RADIATION ABSORPTION IN A BOUNDED PART OF A SPHERICAL PARTICLE

V.A. Babenko

B.I. Stepanov Institute of Physics, National Academy of Sciences, Minsk, Belarus Received March 31, 1998

Absorption power in a bounded internal part of a particle is described by semianalytical expressions obtained on the base of two different approaches (surface Poynting integral and volume integral) within the frameworks of Mie theory applied to a homogeneous sphere. This enables one to estimate heat release from "hotB points. The expressions are simplified with the allowance for contribution from only one resonant mode. The developed algorithms and programs are efficient from the computational viewpoint. Illustrative calculations are performed for water particles excited at laser wavelengths and for some model particles in the presence of morphological absorption resonance.

1. INTRODUCTION

Calculation of absorption power in a bounded part V of a spherical particle is very useful in many problems of nonlinear optics of disperse media, e.g., in studying interaction between high-power electromagnetic radiation and isolated aerosol particles (especially in the presence of the so-called morphologic resonance¹) and in estimating the efficiency of the pump energy conversion in microlasers (see, for instance, Ref. 2). In its most general formulation the problem has no analytical solution. In practice, it is reduced to numerical volume integration of the inner field intensity. This is difficult to be done at small values of the absorption index due to rapidly oscillating structure of the field. However, the problem can be simplified if one takes into account the fact that practically interesting "hot pointsB are on the sphere's large axis coinciding with the direction of the incident wave's propagation.³ In this case, a rotationally symmetric body whose axis coincides with the abovementioned direction can be taken as V.

Let us specify the geometry of the problem. A plane monochromatic (exp $(-i\omega t)$), linearly polarized (the vector **E** oscillates along the *x* axis) electromagnetic wave with the amplitude E_0 falls onto a spherical homogeneous particle of the radius *R* with the complex refractive index $m = N + i\kappa$ (the center of the particle coincides with the origin of a Cartesian, *x*, *y*, *z*, and spherical, *r*, θ , ϕ , coordinate systems) along the positive direction of the *z* axis. The volume *V* is bounded by a cone-shaped surface $S_3(\theta = \Theta)$ and two spherical surfaces $S_1(r = r_1)$ and $S_2(r = r_2)$. For $\Theta = \pi/2$, π , this reduces to the earlier considered cases of a hemisphere⁴ and a concentric layer.^{5,6}

2. SURFACE INTEGRAL

According to Poynting's theorem the absorption power inside a volume bounded by a closed surface $S = S_1 + S_2 + S_3$ is equal to

$$W_{\rm abs} = -\frac{1}{2} \operatorname{Re} \int_{S} \left[\mathbf{E} \times \mathbf{H}^* \right] \cdot \mathbf{n} \, \mathrm{d}S, \tag{1}$$

where **n** is the exterior normal vector to the surface S; * is the complex conjugate; (**E**, **H**) are the electric and magnetic interior fields of the sphere, their components have the form⁷

$$\begin{pmatrix} E_r \\ (\mu_0/\varepsilon_0)^{1/2} H_r \end{pmatrix} = \frac{E_0 \sin\theta}{(m\rho a)^2} \begin{pmatrix} \cos\phi \\ m \sin\phi \end{pmatrix} \sum_{n=1}^{\infty} i^{n-1} \begin{pmatrix} Z_n \\ X_n \end{pmatrix} \pi_n;$$
(2)
$$\begin{pmatrix} E_\theta \\ E_\phi \end{pmatrix} = \frac{E_0}{m\rho a} \begin{pmatrix} \cos\phi \\ -\sin\phi \end{pmatrix} \sum_{n=1}^{\infty} \gamma_n \left[X_n \begin{pmatrix} \pi_n \\ \tau_n \end{pmatrix} - iV_n \begin{pmatrix} \tau_n \\ \pi_n \end{pmatrix} \right];$$
(3)
$$\begin{pmatrix} H_\theta \\ H_\phi \end{pmatrix} = \frac{E_0}{\rho a} \left(\frac{\varepsilon_0}{\mu_0} \right)^{1/2} \begin{pmatrix} \sin\phi \\ \cos\phi \end{pmatrix} \times$$

$$\times \sum_{n=1}^{\infty} \gamma_n \left[Z_n \begin{pmatrix} \pi_n \\ \tau_n \end{pmatrix} - i Y_n \begin{pmatrix} \tau_n \\ \pi_n \end{pmatrix} \right].$$
(4)

Here $\gamma_n = i^n / n(n + 1)$; ε_0 , μ_0 are electric and magnetic constants; $\rho = k_0 R$ is the diffraction parameter; $k_0 = 2\pi / \lambda$ is the wave number in the ambient space; a = r/R is the relative radial coordinate; π_n , τ_n are angular functions⁷ of the argument $\mu = \cos\theta$;

$$X_n(a) = c_n \psi_n(m\rho a) = \frac{im(2n+1) R_n(m\rho a)}{\xi_n(\rho) [G_n(\rho) - mD_n(m\rho)]},$$

$$Y_n(a) = X_n(a) D_n(m\rho a),$$

$$Z_n(a) = d_n \psi_n(m\rho a) = \frac{im(2n+1) R_n(m\rho a)}{\xi_n(\rho) [mG_n(\rho) - D_n(m\rho)]},$$

$$V_n(a) = Z_n(a) D_n(m\rho a)$$

 $D_n(z)$ and $G_n(z)$ are the logarithmic derivatives of the Riccati-Bessel and Riccati-Hankel functions⁷ $\psi_n(z)$, $\xi_n(z)$, respectively; c_n , and d_n are the amplitude coefficients of the interior field of the sphere (in contrast to Ref. 7, these include the factor (2n + 1)); $R_n(m\rho a) = \psi_n(m\rho a)/\psi_n(m\rho)$.

Let us deduce the expressions for W. The integral (1) for the fluxes through $S_{1,2}$ equals

$$W_{1,2} = \frac{a_{1,2}}{2} \operatorname{Re} \int_{0}^{\Theta} \int_{0}^{2\pi} \left(E_{\theta} H_{\phi}^{*} - E_{\phi} H_{\theta}^{*} \right)_{a=a_{1,2}} \sin\theta \, \mathrm{d}\theta \, \mathrm{d}\phi,$$

where $a_{1,2} = r_{1,2}/R$. By substituting the expansions (3)–(4) into this expression, integrating over the angle ϕ , combining the terms, and interchanging the integration and summation, we come to the expression

$$W_{\frac{1}{2}} = \pm A \operatorname{Re} \frac{1}{m} \sum_{n=1}^{\infty} \sum_{l=1}^{\infty} \gamma_n \gamma_l^* \times \left[\alpha_{nl}(a_1) f_{nl}(v) - i\beta_{nl}(a_1) h_{nl}(v) \right],$$

where

$$v = \cos\Theta; \quad A = \pi E_0^2 (\varepsilon_0 / \mu_0)^{1/2} / 2k_0^2;$$

$$\alpha_{nl}(a) = X_n(a) Z_l^*(a) + V_n(a) Y_l^*(a),$$

$$\beta_{nl}(a) = V_n(a) Z_l^*(a) - X_n(a) Y_l^*(a);$$

$$h_{nl}(v) \equiv \int_{v}^{1} H_{nl}(\mu) d\mu = \int_{v}^{1} (\pi_n \pi_l + \tau_n \tau_l) d\mu$$

$$f_{nl}(\nu) = \int_{\nu}^{1} (\pi_n \tau_l + \tau_n \pi_l) \, d\mu = (1 - \nu^2) \, \pi_n(\nu) \, \pi_l(\nu).$$

For $n \neq l$, one can obtain⁸

$$h_{nl}(v) = \frac{(1-v^2)}{(n-l)(n+l+1)} [n(n+1)\pi_n(v)\tau_l(v) - l(l+1)\tau_n(v)\pi_l(v)],$$

as for the case n = l, one can use the approach similar to that developed in Ref. 9. If one introduces an auxiliary indefinite integral $T_n(\mu)/(2n + 1) = \int (1 - \mu^2) \pi_n^2 d\mu$, it is easy to see that $H_{nn}(\mu) = n(n+1) T_n(\mu)/(2n+1) - 1$

 $-(1-\mu^2)\pi_n(\mu)\tau_n(\mu)$. The following recursion relation is valid for the index *n* for the function T_n

$$(n-1) T_n(\mu) = (n+1) T_{n-1}(\mu) +$$

+ $(1-\mu^2) \{ \mu [(n+1) \pi_{n-1}^2 + (n-1) \pi_n^2] - 2n \pi_{n-1} \pi_n \}$

with the initial value $T_1(\mu) = \mu(3 - \mu^2)$. Therefore, using the values $T_1(1)$, $T_1(\nu)$, one can obtain $T_n(1)$ and $T_n(\nu)$, then $m_n(1)$ and $m_n(\nu)$, and, finally, $h_{nn}(\nu) = H_n(1) - H_n(\nu)$ according to the recursion.

Thus, calculation of the integrals $W_{1,2}$ is reduced to calculation of a double series with respect to combinations of cylindrical and Legendre functions. For a cone-shaped boundary S_3 , the Poynting integral has the form

$$W_3 = \frac{R^2}{2} (1 - v^2)^{1/2} \times$$
$$\times \operatorname{Re} \int_{a_1}^{a_2} \int_{0}^{2\pi} \left(E_r H_{\phi}^* - E_{\phi} H_r^* \right)_{\theta = \Theta} a \, \mathrm{d}a \, \mathrm{d}\phi.$$

Substituting the components of the fields (2)–(4) for $\theta = \Theta$ into this expression and integrating over the angle ϕ , we obtain

$$W_{3} = \frac{A}{\rho} (1 - v^{2}) \times$$

 $\times \operatorname{Re} \int_{a_{1}}^{a_{2}} \left[\frac{1}{m^{2}} S_{1}(a) S_{2}^{*}(a) + \frac{1}{|m|^{2}} S_{3}^{*}(a) S_{4}(a) \right] \frac{\mathrm{d}a}{a^{2}}, \quad (5)$

where

$$\begin{pmatrix} S_1(a) \\ S_3(a) \end{pmatrix} = \sum_{n=1}^{\infty} i^{n-1} \pi_n(v) \begin{pmatrix} Z_n(a) \\ X_n(a) \end{pmatrix},$$

$$\begin{pmatrix} S_2(a) \\ S_4(a) \end{pmatrix} = \sum_{n=1}^{\infty} \gamma_n \left[\tau_n(v) \begin{pmatrix} Z_n(a) \\ X_n(a) \end{pmatrix} - i\pi_n(v) \begin{pmatrix} Y_n(a) \\ V_n(a) \end{pmatrix} \right].$$

Here, in contrast to the integrals $W_{1,2}$, it is worthless changing the order of summation and integration as the resulting integrals over quadratic combinations of cylindrical functions have no closed analytical representations and recursion relations with respect to the indices n and l.

Let us consider the computational aspects of the problem. The number of terms in the sums over indices n and l that is necessary for convergence was determined by the following formula:

 $L = \min[f L_W(\rho), f L_W(|m|\rho a)],$

where $L_W(x) = x + 4.05x^{1/3} + 2$ is the estimate of the number of terms in the Mie series in accordance with Ref. 10, and f is the empirical coefficient which exceeds unity in value (our computations of the interior field demonstrates that $f \approx 1.2$). The functions ξ_n , G_n , and R_n are calculated by the ascending

recursion,¹¹ and functions D_n by the descending recursion; the initial values D_L are calculated by the method of continued fractions.¹² The expressions (5) were integrated by the Gaussian quadrature formulas. Numerical experiments demonstrate that double precision is required in calculations at $\kappa < 10^{-5}$, while at $\kappa \approx 10^{-8}$ the computation scheme becomes unstable in some ranges of the ρ value. This is not surprising because, within the frames of the approach, absorption is considered in fact as a difference between the radiation fluxes coming into and out of a given volume. For very small κ , the difference becomes very small as compared with the above-mentioned fluxes what leads to instability of the calculations.

3. VOLUME INTEGRAL

In this situation, another one approach appeared to be useful. The approach uses volume integral. As known, absorption power in a volume V is

$$W_{\rm abs} = \frac{2\pi N\kappa}{\lambda} \left(\frac{\varepsilon_0}{\mu_0}\right)^{1/2} \int_V \left(\mathbf{E} \cdot \mathbf{E}^*\right) \,\mathrm{d}^3 \mathbf{r}. \tag{6}$$

Substituting the expansions (2) and (3) into this expression, integrating over the angle ϕ , and factoring the double sum outside the integral sign, we obtain, after some transformations, that

$$W_{abs} = A \frac{2N\kappa\rho}{|m|^2} \int_{a_1}^{a_2} \sum_{n=1}^{\infty} \sum_{l=1}^{\infty} \left\{ \frac{t_{nl}(\nu)}{|m|^2 \rho^2 a^2} \operatorname{Re} \left(i^{n-1} Z_n Z_l^* \right) + h_{nl}(\nu) \operatorname{Re} \left(\gamma_n \gamma_l^* u_{nl} \right) + f_{nl}(\nu) \operatorname{Re} \left(i\gamma_n \gamma_l^* w_{nl} \right) \right\} da, \quad (7)$$

where

$$u_{nl}(a) = X_{n}(mpa) X_{l}^{*}(mpa) + V_{n}(mpa) V_{l}^{*}(mpa),$$

$$w_{nl}(a) = X_{n}(mpa) X_{l}^{*}(mpa) + V_{n}(mpa) V_{l}^{*}(mpa),$$

$$t_{nl}(v) = \int_{v}^{1} (1 - \mu^{2}) \pi_{n} \pi_{l} d\mu.$$

The function $t_{nl}(\mathbf{v})$ can be represented analytically in the case of $n \neq l$ because

$$\int (1-\mu^2) \pi_n \pi_l d\mu = \frac{(1-\mu^2)(\tau_n \pi_l + \pi_n \tau_l)}{(n-l)(n+l+1)}$$

and for n = l it can be calculated within the recursion for $h_{nn}(v)$.

From the computational point of view, the expression (7) little differs from Eq. (5). Factoring the sums outside the integral sign is also worthless here as the integrals obtained have no analytical

representations. So, like for the W_3 flux in the case of the surface Poynting integral, the linear integral over ain Eq. (7) is to be taken numerically by the Gaussian quadrature. Certainly, this is a significant shortcoming of the approach developed here, but calculation of the linear integral (7) is, nevertheless, incommensurably easier as compared with the initial volume integral (6). Practical realization of the developed algorithms demonstrates that calculations by the program based on the surface integral are preferable at the values of the absorption index $\kappa > 10^{-6}$ as the program is much faster than that based on the volume integral. On the other hand, at a very small $\kappa \approx 10^{-7}$ and lower, the calculations may be performed only by the volume integral; however, relative slowness of this program complicates to some extent the calculations at $\rho > 150$.

4. RESONANCE

According to many papers on studying the morphological resonance, the interior field (at least at the large axis of a particle coinciding with the direction of incident beam propagation and nearby) is determined by the resonance mode under resonance conditions. In this connection, it is interesting to simplify Eq. (7) having in mind that only one resonant mode contributes into the $W_{\rm abs}$.

Let us start with the magnetic resonance. Suppose that only one amplitude coefficient c_n is different from zero. Then Eq. (7) contains only the second term

$$W_{abs}^{(n, mag)} = A \frac{2N\kappa\rho}{|m|^2} \frac{h_{nn}(\nu)}{n^2(n+1)^2} |c_n|^2 \int_{a_1}^{a_2} |\psi_n(m\rho a)|^2 da.$$

Taking into account that

$$\int \psi_n(\alpha x) \ \psi_n(\beta x) \ dx = \frac{1}{\alpha^2 - \beta^2} \times \\ \times \left[\beta \psi_n(\alpha x) \ \psi'_n(\beta x) - \alpha \psi'_n(\alpha x) \ \psi_n(\beta x) \right],$$

we come to the expression

$$W_{abs}^{(n, mag)} = A \frac{h_{nn}(v)}{|m|^2 n^2 (n+1)^2} \operatorname{Im}[m^* X_n(a) Y_n(a)] \Big|_{a_1}^{a_2}.$$
(8)

Let us turn to the electric resonance (only one amplitude coefficient d_n differs from zero). Then, taking into account the ratio between $t_{nn}(\mathbf{v})$ and $h_{nn}(\mathbf{v})$, we obtain

$$W_{abs}^{(n, el)} = A \frac{2N\kappa\rho}{|m|^2 n(n+1)} |d_n|^2 \times \left\{ \frac{h_{nn}(\nu)}{n(n+1)} \int_{a_1}^{a_2} \left[\frac{n(n+1)}{|m|^2 \rho^2 a^2} |\psi_n(m\rho a)|^2 + |\psi'_n(m\rho a)|^2 \right] da - \frac{h_{nn}(\nu)}{n(n+1)} \int_{a_1}^{a_2} \left[\frac{n(n+1)}{|m|^2 \rho^2 a^2} |\psi_n(m\rho a)|^2 + |\psi'_n(m\rho a)|^2 \right] da - \frac{h_{nn}(\nu)}{n(n+1)} \int_{a_1}^{a_2} \left[\frac{h_{nn}(\nu)}{|m|^2 \rho^2 a^2} |\psi_n(m\rho a)|^2 + |\psi'_n(m\rho a)|^2 \right] da - \frac{h_{nn}(\nu)}{n(n+1)} \int_{a_1}^{a_2} \left[\frac{h_{nn}(\nu)}{|m|^2 \rho^2 a^2} |\psi_n(m\rho a)|^2 + \frac{h_{nn}(\nu)}{n(n+1)} \right] da - \frac{h_{nn}(\nu)}{n(n+1)} \int_{a_1}^{a_2} \left[\frac{h_{nn}(\nu)}{|m|^2 \rho^2 a^2} |\psi_n(m\rho a)|^2 + \frac{h_{nn}(\nu)}{n(n+1)} \right] da - \frac{h_{nn}(\nu)}{n(n+1)} \int_{a_1}^{a_2} \left[\frac{h_{nn}(\nu)}{|m|^2 \rho^2 a^2} |\psi_n(m\rho a)|^2 + \frac{h_{nn}(\nu)}{n(n+1)} \right] da - \frac{h_{nn}(\nu)}{n(n+1)} \int_{a_1}^{a_2} \left[\frac{h_{nn}(\nu)}{|m|^2 \rho^2 a^2} |\psi_n(m\rho a)|^2 + \frac{h_{nn}(\nu)}{n(n+1)} \right] da - \frac{h_{nn}(\nu)}{n(n+1)} \int_{a_1}^{a_2} \left[\frac{h_{nn}(\nu)}{|m|^2 \rho^2 a^2} |\psi_n(m\rho a)|^2 + \frac{h_{nn}(\nu)}{n(n+1)} \right] da - \frac{h_{nn}(\nu)}{n(n+1)} \int_{a_1}^{a_2} \left[\frac{h_{nn}(\nu)}{(m+1)} \right] da - \frac{h_{nn}(\nu)}{(m+1)} \int_{a_1}^{a_1} \left[\frac{h_{nn}(\nu)}{(m+1)} \right] da - \frac{h_{nn}(\nu)}{($$

Here the first integral can be taken analytically as

$$\int \left[\psi'_n(\alpha x) \ \psi'_n(\beta x) + \frac{n(n+1)}{x^2 \ \alpha \beta} \ \psi_n(\alpha x) \ \psi_n(\beta x) \right] dx =$$

= $\frac{1}{\alpha^2 - \beta^2} \left[\alpha \psi_n(\alpha x) \ \psi'_n(\beta x) - \beta \psi'_n(\alpha x) \ \psi_n(\beta x) \right],$

while the analytical representation of the second integral is unknown.

Finally, we obtain

$$W_{abs}^{(n, el)} = A \frac{h_{nn}(v)}{|m|^2 n^2 (n+1)^2} \operatorname{Im}[m Z_n(a) V_n^*(a)] \Big|_{a_1}^{a_2} - 2AN\kappa\rho \frac{(1-v^2) \pi_n(v) \tau_n(v)}{|m|^4 n(n+1) \rho} |d_n|^2 \int_{a_1}^{a_2} |\psi_n(m\rho a)|^2 \frac{da}{a^2}.$$
 (9)

It is evident that, to integrate the second term, one should apply the numerical quadrature what is not difficult here.

5. ILLUSTRATIVE RESULTS FOR WATER DROPLETS

To illustrate the possibilities of the proposed semianalytical methods of calculation, below we present some results for water droplets at laser wavelengths $\lambda = 10.6$, 2.36, and 0.69 µm. In our opinion, the ratio η of the mean relative field intensity \overline{B}_V in a bounded volume V to the similar value \overline{B} averaged over the entire volume of a spherical particle is quite a comprehensive measure of absorption in a bounded volume of a particle. In fact, this value demonstrates how strongly the field intensity increases in a bounded volume η to other absorption characteristics are rather evident.

Figures 1 and 2 present the value η as a function of the spherical angle Θ counted from the forward scattering direction, for several values of the diffraction parameter. The volume in the shadow hemisphere was bounded by a cone-shaped surface ($\theta = \Theta$, $\phi = 0 - 2\pi$, $a = a_1 - a_2$) and two spherical surfaces ($a_1 = 0.05$, $\theta = 0 - \Theta$, $\phi = 0 - 2\pi$) and ($a_2 = 1$, $\theta = 0 - \Theta$, $\phi = 0 - 2\pi$). The value Θ varied from 0 to 45°.

In the region of strong absorption ($\lambda = 10.6 \,\mu\text{m}$, see Fig. 1), the values η are very small. For $\rho = 1$, η is 1.05 and in fact does not depend on the angle Θ what is indicative of almost homogeneous distribution of the field. However, already at $\rho = 2 - 5$, a visible maximum appears at $\Theta = 0$. This reflects the appearance of maxima on the large axis of a particle in

the shadow hemisphere. At $\rho = 10$, this maximum disappears, and the values η diminish because the major part of energy begins to release in the illuminated hemisphere. With the further increase in ρ , the values of η continue to fall; thus at $\rho \approx 50$, a small maximum is formed at $\Theta = 2^{\circ}$. Perhaps, this indicates toward a shift of the field maxima off the large axis of the particle.



FIG. 1. The ratio η as a function of Θ angle for spherical water particles (m = 1.73 + i0.0823) at the wavelength $\lambda = 10.6 \mu m$. The figures at the curves are the values of the particle diffraction parameter ρ .



FIG. 2. The same data as in Fig. 1, But for $\lambda = 0.69 \ \mu m$ (a) (m = 1.33 + i3.10⁻⁸) and $\lambda = 2.36 \ \mu m$ (B) (m = 1.274 + i7.6.10⁻⁴) (see Ref. 13).

For the wavelengths $\lambda = 2.36$ and 0.69 µm (see Fig. 2), where water absorption is less by several orders of magnitude, a qualitatively different picture is observed. At small values $\rho \approx 1 - 2$, the ratio η very weakly depends on Θ , but, at $\rho = 5$, a maximum appears at $\Theta = 0^{\circ}$. The values η are much higher than those at the wavelength 10.6 µm. A maximum appearing at $\rho \approx 20 - 50$ at the angle $\Theta = 2 - 3^{\circ}$ can be caused by a shift of field maxima off the large axis.

The above-mentioned functions $\eta(\Theta)$ refer to the case when no resonance occurs. To illustrate influence of the morphological resonance, Fig. 3 presents the functions $\eta(\Theta)$ for a model particle with N = 1.40,

 $\rho = 31.789230$, what corresponds to the first resonance of the amplitude coefficient d_{39} . Calculations have been performed for several values of the absorption index κ (from 10^{-8} to 10^{-3}) and for a particle beyond the resonance ($m = 1.4 + i10^{-8}$, $\rho = 31.80$). If the absorption is rather strong ($\kappa \approx 10^{-3}$), the value η only weakly depends on Θ, in the presence of resonance, as well as at its absence. But under the resonance conditions and decreased κ , a maximum of η appears at $\Theta = 0$. Maximum values of η are very high here: ≈ 25 at $\kappa = 10^{-4}$ and ≈ 37 at $\kappa = 10^{-5}$ and lower.



FIG. 3. The ratios η as functions of the angle Θ for model spherical particles with the refractive index N = 1.4 and diffraction parameter $\rho = 31.789230$. The figures at the curves mean the values of log κ , the dashed line is for a particle with $m = 1.4 + i \cdot 10^{-8}$ and $\rho = 31.80$.

For this model of a resonant particle, the value \overline{B} averaged over the entire sphere is 44 at $\kappa = 10^{-6}$. So we

obtain that, at $\kappa\approx 10^{-6}-10^{-8},$ the mean relative intensity of the interior field in a narrow cone of $\Theta\approx 0.5^\circ$ is $\approx 1600.$

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