Solving diffraction problems by the *T*-matrix and the pattern equations methods

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T-matrix method is compared to the pattern equation method. It is shown that the pattern equation method allows analytical averaging of particle orientation, as well as the *T*-matrix method. However, the pattern equation method is applicable to diffraction problems for a broader class of particle geometry and gives higher accuracy than the *T*-matrix method.

INTRODUCTION

The *T*-matrix method (TMM), proposed by Waterman more than forty years ago [1], is currently commonly used for solving wave diffraction problems arising in optics, radio physics, radio astronomy, etc. [2, 3]. *T* matrix interrelates incident and scattered wave spherical basis expansion coefficients. As such, *T* matrix depends only on physical and geometric characteristics of a scatterer and is absolutely independent on propagation and polarization directions of the incident and scattered fields [2, 3].

The pattern equation method, for the first time proposed in paper [4], also allows obtaining the solution of the diffraction problem in the form similar to TMM, but it is applicable at significantly less stringent restrictions on scatterer geometry. Therefore, it is of interest to compare these two methods.

TMM AND PEM ALGORITHMS

In paper [5], it is shown that TMM is correct only if the scatterer geometry belongs to the class of Rayleigh bodies, i.e. such bodies that all wave field analytic continuation singularities are located inside of the sphere inscribed in a scatterer. Such class of geometries is particularly narrow.

PEM allows to obtain the rigorous diffraction problem solution (i.e. theoretically with any given accuracy) for so called weakly non-convex bodies [4]. All convex bodies are part of this class.

Let us perform a more detailed comparison of both methods. Consider two-dimensional diffraction problem on a scatterer with Dirichlet boundary condition for simplicity. As is well known, the scattered field cylindrical harmonic expansion

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$u^1(\vec{r}) = \sum_{n=-\infty}^{\infty} c_n H_n^{(2)}(kr) e^{in\varphi}$ coefficients c_n are related to the incident field (plane wave, propagating at angle φ_0 to the OX axis) expansion coefficients a_n by the following formula

$$\overline{c} = T\overline{a}\,, \tag{1}$$

where $T = QH^{-1}$, and

$$a_n = -(-i)^n e^{-in\varphi_0}\,, \tag{2}$$

$$Q_{nm} = \int_0^{2\pi} J_n(k\rho(\varphi)) e^{i(m-n)\varphi} d\varphi, \quad H_{nm} = \int_0^{2\pi} H_n^{(2)}(k\rho(\varphi')) e^{i(m-n)\varphi'} d\varphi'. \tag{3}$$

In PEM, similar to Eq. (1) formula is given by:

$$\overline{c} = (I - G)^{-1} \overline{c}^0\,, \tag{4}$$

where I is the identity matrix and matrix G and vector $\overline{c}^0$ elements are given by [4]:

$$G_{nm} = \frac{1}{4} \int_0^{2\pi} J_n(k\rho(\varphi)) \left[ik\rho(\varphi) H_m^{(2)\prime}(k\rho) + m \frac{\rho'(\varphi)}{\rho(\varphi)} H_m^{(2)}(k\rho) \right] e^{i(m-n)\varphi} d\varphi\,, \tag{5}$$

$$c_n^0 = \frac{k}{4} \int_0^{2\pi} J_n(k\rho(\varphi)) \left[\rho(\varphi)\cos(\varphi - \varphi_0) + \rho'(\varphi)\sin(\varphi - \varphi_0) \right] e^{-ik\rho(\varphi)\cos(\varphi-\varphi_0) - in\varphi} d\varphi\,. \tag{6}$$

Obviously, although values c_n^0 are not incident wave cylindrical basis expansion coefficients, but similarly to a_n coefficients in TMM, they depend (functionally) on the incident plane wave angle φ_0 only. As can be seen from Eqs. (5) and (6), in order to find vector $\overline{c}$ in PEM, it is necessary to invert the matrix with much more complex element formulas than in TMM. However, the inverted matrix $(I - G)^{-1}$ is already essentially a T matrix that links vector $\overline{c}^0$, characterizing the incident wave, to the scattered wave coefficients $\overline{c}$, while in TMM, in order to obtain T matrix, it is still necessary to perform matrix Q and H^{-1} multiplication (although those matrices are significantly more simple). Therefore, it is of interest to compare the computation speed and accuracy for both methods.

NUMERICAL RESULTS

As an example, let us consider the diffraction problem for a plane wave with incident angle $\varphi_0 = 0$ on Rayleigh ellipse with semiaxes $ka = 8,\ kc = 11$. We calculate the scattering pattern as:

$$g(\varphi) = \sum_{n=-\infty}^{\infty} c_n i^n e^{in\varphi} . \tag{7}$$

Let us denote $g_N(\varphi)$ - the scattering pattern, obtained by solving the truncated system (when its size is equal to $2N+1 \times 2N+1$). We calculate the difference between the patterns at different N as $\Delta g_{N_1,N_2}^{\max} = \max\left|g_{N_1}(\varphi) - g_{N_2}(\varphi)\right|$. If $\Delta g_{N_1,N_2}^{\max} < 10^{-6}$, i.e. at least 7 significant digits are agreeing in the patterns, we consider that adequate accuracy is achieved and there is no point to increase N any more. Additionally, we assess the graphic overlap of patterns.

The calculated values of $\Delta g_{N_1,N_2}^{\max}$ at different N_1, N_2 for PEM and TMM are given in Table 1.

Table 1.

	PEM	TMM
$\Delta g_{10,15}^{\max}$	$4.7334279 \cdot 10^{-1}$	$4.7133309 \cdot 10^{-1}$
$\Delta g_{15,20}^{\max}$	$6.0765886 \cdot 10^{-4}$	$1.1055532 \cdot 10^{-2}$
$\Delta g_{20,25}^{\max}$	$3.3979730 \cdot 10^{-7}$	$1.7063574 \cdot 10^{-4}$
$\Delta g_{25,30}^{\max}$	$2.4759473 \cdot 10^{-11}$	$1.6644684 \cdot 10^{-6}$
$\Delta g_{30,35}^{\max}$	$8.3348103 \cdot 10^{-14}$	$3.2701861 \cdot 10^{-6}$

As it shows, the PEM has much higher convergence rate and allows obtaining twice as good accuracy than TMM. In PEM, we have reached the desired accuracy of 10^{-6} already at $N = 20$, whereas TMM did not obtain the desired accuracy at all. The highest possible accuracy, which PEM provides for a given scatterer, is $8.3348103 \cdot 10^{-14}$, but TMM achieves only $1.6644684 \cdot 10^{-6}$. As it can be seen, at $N > 35$ for PEM and at $N > 25$ for TMM, the accuracy begins to decrease. This is caused by the increase of special function calculation error, which eventually leads to the failure of the algorithm (see [5]).

Let us now compare the computation time. At $N = 20$, the computation time of PEM is 10.779 seconds and TMM is 9.224 seconds. At $N = 35$, the computation time of PEM is 50.136 seconds and TMM is 21.502 seconds.

We can see that, at smaller N values, the computation time is about the same for both methods, but as N increases, the computation time for PEM becomes significantly longer. The explanation is that in the case of TMM we calculate $(2N+1)^2$ times a rather simple integral Eq. (3), whereas in the case of PEM we calculate $(2N+1)^2$ times a much more complicated integral Eq. (5) plus $2N+1$ times integral Eq. (6). However, during the first 10 seconds using PEM, we obtained the accuracy of 10^{-10}, while using TMM for the same time we obtained only 10^{-5}.

As already mentioned above, the applicability of PEM (any weak non-convex bodies) is much broader than the applicability of TMM (only Rayleigh bodies). This is another major advantage of PEM. Some examples illustrating inapplicability of TMM to non- Rayleigh geometries can be found in [5].

Let us now consider the particle irradiated by a plane wave, incident at random angles φ_0. We can calculate scattering characteristics of the particle averaged by irradiation angles. For example, the single-particle scattering cross section $\langle C_{sca} \rangle$, averaged over the ensemble of random orientations, can be calculated in the *T*-matrix method as [2] $\langle C_{sca} \rangle = \sum_n \sum_m |T_{nm}|^2$ (see also Eq. (1) and Eq. (7)). Similarly, as follows from the equations (4) and (7), in the method of pattern equations the same value can be calculated as $\langle C_{sca} \rangle = \sum_n \sum_m \sum_p |(I-G)^{-1}_{nm}| C_{mp}$, where $C_{mp} = \frac{1}{2\pi} \int_0^{2\pi} c_m^0 c_p^{0*} d\varphi_0$. Our simulations show that equal accuracy of the $\langle C_{sca} \rangle$ requires twice as much computation time using the pattern equation method, relative to the *T*-matrix method.

To summarize, the comparison of PEM and TMM clearly demonstrates that PEM is unconditionally superior to TMM in terms of accuracy and applicability. The price for this is some increase of computation time. The averaging of scattering characteristics by orientation of the particle is similarly simple in both PEM and TMM.

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