Rigorous Derivation of Superposition *T*-matrix Approach from Solution of Inhomogeneous Wave Equation.

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Abstract

The problem of electromagnetic scattering by a system of particles is considered. Starting from the integral solution of the inhomogeneous wave equation, the equations for Green's and transition operators are derived. By expanding the free-space dyadic Green's function in terms of spherical wave functions, equations for determining the matrix elements of the dyadic transition operators for system of particles are obtained. The relations between the matrix elements of the dyadic transition operator and Waterman's T matrix are established.

1 Introduction

Waterman's T-matrix formalism is widely used in acoustic and electromagnetic scattering problems [1]-[4]. For the problem of electromagnetic scattering by aggregated (composite) particles the superposition T-matrix approach has been developed (see, for example [2], [4]).

Alternative methods for treating the electromagnetic scattering problem are the quantum-mechanical potential scattering approach [3], [5] and recently developed self consistent Green's function formalism [6]. In [6] it is shown that, for suitable choice of expansion functions, the matrix elements of interaction operator are related with Waterman's T-matrix.

In this paper we present rigorous and systematic derivation of the superposition T-matrix approach, which directly follows from the inhomogeneous wave equation. Starting from the complete integral solution of the inhomogeneous wave equation for a time harmonic field, we obtain first the equations for the Green's and transition operators. Then, expressing the free space dyadic Green's function in terms of spherical wave functions and separating variables, we find the equation for determining the matrix elements of transition operator $\overleftrightarrow{T}$ for a system of particles using the matrix elements of $\overleftrightarrow{T}$ for isolated particles. We show that for divergence free electric field the matrix elements of $\overleftrightarrow{T}$, expressed in spherical wave functions, directly connected to Waterman's T matrix.

2 Equation for particle-centered matrix elements of the dyadic transition operator $\overleftrightarrow{T}$

Let us consider electromagnetic scattering by a system of nonmagnetic scatterers assuming, as usual, that the scatterers are embedded in an infinite, homogeneous, linear, isotropic, nonmagnetic and nonabsorbing host medium. For this problem, it is well-known that everywhere in space the time harmonic electric field satisfies the inhomogeneous differential equation [2]:

$$\nabla\times\nabla\times\mathbf{E}(\mathbf{r})-k^2\mathbf{E}(\mathbf{r})=\mathbf{J}(\mathbf{r}). \tag{1}$$

Here

$$\mathbf{J}(\mathbf{r})=\mathbf{J}_0(\mathbf{r})+k^2(\tilde{m}^2(\mathbf{r},\omega)-1)\mathbf{E}(\mathbf{r}), \tag{2}$$

$$\mathbf{J}_0(\mathbf{r})=\begin{cases}0, & \mathbf{r}\notin V_{sour},\\ \mathbf{J}_0(\mathbf{r}), & \mathbf{r}\in V_{sour},\end{cases} \tag{3}$$

$$\tilde{m}(\mathbf{r},\omega)=\begin{cases}1, & \mathbf{r}\in V_h,\\ \tilde{m}_i(\mathbf{r},\omega)=\dfrac{m_i(\mathbf{r},\omega)}{m}=\dfrac{k_i(\mathbf{r},\omega)}{k}, & \mathbf{r}\in V_i,\end{cases} \tag{4}$$

where $\mathbf{J}_0(\mathbf{r})$ is a source of radiation, V_{sour} is volume of the source of radiation, V_h and V_i are the volumes of the host medium and the *i*-th particle, respectively, $\tilde{m}_i(\mathbf{r},\omega)$ is the complex refractive index of the *i*-th particle relative to that of the host medium, m and $m_i(\mathbf{r},\omega)$ are the refractive indices of the host medium and the *i*-th particle, respectively. k and $k_i(\mathbf{r},\omega)$ are the wave numbers in the host medium and inside the *i*-th particle, respectively.

The complete solution of Eq.(1) (see, for example [2]) is as follows:

$$\mathbf{E}(\mathbf{r})=\mathbf{E}_{inc}(\mathbf{r})+\int_V \vec{G}_0(\mathbf{r},\mathbf{r}')\vec{U}(\mathbf{r}')\mathbf{E}(\mathbf{r}')d^3\mathbf{r}', \tag{5}$$

where $\vec{G}_0(\mathbf{r},\mathbf{r}')$ is the free space dyadic Green's functions, $\vec{U}(\mathbf{r}')$ is scattering potential [3], [5].

Eq. (5) can be written as follows:

$$\mathbf{E}(\mathbf{r})=\int_V \vec{G}(\mathbf{r},\mathbf{r}_0)\mathbf{J}_0(\mathbf{r}_0)d^3\mathbf{r}_0, \tag{6}$$

where $\vec{G}(\mathbf{r},\mathbf{r}_0)$ is dyadic Green's function for whole system of scatterers. Introducing the transition operator, related with the *i*-th particle and transition operators, related with the *i*-th and *j*-th particles (see for example, [5]), one can write for $\vec{G}(\mathbf{r},\mathbf{r}_0)$:

$$\vec{G}(\mathbf{r},\mathbf{r}_0)=\vec{G}_0(\mathbf{r},\mathbf{r}_0)+\sum_{i,j}\int_{V_i}\int_{V_j}\vec{G}_0(\mathbf{r},\mathbf{r}'_i)\vec{T}_{ij}(\mathbf{r}'_i,\mathbf{r}''_j)\vec{G}_0(\mathbf{r}''_j,\mathbf{r}_0)d^3\mathbf{r}'_i d^3\mathbf{r}''_j. \tag{7}$$

Here $\vec{T}_{ij}(\mathbf{r}'_i,\mathbf{r}''_j)$ is transition operator, related with particles *i* and *j*.

$$\vec{T}_{ij}(\mathbf{r}'_i,\mathbf{r}''_j)=\vec{T}_0^i(\mathbf{r}'_i,\mathbf{r}''_i)\delta_{ij}+\int_{V_i}\vec{T}_0^i(\mathbf{r}'_i,\mathbf{r}'''_i)d^3\mathbf{r}'''_i\sum_{k\neq i}\int_{V_k}\vec{G}_0(\mathbf{r}'''_i,\mathbf{r}''_k)\vec{T}_{kj}(\mathbf{r}''_k,\mathbf{r}''_j)d^3\mathbf{r}''_k. \tag{8}$$

$\vec{T}_0^i(\mathbf{r}'_i,\mathbf{r}'''_i)$ is transition operator, related with particles *i* [3], [5]. Let us separate variables $\mathbf{r}$ and $\mathbf{r}'_i$ ($\mathbf{r}_0$ and $\mathbf{r}''_j$ etc.) in Eqs.(7), (8) and express $\vec{G}_0$ in terms of spherical wave functions. Then Eq.(7) can be written in the following form:

$$\vec{G}(\mathbf{r},\mathbf{r}_0)=\vec{G}_0(\mathbf{r},\mathbf{r}_0)-k^2\sum_{i,j}\sum_{lml'm'}\vec{g}_{lm}^{(1)}(k\mathbf{r}_i)\vec{T}_{lml'm'}^{ij}\vec{g}_{l'm'}^{(2)*T}(k\mathbf{r}_j^0), \tag{9}$$

$$\vec{g}_{lm}^{(1)}(k\mathbf{r}_i)=\left(\vec{I}+\frac{\nabla\otimes\nabla}{k^2}\right)\psi_{lm}^{(1)}(k\mathbf{r}_i), \tag{10}$$

$$\psi_{lm}^{(1)}(k\mathbf{r}_i)=h_l^{(1)}(kr_i)Y_{lm}(\vartheta_i,\varphi_i), \tag{11}$$

$\psi_{lm}^{(1)}(k\mathbf{r}_i)$ are scalar spherical wave functions, $(r_i,\vartheta_i,\varphi_i)$ are spherical coordinates of the radius-vector $\mathbf{r}_i$ in the coordinate system $\{x_i,y_i,z_i\}$ associated with the *i*-th particle.
$\vec{T}_{lml'm'}^{ij}$ are the matrix elements of the dyadic transition operator $\vec{T}_{ij}(\mathbf{R}_i+\mathbf{R}'_i,\mathbf{R}_j+\mathbf{R}''_j)$:

$$\vec{T}_{lml'm'}^{ij}=\int_{V_i}\int_{V_j}Rg\psi_{lm}^*(k\mathbf{R}'_i)\vec{T}_{ij}(\mathbf{R}_i+\mathbf{R}'_i,\mathbf{R}_j+\mathbf{R}''_j)Rg\psi_{l'm'}(k\mathbf{R}''_j)d\mathbf{R}'_i d\mathbf{R}''_j, \tag{12}$$

$$Rg\psi_{lm}(k\mathbf{R}'_i)=j_l(kR'_i)Y_{lm}(\beta'_i,\alpha'_i), \tag{13}$$

where $Rg\psi_{lm}(k\mathbf{R}'_i)$ are scalar regular spherical wave functions.

The matrix $\vec{T}_{lml'm'}^{ij}$ is a tensor of 2-nd rank (dyad) associated with the particles *i* and *j* (the particle-centered matrix). It contains all possible scattering processes occurring while wave propagates from the particle *j* to the particle *i*. The matrices $\vec{T}_{lml'm'}^{ij}$ are independent of the incidence and scattering directions as well as of the polarization state of the incident field. They depend only on the configuration of the system of particles, the properties of the component particles, their orientation, etc.

For the matrix elements $\vec{\vec{T}}^{0i}_{lml'm'}$, associated with isolated particles, we can write similar to (12) the following relation:

$$\vec{\vec{T}}^{0(i)}_{lml'm'} = \int_{V_i}\int_{V_i} Rg\psi^*_{lm}(k\mathbf{R}'_i)\vec{\vec{T}}^i_0(\mathbf{R}_i+\mathbf{R}'_i,\mathbf{R}_i+\mathbf{R}''_i)Rg\psi_{l'm'}(k\mathbf{R}''_i)d\mathbf{R}'_i d\mathbf{R}''_i \,. \tag{14}$$

Using the definitions (12), (14) and the addition theorems for scalar spherical wave functions (see, for example, [7]), from Eq.(8) we have the following equation for matrix $\vec{\vec{T}}^{ij}_{lml'm'}$:

$$\vec{\vec{T}}^{ij}_{lml'm'} = \vec{\vec{T}}^{0(i)}_{lml'm'}\delta_{ij} + \sum_{l_1m_1}\vec{\vec{T}}^{0(i)}_{lml_1m_1}\sum_{k\neq i}\sum_{l_2m_2}\vec{\vec{H}}_{l_1m_1l_2m_2}(k\mathbf{r}_{ki})\vec{\vec{T}}^{kj}_{l_2m_2l'm'}\,, \tag{15}$$

$$\vec{\vec{H}}_{l_1m_1l_2m_2}(k\mathbf{r}_{ki}) = ik(-1)^{l_2+m_2}\sum_{l_3m_3}\vec{\vec{g}}^{(1)}_{l_3m_3}(k\mathbf{r}_{ki})c(l_3m_3\,|\,l_1m_1\,|\,l_2-m_2)\,, \tag{16}$$

$$c(l_3m_3\,|\,l_1m_1\,|\,l_2-m_2) = i^{l_1+l_2-l_3}4\pi\sqrt{\frac{(2l_1+1)(2l_2+1)}{4\pi(2l_3+1)}}C^{l_3\,0}_{l_1\,0\,l_2\,0}C^{l_3m_3}_{l_1m_1l_2-m_2}\,, \tag{17}$$

$C^{l_3\,0}_{l_1\,0\,l_2\,0}$ and $C^{l_3m_3}_{l_1m_1l_2-m_2}$ are Clebsh-Gordan coefficients [7].

2 Relation between Waterman's *T* matrix and the matrix elements of the dyad transition operator $\vec{\vec{T}}$

Eq.(9) for Green's function and Eqs.(12),(14)-(16) for the matrix elements of the transition operators are obtained for the following conditions: the Green's function must satisfy vector wave equation and must be limited at infinity. Thus $\vec{\vec{G}}_0(\mathbf{r},\mathbf{r}_0)$ and $\vec{\vec{G}}(\mathbf{r},\mathbf{r}_0)$ are not divergence free and contain both transverse and longitudinal parts. For the system of uncharged particles electromagnetic field outside of source region is purely transverse. Thus in Eq.(9) and Eqs.(12), (14)-(16) one has left just the divergence free transverse part of $\vec{\vec{G}}_0(\mathbf{r},\mathbf{r}_0)$ and $\vec{\vec{G}}(\mathbf{r},\mathbf{r}_0)$. For the transverse part of Green's function from Eq.(9) we can write following equation:

$$\begin{aligned}\vec{\vec{G}}^{tr}(\mathbf{r},\mathbf{r}_0) = \vec{\vec{G}}^{tr}_0(\mathbf{r},\mathbf{r}_0) + ik\sum_{LML_1M_1}\frac{(-1)^{M_1}}{L(L+1)L_1(L_1+1)}\Big\{T^{11}_{LML_1M_1}\mathbf{M}_{LM}(k\mathbf{r})\otimes\mathbf{M}_{L_1-M_1}(k\mathbf{r}_0)\\ +T^{12}_{LML_1M_1}\mathbf{M}_{LM}(k\mathbf{r})\otimes\mathbf{N}_{L_1-M_1}(k\mathbf{r}_0)+T^{21}_{LML_1M_1}\mathbf{N}_{LM}(k\mathbf{r})\otimes\mathbf{M}_{L_1-M_1}(k\mathbf{r}_0)+T^{22}_{LML_1M_1}\mathbf{N}_{LM}(k\mathbf{r})\otimes\mathbf{N}_{L_1-M_1}(k\mathbf{r}_0)\Big\},\end{aligned} \tag{18}$$

$$T^{11}_{LML_1M_1} = \sqrt{L(L+1)L_1(L_1+1)}\;T^{LL_1}_{LML_1M_1} = ik\int_V\int_V Rg\mathbf{M}^*_{LM}(k\mathbf{R}')\;\vec{\vec{T}}(\mathbf{r}'+\mathbf{R}',\mathbf{r}''+\mathbf{R}'')Rg\mathbf{M}_{L_1M_1}(k\mathbf{R}'')d^3\mathbf{R}'d^3\mathbf{R}'', \tag{19}$$

$$T^{12}_{LML_1M_1} = \sqrt{L(L+1)L_1(L_1+1)}\left(-i\sqrt{\frac{L_1}{2L_1+1}}T^{LL_1+1}_{LML_1M_1} + i\sqrt{\frac{L_1+1}{2L_1+1}}T^{LL_1-1}_{LML_1M_1}\right) = ik\int_V\int_V Rg\mathbf{M}^*_{LM}(k\mathbf{R}')\;\vec{\vec{T}}\;Rg\mathbf{N}_{L_1M_1}(k\mathbf{R}'')d^3\mathbf{R}'d^3\mathbf{R}'', \tag{20}$$

$$T^{21}_{LML_1M_1} = \sqrt{L(L+1)L_1(L_1+1)}\left(i\sqrt{\frac{L}{2L+1}}T^{L+1L_1}_{LML_1M_1} - i\sqrt{\frac{L+1}{2L+1}}T^{L-1L_1}_{LML_1M_1}\right) = ik\int_V\int_V Rg\mathbf{N}^*_{LM}(k\mathbf{R}')\;\vec{\vec{T}}\;Rg\mathbf{M}_{L_1M_1}(k\mathbf{R}'')d^3\mathbf{R}'d^3\mathbf{R}'', \tag{21}$$

$$\begin{aligned}T^{22}_{LML_1M_1} &= \frac{\sqrt{L(L+1)L_1(L_1+1)}}{(2L+1)(2L_1+1)}\left(\sqrt{LL_1}T^{L+1L_1+1}_{LML_1M_1}+\sqrt{(L+1)(L_1+1)}T^{L-1L_1-1}_{LML_1M_1}-\sqrt{L(L_1+1)}T^{L+1L_1-1}_{LML_1M_1}-\sqrt{(L+1)L_1}T^{L-1L_1+1}_{LML_1M_1}\right)\\ &= ik\int_V\int_V Rg\mathbf{N}^*_{LM}(k\mathbf{R}')\;\vec{\vec{T}}(\mathbf{r}'+\mathbf{R}',\mathbf{r}''+\mathbf{R}'')Rg\mathbf{N}_{L_1M_1}(k\mathbf{R}'')d^3\mathbf{R}'d^3\mathbf{R}'',\end{aligned} \tag{22}$$

In Eqs.(19)-(22) the dyadic transition operator $\overleftrightarrow{T}$ for the system of particles is defined by Eq.(8) whereas for isolated particles it is the transition operator related with a particle [5]. $\mathbf{M}_{lm}(k\mathbf{r})$, $\mathbf{N}_{lm}(k\mathbf{r})$ are vector spherical wave functions [2]. In (19)-(22) the matrix elements $T^{ll_1}_{LML_1M_1}$ ($l = L, L\pm 1$) are related with cyclical components $T^{qq_1}_{lml_1m_1}$ (q and q_1 take values $0,\pm 1$)) of $\overleftrightarrow{T}_{lml_1m_1}$ (see Eq.(12), Eq.(14)) by the equations:

$$T^{ll_1}_{LML_1M_1} = ik\sum_{mm_1}\sum_{qq_1}(-1)^{q+q_1}C^{LM}_{lm1-q}C^{L_1M_1}_{l_1m_11-q_1}T^{qq_1}_{lml_1m_1}, \qquad T^{qq_1}_{lml_1m_1} = \frac{1}{ik}\sum_{LML_1M_1}(-1)^{q+q_1}C^{LM}_{lm1-q}C^{L_1M_1}_{l_1m_11-q_1}T^{ll_1}_{LML_1M_1} \tag{23}$$

From Eqs.(5), (6), (18) one can obtain the expansions for scattered and incident fields:

$$\mathbf{E}_{sc}(\mathbf{r}) = \sum_{LM}(p_{LM}\mathbf{M}_{LM}(k\mathbf{r}) + q_{LM}\mathbf{N}_{LM}(k\mathbf{r})), \qquad \mathbf{E}_{inc}(\mathbf{r}') = \sum_{LM}(a_{LM}Rg\mathbf{M}_{LM}(k\mathbf{r}') + b_{LM}Rg\mathbf{N}_{LM}(k\mathbf{r}')), \tag{24}$$

where scattering coefficients are related with expansion coefficients of incident field through the matrix elements (19)-(22) $T^{pn}_{LML_1M_1}$:

$$\begin{pmatrix} p_{LM} \\ q_{LM} \end{pmatrix} = \frac{1}{L(L+1)}\sum_{L_1M_1}\begin{pmatrix} T^{11}_{LML_1M_1} & T^{12}_{LML_1M_1} \\ T^{21}_{LML_1M_1} & T^{22}_{LML_1M_1} \end{pmatrix}\begin{pmatrix} a_{L_1M_1} \\ b_{L_1M_1} \end{pmatrix} \tag{25}$$

Thus the matrix elements of transition operator, which are defined by the relations (19)-(22), are the elements of Waterman's *T* matrix and the matrix elements of $\overleftrightarrow{T}$ defined by the relations (12), (14) are related with Waterman's *T* matrix by relations (19)-(22) and (23). Consequently, for the elements of *T* matrix we have a similar to (15) equation, that allows calculating the *T* matrix for system of particles using *T* matrices for individual particles of the system.

3 Conclusion

In this paper the matrix elements of $\overleftrightarrow{T}$ we expressed in terms of spherical wave functions. As a result, Eq.(15) for the particle-centered *T* matrices ($\mathbf{T}^{ij}$) is obtained for the condition: the smallest spheres circumscribing particles must not overlap with each other. These restrictions are known in the superposition *T*-matrix approach as well [2]. But the expression in terms of spherical wave functions is not the only possible one. For example, other possible expressions are the expressions in terms of spheroidal or cylindrical wave functions. Being expressed in terms of such function the *T* matrices for the cluster of particles must satisfy the following condition: the smallest spheroids (smallest cylinders) circumscribing particles must not overlap with each other. Note that independently of the chosen expansion functions, Eq.(15) for $\mathbf{T}^{ij}$ in the matrix form must be the same, since they are the consequence of more general equations (8) for operators. The key condition is that in the chosen function basis, one could separate variables for the Green's function.

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