$$

where $\mathbf{T}_{\alpha\beta}^1$ is the transition matrix of the inhomogeneous sphere of radius $R_1$. The field scattered by the inhomogeneous sphere of radius $R_2$ is given by

$$\begin{aligned} \mathscr{E}_{\mathrm{s}}(\mathbf{r}) &= \sum_{\alpha} \mathbf{Y}_{\alpha}(\boldsymbol{\Omega}) \mathbf{H}_{\alpha}(r) \mathbf{c}_{\mathrm{s}1\alpha} \\ &+ \frac{\mathrm{j}k_{\mathrm{s}}}{\pi} \sum_{\alpha} \mathbf{Y}_{\alpha}(\boldsymbol{\Omega}) \mathbf{H}_{\alpha}(r) \int_{R_1}^{R_2} \mathbf{J}_{\alpha}^T(r') \mathbf{F}_{\alpha}(r')\, \mathrm{d}r' \\ &= \sum_{\alpha} \mathbf{Y}_{\alpha}(\boldsymbol{\Omega}) \mathbf{H}_{\alpha}(r) \mathbf{c}_{\mathrm{s}\alpha}, \end{aligned} \tag{2.48}$$

with

$$\mathbf{c}_{\mathrm{s}\alpha} = \mathbf{c}_{\mathrm{s}1\alpha} + \frac{\mathrm{j}k_{\mathrm{s}}}{\pi} \int_{R_1}^{R_2} \mathbf{J}_{\alpha}^T(r) \mathbf{F}_{\alpha}(r)\, \mathrm{d}r. \tag{2.49}$$

sphere of radius $R_1$. The third equation in (2.47) gives the expansion coefficients of the field scattered by the inhomogeneous spherical shell and exciting the inhomogeneous sphere of radius $R_1$. Finally, the scattered field (2.48) is a superposition of the fields that are scattered from the individual particles (the inhomogeneous sphere of radius $R_1$ and the spherical shell).

In terms of global matrices, (2.47) and (2.49) read as

$$\begin{aligned} \mathbf{F}(r) &= \mathbf{U}(r) \mathbf{J}(r) \mathbf{c}_0 + \mathbf{U}(r) \mathbf{H}(r) \mathbf{c}_{\mathrm{s}1} \\ &+ \int_{R_1}^{R_2} \mathbf{U}(r) \mathbf{g}(r, r') \mathbf{F}(r')\, \mathrm{d}r', \\ \mathbf{c}_{\mathrm{s}1} &= \mathbf{T}_1 \left( \mathbf{c}_0 + \mathbf{c}_{02} \right), \\ \mathbf{c}_{02} &= \frac{\mathrm{j}k_{\mathrm{s}}}{\pi} \int_{R_1}^{R_2} \mathbf{H}^T(r) \mathbf{F}(r)\, \mathrm{d}r, \end{aligned} \tag{2.50}$$

and

$$\mathbf{c}_{\mathrm{s}} = \mathbf{c}_{\mathrm{s}1} + \frac{\mathrm{j}k_{\mathrm{s}}}{\pi} \int_{R_1}^{R_2} \mathbf{J}^T(r) \mathbf{F}(r)\, \mathrm{d}r \tag{2.51}$$

respectively, while the $\mathbf{T}$-matrix equation takes the form $\mathbf{c}_{\mathrm{s}} = \mathbf{T}\mathbf{c}_0$.

In (2.50) we choose $R_1 = R - \Delta R$ and $R_2 = R$, set $r = R$ and $\mathbf{T}_1 = \mathbf{T}(R - \Delta R)$, and apply the right-endpoint quadrature formula to compute the integrals $\int_{R-\Delta R}^{R} \cdots \mathrm{d}r$. Solving the resulting matrix equations yields the following representation for the $\mathbf{T}$ matrix of the inhomogeneous sphere of radius $R$:

$$\begin{aligned} \mathbf{T}(R) &= \mathbf{T}(R - \Delta R) \\ &+ \frac{\mathrm{j}k_{\mathrm{s}}}{\pi} \Delta R \left[ \mathbf{T}(R - \Delta R) \mathbf{H}^T + \mathbf{J}^T \right] \\ &\times \left[ \mathbf{I} - \Delta R \mathbf{U} \mathbf{g} - \frac{\mathrm{j}k_{\mathrm{s}}}{\pi} \Delta R \mathbf{U} \mathbf{H} \mathbf{T}(R - \Delta R) \mathbf{H}^T \right]^{-1} \\ &\times \mathbf{U} \left[ \mathbf{J} + \mathbf{H} \mathbf{T}(R - \Delta R) \right]. \end{aligned} \tag{2.52}$$

In terms of the matrix $\mathbf{Q}$ defined in (2.29), the recurrence relation (2.52) becomes

$$\begin{aligned} \mathbf{T}(R) &= \mathbf{T}(R - \Delta R) + \frac{\mathrm{j}k_{\mathrm{s}}}{\pi} \left[ \mathbf{T}(R - \Delta R) \mathbf{H}^T + \mathbf{J}^T \right] \\ &\times \left[ \mathbf{I} - \frac{\mathrm{j}k_{\mathrm{s}}}{\pi} \mathbf{Q} \mathbf{H} \mathbf{T}(R - \Delta R) \mathbf{H}^T \right]^{-1} \\ &\times \mathbf{Q} \left[ \mathbf{J} + \mathbf{H} \mathbf{T}(R - \Delta R) \right]. \end{aligned} \tag{2.53}$$

$\mathbf{T} = \mathbf{T}(R)$, $\mathbf{T}_1 = \mathbf{T}(R - \triangle R)$, and

$$\left(\mathbf{I} - \mathbf{T}_1\overline{\mathbf{Q}}_{22}\right)^{-1} = \mathbf{I} + \mathbf{A}, \tag{2.54}$$

where

$$\mathbf{A} = \mathbf{T}_1\overline{\mathbf{Q}}_{22}\left(\mathbf{I} - \mathbf{T}_1\overline{\mathbf{Q}}_{22}\right)^{-1}, \tag{2.55}$$

and performing the matrix multiplications in (2.40) we obtain

$$\begin{aligned}\mathbf{T} = \mathbf{T}_1 &+ \overline{\mathbf{Q}}_{11} + \mathbf{T}_1\overline{\mathbf{Q}}_{21} + \overline{\mathbf{Q}}_{12}\mathbf{T}_1 + \overline{\mathbf{Q}}_{12}\mathbf{T}_1\overline{\mathbf{Q}}_{21} \\ &+ \mathbf{A}\mathbf{T}_1 + \mathbf{A}\mathbf{T}_1\overline{\mathbf{Q}}_{21} + \overline{\mathbf{Q}}_{12}\mathbf{A}\mathbf{T}_1 + \overline{\mathbf{Q}}_{12}\mathbf{A}\mathbf{T}_1\overline{\mathbf{Q}}_{21}.\end{aligned} \tag{2.56}$$

Similarly, setting $\alpha = \mathrm{j}k_s/\pi$, and

$$\left(\mathbf{I} - \alpha\mathbf{Q}\mathbf{H}\mathbf{T}_1\mathbf{H}^T\right)^{-1} = \mathbf{I} + \mathbf{B}, \tag{2.57}$$

where

$$\mathbf{B} = \alpha\mathbf{Q}\mathbf{H}\mathbf{T}_1\mathbf{H}^T\left(\mathbf{I} - \alpha\mathbf{Q}\mathbf{H}\mathbf{T}_1\mathbf{H}^T\right)^{-1}, \tag{2.58}$$

we express the recurrence relation (2.53) as

$$\begin{aligned}\mathbf{T} = \mathbf{T}_1 &+ \overline{\mathbf{Q}}_{11} + \mathbf{T}_1\overline{\mathbf{Q}}_{21} + \overline{\mathbf{Q}}_{12}\mathbf{T}_1 + \mathbf{T}_1\overline{\mathbf{Q}}_{22}\mathbf{T}_1 \\ &+ \alpha\mathbf{T}_1\mathbf{H}^T\mathbf{B}\mathbf{Q}\mathbf{J} + \alpha\mathbf{T}_1\mathbf{H}^T\mathbf{B}\mathbf{Q}\mathbf{H}\mathbf{T}_1 \\ &+ \alpha\mathbf{J}^T\mathbf{B}\mathbf{Q}\mathbf{J} + \alpha\mathbf{J}^T\mathbf{B}\mathbf{Q}\mathbf{H}\mathbf{T}_1.\end{aligned} \tag{2.59}$$

Using the matrix identity

$$\mathbf{X}\left(\mathbf{I} - \mathbf{Y}\mathbf{X}\right)^{-1} = \left(\mathbf{I} - \mathbf{X}\mathbf{Y}\right)^{-1}\mathbf{X}, \tag{2.60}$$

where $\mathbf{X}$ and $\mathbf{Y}$ are rectangular matrices, but $\mathbf{XY}$ and $\mathbf{YX}$ are square matrices, and taking into account the definition of the matrices $\overline{\mathbf{Q}}_{11}$, $\overline{\mathbf{Q}}_{12}$, $\overline{\mathbf{Q}}_{21}$ and $\overline{\mathbf{Q}}_{22}$, we find the following identities:

$$\begin{aligned}\alpha\mathbf{T}_1\mathbf{H}^T\mathbf{B}\mathbf{Q}\mathbf{J} &= \mathbf{A}\mathbf{T}_1\overline{\mathbf{Q}}_{21}, \\ \alpha\mathbf{T}_1\mathbf{H}^T\mathbf{B}\mathbf{Q}\mathbf{H}\mathbf{T}_1 &= \mathbf{A}\mathbf{T}_1 - \mathbf{T}_1\overline{\mathbf{Q}}_{22}\mathbf{T}_1, \\ \alpha\mathbf{J}^T\mathbf{B}\mathbf{Q}\mathbf{J} &= \overline{\mathbf{Q}}_{12}\mathbf{T}_1\overline{\mathbf{Q}}_{21} + \overline{\mathbf{Q}}_{12}\mathbf{A}\mathbf{T}_1\overline{\mathbf{Q}}_{21}, \\ \alpha\mathbf{J}^T\mathbf{B}\mathbf{Q}\mathbf{H}\mathbf{T}_1 &= \overline{\mathbf{Q}}_{12}\mathbf{A}\mathbf{T}_1.\end{aligned} \tag{2.61}$$

Substituting (2.61) into (2.59) yields (2.56), and the proof is finished.

and (2.40) have been established by using an integral approach in conjunction with the invariant imbedding procedure, while the recurrence (2.52) has been derived by using an integral-matrix approach. The recurrence (2.40) requires two matrix inversions because the computation of the matrix $\mathbf{Q}$ demands an additional inversion step, while the recurrences (2.26) and (2.52) requires only one matrix inversion. Thus, (2.52) is more efficient than (2.40) in terms of the computational speed.

## 2.3 Conclusions

In this chapter, we revised the theoretical foundation of the invariant imbedding **T**-matrix method and established the connection with the superposition **T**-matrix method. Moreover, we derived two new recurrence relations for the **T** matrix: recurrence (2.26) which is essentially the modified Davison-Maki method with Pade approximation to the matrix exponential for solving Riccati differential equations, and recurrence (2.52) which has been obtained by using an integral-matrix approach. Although recurrence (2.52) will not dramatically increase the computation speed (as compared to Johnson's recurrence (2.40)), it appears to be of beneficial use for particles with very large size parameters. As a matter of fact, any numerical method for solving Riccati differential equations can be used to design new recurrence relations. Here we think about methods which transform Riccati differential equation into two coupled nonlinear equations (Chandrasekhar system), methods based on the superposition property of the Riccati solutions, and matrix versions of the ordinary differential equations methods.

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