Energy Invariants to Composition Rules for Scattering and Transfer Matrices of Propagating and Evanescent Waves in Dielectric Structures

Y. N. Barabanenkov

Institute of Radioengineering and Electronics of Russian Academy of Sciences, Russia

M. Y. Barabanenkov

Institute of Microelectronics Technology and High Purity Materials of Russian Academy of Sciences, Russia

Abstract—We present as a basis to modern wave multiple scettering theory an extended unitarity for the S-scattering matrix and an extended pseudo-unitarity for the transfer matrix of propagating and evanescent (near field) electromagnetic waves in a volume or surface lossless dielectric structure with spatial inhomogeneities of any dimension. The formalism of angular spectrum wave amplitudes is used. The presented extended unitarity and pseudo-unitarity are shown to be energy invariants to composition rules for the S-matrix and the transfer matrix, respectively. From composition rules, we derive a complete system of nonlinear differential equations for blocks of the S-matrix, with Riccati equation being a main one, and a linear equation for the transfer matrix.

Section 1.

During the last one and half decade the wave multiple scattering theory based on composition rule [1] for scattering operator (T-matrix) was reformulated in terms of virtual splitting the volume or surface inhomogeneous dielectric structure into a stack of elementary layers (slices), with slices being perpendicular to an embedding parameter and separated by splits, which may be vanishingly thin. In result using the Sommerfeld-Weyl angular-spectrum decomposition of wave amplitudes, a system of exact equations (transfer relation) [2] was obtained for the operator wave reflection and transmission coefficients of the structure and the operator wave amplitudes of waves in splits between slices (local fields).

The report aims to show that the recently derived, at study the effect of energy emission from an evanescent wave, extended unitarity of the 2×2 block S-scattering matrix [3] is an energy invariant to a specific composition rule for S-matrix, which is a consequence from the transfer relations. This composition rule describes the incremental change of S-matrix of subsystem of slices upon attachment an additional subsystem of slices. In the case of infinitesimally thin attached slice, we obtain a complete system of nonlinear differential equations for blocks of the S-matrix, with Riccati equation being a main one and taking into account a strong singularity of the electric field Green tensor function in a background. The S-matrix is closely related to the transfer matrix, for which we derive a linear equation with an energy invariant in the form of an extended pseudo-unitarity of the transfer matrix.

Section 2.

Let a volume or surface dielectric structure with scalar dielectric permittivity $\epsilon(\vec{r})$ occupies a region between planes z = 0 and z = L of Cartesian coordinate system x, y, z. The electric field of monochromatic electromagnetic wave to be incident onto the left boundary plane z = 0 is written as (see details in [2] and [3]) $(2\pi)^{-2} \int d\vec{k}_{\perp} \exp(i\vec{k}_{\perp}\vec{r}_{\perp})E_{\alpha}^{\circ}(\vec{k}_{\perp})\exp(i\gamma_{k}z)$. Here \vec{k}_{\perp} is the transverse to the z axis component of a wave vector \vec{k} , and the angular spectrum amplitude $E_{\alpha}^{\circ}(\vec{k}_{\perp})$ of the incident electric field describes either propagating or evanescent wave, depending on $k_{\perp} < k_{\circ}$ and $\gamma_{k} = \sqrt{k_{\circ}^{2} - k_{\perp}^{2}}$ is real or $k_{\perp} > k_{\circ}$ and $\gamma_{k} = i\sqrt{k_{\perp}^{2} - k_{\circ}^{2}}$ is purely imaginary quantity, respectively. The quantity k_{\circ} is the wave number in a background with dielectric permittivity ϵ_{\circ} . The angular spectrum amplitudes of electric field, transmitted through and reflected from the structure, are written in terms of the tensor operator transmission $A_{\alpha\beta}(\vec{k}_{\perp}, \vec{k'}_{\perp}) E_{\beta}^{\circ}(\vec{k'}_{\perp})$ and $(2\pi)^{-2} \int d\vec{k}_{\perp} B_{\alpha\beta}(\vec{k}_{\perp}, \vec{k'}_{\perp}) E_{\beta}^{\circ}(\vec{k'}_{\perp})$, respectively. An electromagnetic wave may be incident upon the right boundary plane z = L with angular spectrum amplitude $\tilde{E}_{\alpha}^{\circ}(\vec{k}_{\perp})$. In this case the angular spectrum amplitudes of electric field, transmitted through and reflected from the structure, are written in terms of the tensor operator transmission $\tilde{A}_{\alpha\beta}(\vec{k}_{\perp}, \vec{k'}_{\perp})$ and reflection $\tilde{B}_{\alpha\beta}(\vec{k}_{\perp}, \vec{k'}_{\perp})$ coefficients of plane wave.

The 2×2 block S-matrix of the structure is defined in terms of the above tensor coefficients of wave transmission through and reflection from structure as follows

$$S = \left(\begin{array}{cc} A & \tilde{B} \\ B & \tilde{A} \end{array}\right) \tag{1}$$

Physically the S-matrix transforms the angular spectrum amplitudes of incident forward and backward going waves, with respect to positive direction of the z axis,into the angular spectrum amplitudes of scattered forward and backward going waves.

Section 3.

Split virtually the dielectric structure under consideration into a stack of n slices with splits between them, as in Fig. 1 of [2]. According to this reference, the composition rule [1] for the scattering operator (*T*-matrix) together with condition of non-overlapping the slices lead to a mixed system of exact equations-transfer relations for blocks of the *S*-matrices of subsystems of slices and amplitudes of local waves inside splits. As doing so the tensor coefficients of the local fields waves in splits can be eliminated from the transfer relations and expressed in terms of blocks of the *S*-matrices, $S_{1,m}$ and $S_{m+1,n}$. After this elimination, the transfer relations give the separate system of recurrent equations that describes the incremental change of the *S*-matrix of subsystem of slices with numbers $1, \ldots, m$ upon attachment of additional subsystem of slices with numbers $m+1, \ldots, n$. This system of recurrent equations has been got in [2] for the case of 2D dielectric structure and TE polarization, with m = n - 1, and for general case has a form

$$A_{1,n} = A_{m+1,n} (I - \tilde{B}_{1,m} B_{m+1,n})^{-1} A_{1,m},$$

$$B_{1,n} = B_{1,m} + \tilde{A}_{1,m} B_{m+1,n} (I - \tilde{B}_{1,m} B_{m+1,n})^{-1} A_{1,m}$$
(2)

and

$$\tilde{A}_{1,n} = \tilde{A}_{1,m} (\tilde{I} - B_{m+1,n} \tilde{B}_{1,m})^{-1} \tilde{A}_{m+1,n},
\tilde{B}_{1,n} = \tilde{B}_{m+1,n} + A_{m+1,n} \tilde{B}_{1,m} (\tilde{I} - B_{m+1,n} \tilde{B}_{1,m})^{-1} \tilde{A}_{m+1,n}$$
(3)

The symbols I and \tilde{I} denote some identity tensor operators, $I_{\alpha\beta}(\vec{k}_{\perp}, \vec{k'}_{\perp}) = P_{\alpha\beta}^{tr}(\hat{k}^+)\delta_{\vec{k}_{\perp},\vec{k'}_{\perp}}$ and $\tilde{I}_{\alpha\beta}(\vec{k}_{\perp}, \vec{k'}_{\perp}) = P_{\alpha\beta}^{tr}(\hat{k}^-)\delta_{\vec{k}_{\perp},\vec{k'}_{\perp}}$, acting in the subspaces of transverse inhomogeneous plane waves going forward and backward with the wave vectors $\vec{k}^{\pm} = \vec{k}_{\perp} \pm \gamma_k \hat{z}$, respectively, where \hat{z} is the unit vector along the z axis. Besides, the units vectors along these wave vectors are defined by, $\hat{k}^{\pm} = \hat{k}^{\pm}/k_{\circ}$, and a tensor, $P_{\alpha\beta}^{tr}(\hat{k})$, means the orthogonal projector in direction perpendicular to the unit vector \hat{k} . One should note here that in the scalar case a system of recurrent equations similar to Eqs. (2, 3) has been got by Redheffer [4] as the functional relations (semigroup property) associated with the Riccati system of equations for the reflection and transmission coefficients of waves propagating in transmission lines. In this case, Regheffer has introduced an useful notion star product, (*), of the scattering matrices, which enables us to rewrite the above system of recurrent Eqs. (2, 3) shortly as $S_{1,n} = S_{1,m} * S_{m+1,n}$.

Section 4.

Turn to the composition rule for S-matrix in Eqs. (2,3) and consider the case of thin attached nth slice, m = n-1. We introduce a useful renormalized version **S** of the scattering matrix (1) putting $\mathbf{S} = \text{diag}(\gamma^{1/2}, \gamma^{1/2})S$ $\text{diag}(\gamma^{-1/2}, \gamma^{-1/2})$ and suppose the S-matrix of the nth slice to be small deviated from an identity matrix, $\mathbf{I} = \text{diag}(I, \tilde{I})$, and subject to a condition, $\mathbf{S}_{n,n} = \mathbf{I} + \delta \mathbf{S} \Delta \mathbf{z}$. Here a thickness Δz of the nth slice tends to zero and an infinitesimal scattering matrix δS is obtained by a solution to the Lippman-Schwinger equation for T-matrix in the form $(\mathbf{U}^{++}, \mathbf{U}^{+-})$

$$\delta \mathbf{S} = \begin{pmatrix} \mathbf{U}^{++} & \mathbf{U}^{+-} \\ \mathbf{U}^{-+} & \mathbf{U}^{--} \end{pmatrix}$$
(4)

The blocks of this infinitesimal scattering matrix are given by

$$\mathbf{U}_{\alpha\beta}^{\xi\eta}(\vec{k}_{\perp},\vec{k'}_{\perp};z) = \frac{1}{2i} \exp\left[-i(\xi\gamma_k - \eta\gamma_{k'})z\right] \frac{1}{\sqrt{\gamma_k}} U_{\alpha\beta}^{\xi\eta}(\vec{k}_{\perp},\vec{k'}_{\perp};z) \frac{1}{\sqrt{\gamma_{k'}}}$$
(5)

with

$$U^{\xi\eta}_{\alpha\beta}(\vec{k}_{\perp},\vec{k'}_{\perp};z) = P^{tr}_{\alpha\mu}(\hat{k}^{\xi})U_{\mu\nu}(\vec{k}_{\perp}-\vec{k'}_{\perp},z)P^{tr}_{\nu\beta}(\hat{k}^{\eta'})$$
$$U_{\alpha\beta}(\vec{k}_{\perp},z) = V(\vec{k}_{\perp},z)(\hat{x}_{\alpha}\hat{x}_{\beta}+\hat{y}_{\alpha}\hat{y}_{\beta})+v(\vec{k}_{\perp},z)\hat{z}_{\alpha}\hat{z}_{\beta}$$

where $\xi, \eta = \pm, V(\vec{k}_{\perp}, z)$ and $v(\vec{k}_{\perp}, z)$ are the spatial Fourier transforms of the scalar potential $V(\vec{r}) = -k_{\circ}^{2}[\epsilon(\vec{r}) - \epsilon_{\circ}]/\epsilon_{\circ}$ and a function $v(\vec{r}) = -k_{\circ}^{2}[\epsilon(\vec{r}) - \epsilon_{\circ}]/\epsilon(\vec{r})$, respectively, with respect to transverse to the z axis component

of the position vector, \hat{x} and \hat{y} are unit vectors along the x and y axes, respectively. Substituting the obtained asymptotics for the S-matrix of thin nth slice into composition rule in Eqs. (2), (3) gives the following systems of differential equations for blocks of the S-matrix

$$\frac{d\mathbf{B}}{dz} = \mathbf{U}^{+-} + \mathbf{U}^{++}\tilde{\mathbf{B}} + \tilde{\mathbf{B}}\mathbf{U}^{--} + \tilde{\mathbf{B}}\mathbf{U}^{-+}\tilde{\mathbf{B}}, \qquad \tilde{\mathbf{B}}(z=\mathbf{0}) = \mathbf{0}$$
(6)

$$\frac{d\mathbf{A}}{dz} = \tilde{\mathbf{A}}(\mathbf{U}^{--} + \mathbf{U}^{-+}\tilde{\mathbf{B}}), \qquad \tilde{\mathbf{A}}(z=0) = \tilde{I}$$
(7)

$$\frac{d\mathbf{A}}{dz} = (\tilde{\mathbf{B}}\mathbf{U}^{-+} + \mathbf{U}^{++})\mathbf{A}, \qquad \mathbf{A}(z=\mathbf{0}) = I$$
(8)

$$\frac{d\mathbf{B}}{dz} = \tilde{\mathbf{A}}\mathbf{U}^{-+}\mathbf{A}, \qquad \mathbf{B}(z=\mathbf{0}) = \mathbf{0}$$
(9)

Klyatskin [5] derived a matrix Riccati equation similar to Eq. (6) in scalar case.

Section 5.

By straightforward calculation, one can verify that the infinitesimal scattering matrix (4) satisfies the following extended unitarity condition

$$\mathbf{H}^{pr} + i\mathbf{H}^{ev}\Sigma_x)\delta\mathbf{S} + [(\mathbf{H}^{pr} + i\mathbf{H}^{ev}\Sigma_x)\delta\mathbf{S}]^{\dagger} = 0$$
(10)

where \mathbf{H}^{pr} and \mathbf{H}^{ev} denote projectors on propagating and evanescent waves, respectively, and $\Sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ is a block Pauli matrix (see [3]). On the other hand, one can also prove that the *star product* of two S-matrices does satisfies the extended unitarity from [3] in the form

$$\mathbf{H}^{pr}\mathbf{S})^{\dagger}(\mathbf{H}^{pr}\mathbf{S}) = \mathbf{H}^{pr}\mathbf{I}\mathbf{H}^{pr} - i[\mathbf{H}^{ev}\Sigma_{x}\mathbf{S} - (\mathbf{H}^{ev}\Sigma_{x}\mathbf{S})^{\dagger}]$$
(11)

if the both S-matrices satisfy (11) separately. Bearing in mind that the star product is associative [4], we conclude that a solution to the derived Riccati system of equations satisfies the extended unitarity (11).

Section 6.

The transfer matrix \mathbf{M} transforms, in different from the \mathbf{S} -matrix, the angular spectrum amplitudes of forward and backward going waves on the left side of the structure into ones on the right side of the structure. This definition gives the known relation between matrices under consideration (see, e. g., [2]) and leads from the derived Riccati-system of equations to the following linear differential equation for the transfer matrix

$$\frac{d\mathbf{M}}{dz} = \Sigma_z \delta \mathbf{S} \mathbf{M}, \qquad \mathbf{M}(z=0) = \mathbf{I}$$
(12)

were $\Sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$ is a block Pauli matrix. Starting with the extended unitarity (10) for the infinitesimal scattering matrix one can verify by direct differentiation that a solution to the obtained linear equation has an energy invariat in a form of the following extended pseudu-nitarity for the transfer matrix

$$\mathbf{I}^{\dagger}\Sigma_{z}(\mathbf{H}^{pr} - i\Sigma_{x}\mathbf{H}^{ev})\mathbf{M} = \Sigma_{z}(\mathbf{H}^{pr} - i\Sigma_{x}\mathbf{H}^{ev})$$
(13)

This extended pseudu-unitarity for the transfer matrix generalizes the known pseudu-unitarity constraint [6] on the case when evanescent waves may be present.

7. Conclusion

Summarizing, the presented complete system of differential equations for blocks of the S-matrix and differential equation for the transfer matrix together with their energy invariants can be considered as an analytical basis to incorporate the modern theory of electromagnetic wave multiple scattering by dielectric structures with near field effects.

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