ISSN 0027-1349, Moscow University Physics Bulletin, 2015, Vol. 70, No. 4, pp. 258–262. © Allerton Press, Inc., 2015.
Original Russian Text © Yu.A. Eremin, A.G. Sveshnikov, 2015, published in Vestnik Moskovskogo Universiteta. Fizika, 2015, No. 4, pp. 43–46.

OPTICS AND SPECTROSCOPY. LASER PHYSICS

An Optical Theorem for Local Sources in Diffraction Theory

Yu. A. Eremin[a] and A. G. Sveshnikov[b]

[a] *Department of Computational Mathematics and Cybernetics, Moscow State University, Moscow, 119991 Russia*
[b] *Department of Physics, Moscow State University, 119991 Russia*
e-mail: eremin@cs.msu.ru, sveshnikov@phys.msu.ru

Received February 20, 2015; in final form, April 29, 2015

Abstract—The optical theorem is generalized for the case of excitation of local structures by point sources. It is shown that an essential parameter, the Purcell factor, can be represented in analytical form. The results are generalized for the case of an interface between two semi-spaces. These results are of paramount importance for averaging of the coefficient of fluorescence amplification and the efficiency of an optical antenna by the position of an excitation source.

Keywords: optical theorem, local source, Purcell factor.

DOI: 10.3103/S0027134915040086

INTRODUCTION

The optical theorem (OT) is a relationship that connects an entire scattering cross section, an absorption cross section, and the so-called extinction cross section [1]. This concept appeared for the first time in [2]. The extinction cross section describes the interaction between incident external radiation, for example, a plane wave, and a scattered field in the direction of a transmitted wave. Therefore, the OT can be written as follows:

$$C_{ext} = C_{sc} + C_{abs}, \tag{1}$$

where C_{sc}, C_{abs} are the scattering and absorption cross sections, respectively. The OT is used in many applications of the diffraction theory of waves [3, 4]. Generalizations of the OT in the case of diffraction of a plane wave on a local body in the presence of a semi-space are known [5, 6]. In computational diffraction it is applied for the estimation of the correctness of a computer modulus via the calculation of the discrepancy of relationship (1) [7, 8]. Recently, researchers are interested in analysis of the fluorescence processes in the presence of plasmon structures. These structures, plasmon particles, provide a considerable increase in the intensity of optical radiation [9–11]. In this case it is necessary to analyze the scattering and absorption characteristics of plasmon structures upon excitation by a local source (fluorescent molecule) that is located immediately adjacent to a similar structure. The amplification factor of fluorescence is usually averaged by the position of a local source, which requires repeated calculations of the scattering and absorption cross sections. Another field in which the excitation of a plasmon structure by a point source is considered is the design of optical antennas [12–14]. For the optimization of the efficiency of an optical antenna [14], it is necessary to repeatedly solve the problem of the excitation of a cluster of plasmon particles by a point emitter that changes its position. At the same time, the necessity for the multiple calculation of the amplifying factor of fluorescence and efficiency of the optical antenna leads to the necessity of the calculation of the absorption cross section, which is very difficult under the regime of plasmon resonance, when the relative field strength near particles increases by 10^8–10^{10} times [15, 16].

In this work, the problem of the diffraction of a point source on a local body either in free space R^3 or in the presence of a semi-space is considered. It is shown that a relationship that is similar to (1) exists, which makes it possible to calculate the amplification factor of the fluorescence and the efficiency of an optical antenna without calculating of the absorption cross section, which considerably decreases calculation expenses.

1. THE OPTICAL THEOREM FOR LOCAL SOURCES IN FREE SPACE

We will consider the mathematic statement of the problem of the diffraction field of a point source that is located at the point $M_0 \in R^3$ on a local permeable body D_i that has a smooth surface $S \in C^{(2,\alpha)}$. It is assumed that the mathematical statement of the problem is

$$\begin{gathered} \Delta U_0 + k_0^2 U_0 = -\delta(M, M_0), \quad M_0 \in D_0 := R^3/\bar{D}_i; \\ \Delta U_i + k_i^2 U_i = 0, \quad M \in D_i; \\ [U(P)] = [\partial U(P)/\partial n] = 0, \quad P \in S; \end{gathered} \tag{2}$$

$$\frac{\partial U_0}{\partial r} + jk_0 U_0 = o(1/r), \quad r := |M| \longrightarrow \infty.$$

Here [.] indicates to a jump in the field upon a transition over S and n is normal to the surface S. $\mathrm{Im} k_i^2 < 0$, which corresponds to the time dependence of $\exp\{j\omega t\}$. It is known that problem (1) has only one solution [17].

We will choose the origin of the coordinates at a point of the source M_0; we surround the diffuser by a sphere of radius R with its center in the origin of the coordinates that contain D_i. We will designate the area in space that is outlined by the sphere Σ_R and the surface S by D_R. We will apply the second Green formula to U_0 and U_0^* inside D_R:

$$\int_{D_R} (\Delta U_0 U_0^* - \Delta U_0^* U_0) d\tau = \int_{\Sigma_R + S} \left\{ \frac{\partial U_0}{\partial n} U_0^* - \frac{\partial U_0^*}{\partial n} U_0 \right\} d\sigma, \quad (3)$$

where $\frac{\partial}{\partial n}$ is the normal derivative to the respective surface directed outside of D_R. The left side of (3) is transformed regarding (2) as

$$\int_{D_R} (\Delta U_0 U_0^* - \Delta U_0^* U_0) d\tau = 2j \mathrm{Im} U_0(M_0). \quad (4)$$

The right part of (3) can be written as

$$2j \mathrm{Im} \int_{\Sigma_R} \frac{\partial U_0}{\partial n} U_0^* d\sigma - 2j \mathrm{Im} \int_S \frac{\partial U_0}{\partial n^+} U_0^* d\sigma,$$

where $\frac{\partial}{\partial n^+}$ is the normal derivative by the external normal to D_i. We will consider the first integral. Due to the radiation conditions, we obtain

$$\lim_{R \to \infty} \int_{\Sigma_R} \frac{\partial U_0}{\partial r} U_0^* d\sigma = -jk_0 \lim_{R \to \infty} \int_{\Sigma_R} |U_0|^2 d\sigma_r.$$

Taking the fact into account that (3) is true for any $R \longrightarrow \infty$, and using the determination for the directional pattern of the field U_0 [17],

$$U_0(M) = \frac{e^{-jk_0 r}}{k_0 r} F(\vartheta, \varphi) + o(1/r), \quad r \longrightarrow \infty.$$

We obtain

$$\lim_{R \to \infty} \int_{\Sigma_R} |U_0|^2 d\sigma_r = \frac{1}{k_0^2} \int_{\Omega} |F(\vartheta, \varphi)|^2 d\omega, \quad (5)$$

where Ω is a unit sphere. Therefore,

$$\mathrm{Im} \lim_{R \to \infty} \int_{\Sigma_R} \frac{\partial U_0}{\partial r} U_0^* d\sigma = -\frac{1}{k_0} \int_{\Omega} |F|^2 d\omega. \quad (6)$$

We will now apply the second Green formula to U_i and U_i^* inside D_i:

$$\int_{D_i} (\Delta U_i U_i^* - \Delta U_i^* U_i) d\tau = \int_S \left\{ \frac{\partial U_i}{\partial n^+} U_i^* - \frac{\partial U_i^*}{\partial n^+} U_i \right\} d\sigma.$$

Transforming the last relationship and using the field conjugation conditions on S, we have

$$\mathrm{Im} k_i^2 \int_{D_i} |U_i|^2 d\tau = \mathrm{Im} \int_S \frac{\partial U_0}{\partial n} U_i^* d\sigma. \quad (7)$$

Taking the obtained relationships (4)–(7) into account we have

$$\mathrm{Im} U_0(M_0) = -\frac{1}{k_0} \int_{\Omega} |F|^2 d\omega - \left|\mathrm{Im} k_i^2\right| \int_{D_i} |U_i|^2 d\tau. \quad (8)$$

We will describe in detail the left part, taking the fact into account that $U_0(M) = U_0^s(M) + \frac{e^{-jk_0 R_{MM_0}}}{4\pi R_{MM_0}}$. Here U_0^s is the scattered field. Then

$$\lim_{M \to M_0} U_0(M) = U_0^s(M_0) - \frac{k_0}{4\pi}.$$

Finally, the OT for the local source of external excitation takes a form that is absolutely similar to (1)

$$\frac{1}{4\pi} - \frac{1}{k_0} \mathrm{Im} U_0^s(M_0) = \frac{1}{k_0^2} \int_{\Omega} |F|^2 d\omega + \frac{\left|\mathrm{Im} k_i^2\right|}{k_0} \int_{D_i} |U_i|^2 d\tau. \quad (9)$$

As before, $U_0^s(M_0)$ is nothing other than the term that describes the interaction between the scattered field and the external radiation of the local source.

As a consequence, in the case of the absence of local heterogeneity of D_i, the entire scattering cross section of a point source $\frac{e^{-jk_0 R_{MM_0}}}{4\pi R_{MM_0}}$ is

$$\frac{1}{4\pi} = \frac{1}{k_0^2} \int_{\Omega} |F^0|^2 d\omega.$$

In the studies of the effect of plasmon structures on a fluorescent molecule, the Purcell factor is usually estimated, which is [14]

$$F_p = \frac{\sigma_{sc} + \sigma_{abs}}{\sigma_{sc}^0},$$

where σ_{sc}^0 is the scattering cross section of the source in the absence of heterogeneity. Then, in view of these results, we have

$$F_p = 1 - \frac{4\pi}{k_0^2} \operatorname{Im} U_0^s(M_0). \tag{10}$$

Therefore, it is not necessary to calculate the scattering and absorption cross sections, σ_{sc} and σ_{abs}, and the Purcell factor can be expressed using the value of the scattered field at only one point, the point where the local radiation source is located. It should be noted that such a circumstance is especially important, since the Purcell factor is usually averaged over many positions of a point source.

2. THE OPTICAL THEOREM FOR LOCAL SOURCES IN THE PRESENCE OF A TRANSPARENT SEMI-SPACE

We will consider a mathematical statement of the diffraction problem for the field of a point source set at the point M_0 on a local permeable body D_i with a smooth surface $S \in C^{(2,\alpha)}$. It is assumed that all of the $\Re^3$ space is divided by the plane Ξ, $(z = 0)$ into two semi-spaces D_l with the wavenumbers k_l, $l = 0,1$. We will assume that the source is in the upper semi-space, D_0, $(z > 0)$ on the Z-axis at the point $(0, 0, z_0)$. Then, the mathematical statement of the problem can be written as:

$$\begin{gathered}\Delta U_0 + k_0^2 U_0 = -\delta(M, M_0), \quad M_0 \in D_0;\\ \Delta U_i + k_i^2 U_i = 0, \quad M \in D_i;\\ \Delta U_1 + k_1^2 U_1 = 0, \quad M \in D_1;\\ [U(P)] = [\partial U(P)/\partial n] = 0, \quad P \in S;\\ [U(Q)] = [\partial U(Q)/\partial z] = 0, \quad Q \in \Xi;\\ \frac{\partial U_l}{\partial r} + jk_l U_l = o(1/r), \quad l = 0, 1, \quad r := |M| \longrightarrow \infty.\end{gathered} \tag{11}$$

We will assume that $\operatorname{Im} k_i^2 < 0$, and $\operatorname{Im} k_l^2 = 0$, $l = 0.1$. Then, the problem (11) has a unique solution.

In this case the origin of the coordinates is chosen on the Ξ plane. We will perform all constructions in the same manner as that in the previous section, only taking different moments into account. We will choose the sphere Σ_R with the center at the origin of the coordinates such that it would include the source and the diffuser D_i inside. We will designate the circle cut by the sphere on the plane Ξ, as C_R. We will designate the space inside the sphere Σ_R as D_R. It consists of two semi-spheres $D_R = D_R^+ \cup D_R^-$, each of which is limited by two surfaces $\Sigma_R^+ \cup C_R$ and $\Sigma_R^- \cup C_R$. Applying the second Green formula inside D_R^+ to U_0 and U_0^*, we have

$$2j \operatorname{Im} U_0(M_0) = 2j \operatorname{Im}\left\{ \int_{\Sigma_R^+} \frac{\partial U_0}{\partial n} U_0^* d\sigma - \int_S \frac{\partial U_0}{\partial n^+} U_0^* d\sigma - \int_{C_R} \frac{\partial U_0}{\partial z} U_0^* d\sigma \right\}. \tag{12}$$

By applying the second Green formula to U_1 and U_1^* in D_R^-, we have

$$\operatorname{Im} \int_{\Sigma_R^-} \frac{\partial U_1}{\partial r} U_1^* d\sigma + \operatorname{Im} \int_{C_R} \frac{\partial U_1}{\partial z} U_1^* d\sigma = 0. \tag{13}$$

Similarly to the previous case, we obtain the following expressions for the integrals by the remote semi-spheres $\Sigma_R^\pm$:

$$\operatorname{Im} \lim_{R \to \infty} \int_{\Sigma_R^\pm} \frac{\partial U_l}{\partial n} U_l^* d\sigma = -\frac{1}{k_l} \int_{\Omega^\pm} |F_l|^2 d\omega, \tag{14}$$

where $F_1(\vartheta, \varphi)$ are the diagrams of field scattering U_l, $l = 0, 1$ on unit semi-spheres $\Omega^\pm$. Taking (13)–(14) and (7)–(8) into account and the conjugation conditions for the fields on C_R, we have

$$\lim_{M \to M_0} \operatorname{Im} U_0(M) = -\frac{1}{k_0} \int_{\Omega^+} |F_0|^2 d\omega - \left|\operatorname{Im} k_i^2\right| \int_{D_i} |U_i|^2 d\tau - \frac{1}{k_1} \int_{\Omega^+} |F_1|^2 d\omega. \tag{15}$$

Here, it seems that the same approach could be applied as in the previous case; however, in the case of the presence of a semi-space or layered medium, the solution to the diffraction problem is built in another way [18]. In particular, the entire field is divided into the field of a source, which meets the conjunction conditions on Ξ plane, and a scattered field, which also should meet these conditions. Therefore, in this case the field in the upper half-plane $U_0(M) = U_0^s(M) + U_0^0(M)$, where U_0^0 is the field of the source that meets the conjugation conditions on Ξ plane.

This is represented in the form of a Sommerfeld integral [19]:

$$U_0^0(M, M_0) = \frac{1}{4\pi}\int_0^\infty J_0(\lambda r)\nu(\lambda, z, z_0)\lambda d\lambda, \quad (16)$$

where $J_0(.)$ is the Bessel function, $r^2 = \rho^2 + (z - z_0)^2$, and ν is a spectral function, which provides fulfillment of the conjugation conditions at $z = 0$ [20]. It has the following form:

$$\nu(\lambda, z, z_0) = \begin{cases} \dfrac{\exp(-\eta_0|z - z_0|)}{\eta_0} + \dfrac{\eta_0 - \eta_1}{\eta_0 + \eta_1} \\ \times \dfrac{\exp(-\eta_0|z - z_0|)}{\eta_0}, \quad z \ge 0 \\ \dfrac{2\eta_0}{\eta_0 + \eta_1}\dfrac{\exp\{\eta_1 z - \eta_0 z_0\}}{\eta_0}, \quad z \le 0 \end{cases} \quad (17)$$

$$z_0 > 0,$$

here $\eta_l^2 = \lambda^2 - k_l^2$, $l = 0, 1$. It should be noted that the first term in (17) corresponds to the fundamental solution to the Helmholtz equation in free space. Then

$$\lim_{M \to M_0} \operatorname{Im} U_0(M) = \operatorname{Im} U_0^s(M_0) - \frac{k_0}{4\pi} + \frac{1}{4\pi}\lim_{M \to M_0} \operatorname{Im}\int_0^\infty J_0(\lambda r)\tilde{\nu}(\lambda, z, z_0)\lambda d\lambda, \quad (18)$$

where $\tilde{\nu}$ is the second term in the first line of (17). We will consider the last integral in (18) in more detail:

$$\lim_{M \to M_0} \operatorname{Im}\int_0^\infty J_0(\lambda r)\tilde{\nu}(\lambda, z, z_0)\lambda d\lambda = \operatorname{Im}\int_0^\infty \tilde{\nu}(\lambda, z, z_0)\lambda d\lambda = \operatorname{Im}\int_0^\infty \frac{\eta_0 - \eta_1}{\eta_0 + \eta_1}\frac{\exp\{-2z_0\eta_0\}}{\eta_0}\lambda d\lambda. \quad (19)$$

On the condition that $k_1^2 > k_0^2$ (the lower space is denser), we have

$$\operatorname{Im}\int_0^\infty \frac{\eta_0 - \eta_1}{\eta_0 + \eta_1}\frac{\exp\{-2z_0\eta_0\}}{\eta_0}\lambda d\lambda = \operatorname{Im}\int_0^{k_1} \frac{\eta_0 - \eta_1}{\eta_0 + \eta_1}\frac{\exp\{-2z_0\eta_0\}}{\eta_0}\lambda d\lambda.$$

Thus, the optical theorem for a local source takes the form

$$\frac{1}{4\pi} - \frac{1}{4\pi k_0}\operatorname{Im}\int_0^{k_1} \frac{\eta_0 - \eta_1}{\eta_0 + \eta_1}\frac{\exp\{-2z_0\eta_0\}}{\eta_0}\lambda d\lambda$$

$$-\frac{1}{k_0}\operatorname{Im} U_0^s(M_0) = \frac{1}{k_0^2}\int_{\Omega^+}|F_0|^2 d\omega + \frac{1}{k_1 k_0}\int_{\Omega^-}|F_1|^2 d\omega + \frac{|\operatorname{Im} k_i^2|}{k_0}\int_{D_i}|U_i|^2 d\tau. \quad (20)$$

In this case, in absence of the heterogeneity D_i for the point source, we have

$$\frac{1}{4\pi} - \frac{1}{4\pi k_0}\operatorname{Im}\int_0^{k_1} \frac{\eta_0 - \eta_1}{\eta_0 + \eta_1}\frac{\exp\{-2z_0\eta_0\}}{\eta_0}\lambda d\lambda = \frac{1}{k_0^2}\int_{\Omega^+}|F_0^0|^2 d\omega + \frac{1}{k_1 k_0}\int_{\Omega^-}|F_1^0|^2 d\omega. \quad (21)$$

Then, in view of these results, we have for Purcell factor the following expression

$$F_P = 1 - \frac{4\pi}{k_0}\operatorname{Im} U_0^s(M_0) \Big/ \left(1 - \frac{1}{k_0}\operatorname{Im}\int_0^{k_1} \frac{\eta_0 - \eta_1}{\eta_0 + \eta_1} \times \frac{\exp\{-2z_0\eta_0\}}{\eta_0}\lambda d\lambda\right). \quad (22)$$

As is seen from the latter relationship, if $k_1 \longrightarrow k_0$, formula (22) automatically is transformed into the previously obtained relationship, since $\eta_1 \longrightarrow \eta_0$.

CONCLUSIONS

In this work the optical theorem is generalized in the case of the excitation of local structures by a point source, including the case where the entire space is divided into two semi-spaces with different characteristics. It was shown that the obtained relationship makes it possible to calculate the sum of the scattering and absorption cross sections in a closed analytical form by calculating just the scattered field at a unique point. These results are of paramount importance for considering the excitation of plasmon structures, since they decrease the cost of the averaging procedure of the amplification factor of fluorescence considerably and that for calculating the efficiency of an optical antenna by the position of a source.

REFERENCES

1. R. G. Newton, J. Phys. **44**, 639 (1976).
2. J. D. Jackson, *Classical Electrodynamics* (Wiley, New York, 1962).
3. M. I. Mishchenko, L. D. Travis, and A. A. Lacis, *Scattering, Absorption, and Emission of Light by Small Particles* (Cambridge Univ. Press, Cambridge, 2002).
4. M. I. Mishchenko, J. Quant. Spectrosc. Radiat. Transfer **101**, 404 (2006).

5. Yu. A. Eremin, Differ. Equations **43**, 1194 (2007).
6. P. S. Carney, J. C. Schotland, and E. Wolf, Phys. Rev. E **70**, 036611 (2004).
7. D. W. Mackowski, J. Opt. Soc. Am. A **11**, 2851 (1994).
8. V. G. Farafonov and V. B. Il'in, *Light Dispersion by Heterogeneous Non-Spherical Particles* (VVM, St. Petersburg, 2009).
9. P. Anger, P. Bharadwaj, and L. Novotny, Phys. Rev. Lett. **96**, 113002 (2006). http://dx.doi.org10.1103/PhysRevLett.96.113002
10. J.-W. Liaw, H.-Y. Tsai, and C.-H. Huang, Plasmonics **7**, 543 (2012). doi 10.1007/s11468-012-9341-9
11. J.-W. Liaw and C.-Y. Jiang, J. Quant. Spectrosc. Radiat. Transfer **114**, 56 (2013). doi 101016/j.jqsrt/2012.08.024
12. L. Novotny and N. van de Hulst, Nat. Photonics **5**, 83 (2011). doi: 10.1038/nphoton.2010.237
13. L. Tang, S. E. Kocabas, S. Latif, A. K. Okyay, D. S. Ly-Gagnon, K. C. Saraswat, and D. A. B. Miller, Nat. Photonics **2**, 226 (2008).
14. L. Novotny and B. Hecht, *Principles of Nano-Optics* (Cambridge Univ. Press, Cambridge, 2006).
15. J.-W. Liaw, C.-S. Chen, and J.-H. Chen, J. Quant. Spectrosc. Radiat. Transfer **111**, 454 (2010).
16. Yu. A. Eremin, N. V. Grishina, E. Eremina, and T. Wriedt, J. Mod. Opt. **60**, 529 (2013). doi 10.1080/09500340.2013.794393
17. D. Colton and R. Kress, *Integral Equation Methods in Scattering Theory* (Wiley, New York, 1983).
18. Yu. A. Eremin and A. G. Sveshnikov, Moscow Univ. Phys. Bull. **68**, 443 (2013). doi: 10.3103/S0027134913060039
19. V. I. Dmitriev and E. V. Zakharov, *Integral Equation Methods in Computer Electrodynamics* (MAKS, Moscow, 2008) [in Russian].
20. A. V. Baryshev and Yu. A. Eremin, Mat. Model. **22** (5), 122 (2010). http://mi.mathnet.ru/mm2978

Translated by E. Borisenko