Analytical Green's function of the radiative transfer radiance for the infinite medium

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An analytical solution of the radiative transfer equation for the radiance caused by an isotropic source which is located in an infinitely extended medium was derived using the P_N method. The results were compared with Monte Carlo simulations and excellent agreement was found. In addition, the radiance of the SP_N approximation for the same geometry was derived. Comparison with Monte Carlo simulations showed that the SP_N radiance, although being more exact than the radiance derived from diffusion theory, has relatively large errors in many relevant cases.

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I. INTRODUCTION

The radiative transfer equation (RTE) is often used as a model for describing different processes in physics such as neutron transport or light propagation in biological tissue or in the atmosphere [1]. In the literature, solutions of the RTE are usually based on numerical methods such as the discrete ordinates method or Monte Carlo simulations [2]. Analytical solutions of the three-dimensional RTE are known only for the case of isotropic scattering [2–4], although these solutions have many advantages in relation to the accuracy and speediness compared to the numerical techniques. Recently, we derived the fluence of the RTE for an isotropic source, which is located in an infinitely extended scattering medium, for the case of anisotropic scattering [5]. The obtained solutions are easily programed, fast, and were successfully verified with Monte Carlo simulations.

Lately, the simplified spherical harmonics equations (SP_N equations) [6] were introduced in the field of biomedical optics for describing the light propagation in scattering media [7]. Despite being an approximation of the RTE, the SP_N equations deliver more precise results than the often used diffusion equation [1]. Similar to the RTE, the SP_N equations have been solved only numerically [7]. Recently, we derived an analytical solution for the fluence of an isotropic source in an infinite medium and compared it to Monte Carlo simulations showing good agreement even for a relatively large absorption coefficient [8].

In this study the derivation of analytical expressions for the radiance in an infinitely extended medium caused by an isotropic point source is presented using the RTE and the SP_N equations for an arbitrary rotationally symmetric phase function. The obtained solutions are given in the form of recursion relations that can be efficiently computed. The analytical solutions were compared to Monte Carlo simulations and the diffusion theory. The solution of the RTE shows excellent agreement with the Monte Carlo method, whereas the SP_N radiance and especially the diffusion radiance have relatively large errors compared to Monte Carlo simulations.

II. THEORY

A. Radiative transfer equation

The RTE for the radiance $\psi(r,\tau_r)$ in spherical coordinates is given by [9]

$$\tau_r \frac{\partial}{\partial r}\psi(r,\tau_r) + \frac{1-\tau_r^2}{r}\frac{\partial}{\partial \tau_r}\psi(r,\tau_r) + \mu_t \psi(r,\tau_r) = \mu_s \int_{4\pi} f(\boldsymbol{\Omega}\cdot\boldsymbol{\Omega}')\psi(r,\tau_r')\,d\boldsymbol{\Omega}' + S(r,\tau_r), \quad (1)$$

where $\mu_t = \mu_a + \mu_s$ is the total attenuation coefficient, μ_a the absorption coefficient, and μ_s the scattering coefficient. The cosine of the angle between the direction of propagation $\boldsymbol{\Omega}$ and unit vector $\hat{\boldsymbol{r}}$ of position $\boldsymbol{r}$ is defined as $\tau_r = \boldsymbol{\Omega}\cdot\hat{\boldsymbol{r}}$. The internal light source density is given by $S(r,\tau_r)$. An arbitrary phase function f without azimuth angle dependence is applied. By expanding f in Legendre polynomials P_n one obtains [7]

$$f(\cos\theta) = \sum_{n=0}^{\infty} \frac{2n+1}{4\pi} f_n P_n(\cos\theta). \quad (2)$$

The expansion coefficients are defined as

$$f_n = 2\pi \int_{-1}^{1} f(\tau) P_n(\tau)\,d\tau. \quad (3)$$

Two different phase functions are used for the comparison of the obtained analytical solutions with Monte Carlo simulation. The Henyey-Greenstein phase function

$$f(\cos\theta) = \frac{1}{4\pi}\frac{1-g^2}{(1+g^2-2g\cos\theta)^{3/2}}, \quad (4)$$

with the coefficients for the Legendre polynomial expansion $f_n = g^n$, and the Rayleigh function

$$f(\cos\theta) = \frac{3}{16\pi}(1+\cos^2\theta), \quad (5)$$

are applied [10]. In the latter case the coefficients are $f_n = \delta_{n,0} + 1/10 \cdot \delta_{n,2}$. The P_N method is used for solving Eq. (1). In this theory the angular quantities are expanded in spherical harmonics. For the case of spherical symmetry, the radiance is given by

$$\psi(r,\tau_r) = \sum_{n=0}^{\infty} \frac{2n+1}{4\pi}\phi_n(r)P_n(\tau_r), \tag{6}$$

and $\phi_n(r)$ are the Legendre moments. The corresponding P_N equations are obtained by truncating this expansion for the radiance in Eq. (1), multiplying both sides with $P_m(\tau_r)$ and using the orthogonality properties and recursion relations between Legendre polynomials. The result is given by the following set of infinite ordinary differential equations for $n \geqslant 0$ [9]

$$\frac{n+1}{2n+1}\left[\frac{d}{dr}+\frac{n+2}{r}\right]\phi_{n+1}(r) + \frac{n}{2n+1}\left[\frac{d}{dr}-\frac{n-1}{r}\right]\phi_{n-1}(r) + \mu_{an}\phi_n(r) = S(r)\delta_{n,0}, \tag{7}$$

where $\mu_{an} = \mu_a + (1-f_n)\mu_s$ are the nth-order absorption coefficients. Taking the first $N+1$ equations for $n = 0,\ldots,N$ (N odd) and setting $\phi_{N+1}(r) = 0$ the radiance is given by the expression [9]

$$\psi(r,\tau_r) = \sum_{n=0}^{N} \frac{2n+1}{4\pi}\phi_n(r)P_n(\tau_r). \tag{8}$$

The Green's function of Eq. (7) is obtained by using an isotropic source distribution $S(r) = \delta(r)/(4\pi r^2)$ located in an infinitely extended scattering medium. In our recent paper we derived the first-order moment $\phi_0(r)$, which equals the fluence [5].

It can be shown that an appropriate ansatz for obtaining all Legendre moments except the highest-order moment is made by (see Appendix)

$$\phi_n(r) = \frac{1}{4\pi}\sum_{i=1}^{\frac{N+1}{2}} \nu_i A_i H_n(\nu_i) k_n(\nu_i r), \qquad n = 0,\ldots,N, \tag{9}$$

where $k_n(x)$ are the nth-order modified spherical Bessel functions of the second kind. The meaning of the values A_i, $H_n(\nu_i)$, and ν_i is explained after Eq. (14). The first two orders of these special functions are given by $k_0(x) = x^{-1}e^{-x}$ and $k_1(x) = (x^{-2}+x^{-1})e^{-x}$. Higher orders can be obtained by using the upward recursion

$$k_{n+1}(x) = \frac{2n+1}{x}k_n(x) + k_{n-1}(x). \tag{10}$$

The substitution of this ansatz in the P_N equations and the use of Eq. (10) leads to the relation (see Appendix)

$$H_{n-1}(\nu_i) = \frac{1}{n}\left[\frac{2n+1}{\nu_i}\mu_{an}H_n(\nu_i) - (n+1)H_{n+1}(\nu_i)\right], \tag{11}$$

with $H_N(\nu_i) = \nu_i^N N!/P(\lambda_i)$ and $H_{N+1}(\nu_i) = 0$. The values of $P(\lambda_i)$, A_i, and ν_i can be found as follows. By setting $\mathcal{D}_1(\lambda)=1$ and $\mathcal{D}_2(\lambda)=3\mu_{a1}$, the use of the recursively defined polynomials

$$\mathcal{D}_{n+1}(\lambda) = (2n+1)\mu_{an}\mathcal{D}_n(\lambda) + \lambda n^2\mathcal{D}_{n-1}(\lambda), \tag{12}$$

for $n = 2,\ldots,N$ leads to the first polynomial $P(\lambda)$

$$\mathcal{D}_{N+1}(\lambda) = P(\lambda) = \sum_{l=0}^{\frac{N-1}{2}} a_l\lambda^l. \tag{13}$$

For $\mathcal{D}_0(\lambda)=1$ and $\mathcal{D}_1(\lambda)=\mu_a$ Eq. (12) used for $n = 1,\ldots,N$ defines the second polynomial $Q(\lambda)$ as

$$\mathcal{D}_{N+1}(\lambda) = Q(\lambda) = \sum_{l=0}^{\frac{N+1}{2}} b_l\lambda^l. \tag{14}$$

The polynomial equation $Q(\lambda) = 0$ gives all in all $(N+1)/2$ negative real valued zeros λ_i. These zeros are used for defining the values $\nu_i = \sqrt{-\lambda_i}$. The coefficients A_i are determined as

$$A_i = \frac{1}{b_{\frac{N+1}{2}}}\frac{P(\lambda_i)}{\prod_{n=1,\,n\neq i}^{\frac{N-1}{2}}(\lambda_i-\lambda_n)}. \tag{15}$$

Note that for $N = 1$ Eq. (15) becomes $A_1 = 3\mu_{a1} = 1/D$, where D is the diffusion coefficient. The given formulas are based on the derivation of the Green's function for the infinite space fluence. More background information and a detailed derivation of these formulas can be obtained in Ref. [5]. There, also the analytical formulas are given for solving the fourth-order polynomial equation required for the radiance calculation in the P_7 approximation. The radiance can be evaluated with Eq. (8) using these Legendre moments.

Similar to the scaling principle applied in the Monte Carlo method [11] it is possible to obtain such a relation within the P_N theory. By scaling the absorption and scattering coefficients with the factor $\sigma \in \mathbb{R}$ the resulting radiance of Eq. (8) within the P_N theory becomes (see Appendix)

$$\tilde{\psi}(r,\tau_r) = \sigma^2\psi(\sigma r,\tau_r). \tag{16}$$

B. Simplified spherical harmonics equations

The SP_N equations are given by a system of coupled diffusion-like equations for even-order Legendre moments ($n = 0,2,\ldots,N-1$) (N being odd)

$$\frac{1}{\mu_{an+1}}\frac{n+1}{2n+1}\nabla^2\left[\frac{n+1}{2n+3}\phi_{n+2}(r) + \frac{n+1}{2n+3}\phi_n(r)\right] + \frac{1}{\mu_{an-1}}\frac{n}{2n+1}\nabla^2\left[\frac{n}{2n-1}\phi_n(r) + \frac{n-1}{2n-1}\phi_{n-2}(r)\right] - \mu_{an}\phi_n(r) = -S(r)\delta_{n,0}. \tag{17}$$

The odd-order moments for $n = 1,3,\ldots,N$ are given by [7]

$$\phi_n(r) = -\frac{1}{\mu_{an}}\frac{d}{dr}\left[\frac{n+1}{2n+1}\phi_{n+1}(r) + \frac{n}{2n+1}\phi_{n-1}(r)\right]. \tag{18}$$

A similar approach as shown for the P_N theory gives the Legendre moments for $n = 1,\ldots,N$ as (see Appendix)

$$\phi_n(r) = \frac{1}{4\pi}\sum_{i=1}^{\frac{N+1}{2}} \nu_i A_i H_n(\nu_i)\begin{cases} k_0(\nu_i r), & n \text{ even},\\ k_1(\nu_i r), & n \text{ odd},\end{cases} \tag{19}$$

within the SP_N theory. Note that $\phi_0(r)$ within the SP_N theory is the same as for the P_N equations. Again the Legendre moments are applied for the calculation of the radiance with Eq. (8). The coefficients A_i and υ_i are the same as those used for the solution of the P_N equations.

C. Diffusion equation

The radiance within the diffusion theory is given by a sum of the first two Legendre moments [1]

$$\psi(\vec{r},\tau_r) = \frac{1}{4\pi}\phi_0(r) + \frac{3}{4\pi}\phi_1(r)\tau_r. \quad (20)$$

The fluence obtained from the diffusion equation is [12]

$$\phi_0(r) = \frac{e^{-\mu_{\mathrm{eff}} r}}{4\pi Dr}, \quad \mu_{\mathrm{eff}} = \sqrt{\frac{\mu_a}{D}}. \quad (21)$$

By setting $\nu_1 = \mu_{\mathrm{eff}}$, $A_1 = 3\mu_{a1}$, and $H_1(\nu_1) = \nu_1/(3\mu_{a1})$, Eq. (9) gives the first-order Legendre moment in the diffusion theory as

$$\phi_1(r) = \frac{e^{-\mu_{\mathrm{eff}} r}}{4\pi r^2}(1 + \mu_{\mathrm{eff}} r). \quad (22)$$

D. Monte Carlo method

To validate the derived analytical solutions the radiance was compared with results obtained from Monte Carlo simulations. The Monte Carlo method simulates the propagation of photons through the scattering medium using appropriate probability functions and the random number generator of the computer. In the limit of an infinitely large number of photons used in the simulations, the Monte Carlo method is an exact solution of the RTE. Our existing code was modified to be able to calculate the angle-resolved radiance, similar to what was described in the literature [13]. The Monte Carlo code itself was successfully (with a relative difference smaller than 10^{-6}) verified by comparison with simple, but exact analytical solutions of RTE [14]. For example, we showed that the average of the squared distance d between an isotropic source and the location of absorption in an infinitely extended medium equals

$$\langle d^2 \rangle = \frac{2}{\mu_a(\mu_a + \mu_s')}. \quad (23)$$

We note that this and further equations derived in Ref. [14] permit not only to verify the Monte Carlo code, but also the applied random number generator.

III. RESULTS

In this section the derived analytical solutions are compared with Monte Carlo simulations and the diffusion theory. When the results obtained from the P_N equations converge to the same values for increasing N they are denoted as P_∞. Figure 1 shows the radiance versus angle in an infinitely extended medium which is illuminated by an isotropic point source obtained from different theories. The Henyey-Greenstein function with $g = 0$ is applied as the phase function. The radiance calculated with the solution of the diffusion theory (open circles), the P_3 equations (dashed-dotted curve), the SP_3-approximation (dashed curve), the Monte Carlo method (solid noisy curve), and P_∞ equations (solid curve) are shown.

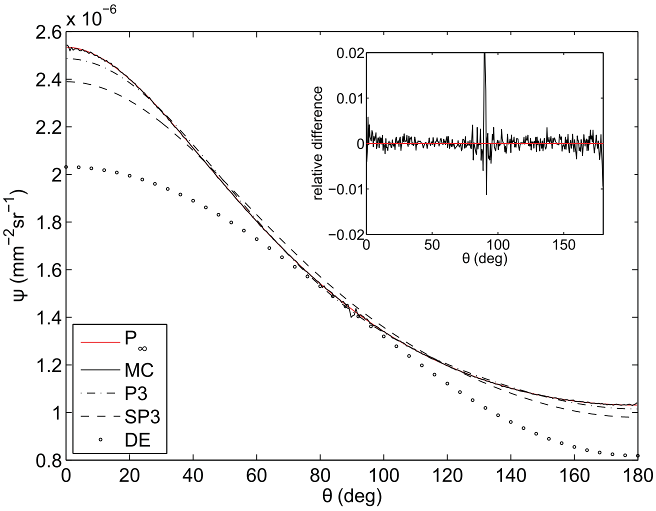

FIG. 1. (Color online) Radiance in an infinitely extended scattering medium for an isotropic point source obtained from different theories, see legend. The optical properties are $\mu_s' = 2.0\,\mathrm{mm}^{-1}$, $\mu_a = 0.1\,\mathrm{mm}^{-1}$, and $g = 0$. The distance to the isotropic point source is $r = 10\,\mathrm{mm}$. The inset shows the relative difference of P_∞ compared to the Monte Carlo method.

It can be seen that the derived analytical solution of the P_N equations converge to the exact solution of the RTE. The relative differences between the results obtained with the Monte Carlo simulations and the P_∞ equations are in the range of 0.001, as is shown in the inset. These differences can be made arbitrarily small by increasing the number of photons used in the Monte Carlo simulations. The radiance of the SP_3 equations shows larger differences than the result obtained from the P_3 equations, whereas the differences between the diffusion theory and the radiative transfer theory are much larger.

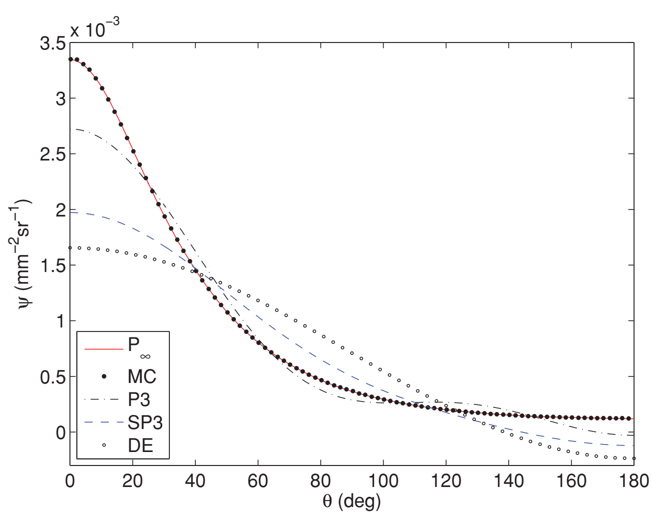

FIG. 2. (Color online) Radiance in an infinitely extended scattering medium for an isotropic point source obtained from different theories, see legend. The optical properties are $\mu_s' = 1.0\,\mathrm{mm}^{-1}$, $\mu_a = 0.5\,\mathrm{mm}^{-1}$, and $g = 0.9$. The distance to the isotropic point source is $r = 2\,\mathrm{mm}$.

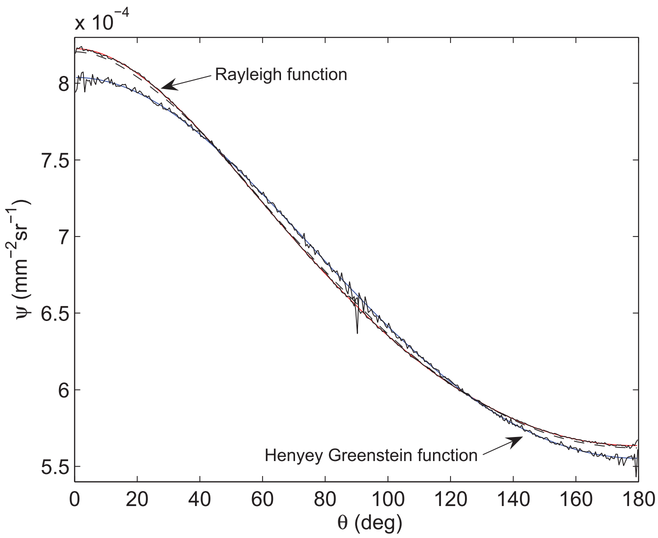

FIG. 3. (Color online) Radiance in an infinitely extended scattering medium for an isotropic point source obtained for two different phase functions. The optical properties are $\mu_s' = 2.0\,\text{mm}^{-1}$, $\mu_a = 0.01\,\text{mm}^{-1}$, and $g = 0.9$. The distance to the isotropic point source is $r = 8\,\text{mm}$. The dashed curve shows the radiance for the Henyey-Greenstein function with $g = 0$.

For the next comparison the optical and geometrical parameters are changed. Again, the Henyey-Greenstein function was applied, but for a different anisotropic factor ($g = 0.9$). Figure 2 shows the result of this comparison using the same theories as in Fig. 1. Note that now, for better visualization, the Monte Carlo results are depicted as filled circles. It can be seen that the P_∞ solution is again very close to the Monte Carlo simulation, whereas P_3, SP_3, and especially the diffusion theory exhibit significant errors compared to the solutions of the RTE. For large angles the radiance calculated by these theories is even negative.

Figure 3 shows the radiance of the P_∞ solution (solid curves) and the Monte Carlo method (noisy curves) for two different phase functions. The comparison using a Henyey-Greenstein function with $g = 0.9$ and a Rayleigh function ($g = 0$) shows, again, excellent agreement between the two solutions. It can also be seen that, even at relatively large distances from the source ($\mu_s' \cdot r = 16$), there is an influence of the phase function on the radiance. In addition, the P_∞ solution using the Henyey-Greenstein function for $g = 0$ (dashed curve) was plotted showing smaller, but still significant differences to the radiance calculated with the Rayleigh function although both phase functions have the same anisotropy factor.

IV. SUMMARY AND DISCUSSION

An analytical solution of the RTE for the radiance caused by an isotropic source which is located in an infinitely extended anisotropic scattering medium was derived using the P_N method. The calculation is based on the results recently obtained for the fluence in an infinitely extended medium by solving the RTE [5]. In addition, the radiance of the SP_N equations was derived. The radiance calculated with both theories and those obtained with the Monte Carlo method and diffusion equation were compared. An excellent agreement was obtained between the P_N solution and the Monte Carlo method for both investigated phase functions, the Henyey-Greenstein function, and the Rayleigh function. The radiance calculated with the SP_N approximations and, especially, that of the diffusion approximation showed relatively large errors compared to solutions of the RTE. We note that, in general, the differences obtained for the radiance are larger than those calculated for the fluence. The fluence obtained from the SP_N equations shows good agreement with the RTE fluence [5].

The presented formulas are solutions in the steady-state domain. They are the base for deriving the solutions for the important cases of the frequency and time-domain radiance. By using the modified nth-order absorption coefficients $\mu_{an} = \mu_a + (1 - f_n)\mu_s + j\omega/c$ the corresponding solutions can be obtained for the frequency domain [5]. For the time-domain radiance, in addition, the inverse Fourier transform has to be applied.

For small values of $r(\mu_s + \mu_a)$ a significant part of the radiance consists of unscattered photons, which produces a delta peak of the radiance at angle $\theta = 0$. This has to be considered when evaluating Eq. (6) because higher-order terms are needed for reaching convergence.

As an example, the derived solutions can be applied to retrieve the optical properties by means of a single fiber which is used to measure the radiance inside scattering media caused by an isotropically emitting fiber [15,16]. An application is, for example, the monitoring of drug concentrations during photodynamic therapy. In the literature, the P_3 approximation was used for these calculations. However, as can be seen in Figs. 1 and 2 in many cases the P_3 solution, although being much more exact than the diffusion equation, might still cause significant errors due to its approximations. Thus, higher-order solutions of P_N have to be applied. The advantage of using P_∞ compared to Monte Carlo simulation is that they are many orders of magnitude faster, allowing the convenient retrieval of the optical properties in a nonlinear regression.

Finally, the obtained formulas can be used as a starting point to derive analytical solutions of the RTE for finite geometries which include the boundary condition at the interface to nonscattering media.

ACKNOWLEDGMENT

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APPENDIX

1. Legendre moments of the spherically symmetric P_N equations

In the following, the correctness of Eq. (9) is proved via complete induction. The base of induction is given by the lowest-order Legendre moment $\phi_0(r)$. This calculation was done explicitly in our earlier publication [5]. The correctness of the Legendre moments is assumed until the moment $\phi_n(r)$. The induction step is made by solving the corresponding P_N equation for obtaining the moment $\phi_{n+1}(r)$. For an arbitrary $n > 1$ the corresponding P_N equation is given by, see Eq. (7),

$$(n+1)\left[\frac{d}{dr}+\frac{n+2}{r}\right]\phi_{n+1}(r) = n\left[\frac{n-1}{r}-\frac{d}{dr}\right]\phi_{n-1}(r)-(2n+1)\mu_{an}\phi_n(r). \quad \text{(A1)}$$

The given ordinary differential equation in $\phi_{n+1}(r)$ can by solved by using the method of variation of the constant. The solution of the homogeneous equation

$$\frac{d}{dr}\phi^{(h)}_{n+1}(r)+\frac{n+2}{r}\phi^{(h)}_{n+1}(r)=0, \quad \text{(A2)}$$

is

$$\phi^{(h)}_{n+1}(r)=\frac{C}{r^{n+2}}, \quad \text{(A3)}$$

where C is an arbitrary constant. The ansatz for the unknown Legendre moment is given by variation of C

$$\phi_{n+1}(r)=\frac{C(r)}{r^{n+2}}. \quad \text{(A4)}$$

The derivative is obtained as

$$\frac{d}{dr}\phi_{n+1}(r)=\frac{1}{r^{n+2}}\frac{d}{dr}C(r)-\frac{n+2}{r^{n+3}}C(r). \quad \text{(A5)}$$

In the following calculation the derivative of the modified spherical Bessel function of the second kind

$$k'_n(x)=-k_{n+1}(x)+\frac{n}{x}k_n(x), \quad \text{(A6)}$$

is used. The first part of the right-hand side of the P_N equation [see Eq. (A1)] becomes

$$\left(\frac{n-1}{r}-\frac{d}{dr}\right)\phi_{n-1}(r)=\frac{1}{4\pi}\sum_{i=1}^{\frac{N+1}{2}}\nu_i A_i H_{n-1}(\nu_i)\nu_i k_n(\nu_i r), \quad \text{(A7)}$$

where Eqs. (A6) and (9) are used. The simplified version of the differential equation, Eq. (A1), for the unknown varied constant becomes

$$\frac{1}{r^{n+2}}\frac{d}{dr}C(r)=\frac{1}{4\pi}\sum_{i=1}^{\frac{N+1}{2}}\frac{\nu_i A_i}{n+1}[\nu_i n H_{n-1}(\nu_i) - (2n+1)\mu_{an}H_n(\nu_i)]k_n(\nu_i r). \quad \text{(A8)}$$

This equation can be integrated directly as follows

$$C(r)=\frac{1}{4\pi}\sum_{i=1}^{\frac{N+1}{2}}\frac{\nu_i A_i}{n+1}[\nu_i n H_{n-1}(\nu_i)-(2n+1)\mu_{an}H_n(\nu_i)] \times\int r^{n+2}k_n(\nu_i r)dr. \quad \text{(A9)}$$

The calculation of the integral can be done by following consideration

$$\begin{aligned}\frac{d}{dr}[r^{n+2}k_{n+1}(\nu_i r)] &= r^{n+2}\nu_i\left[-k_{n+2}(\nu_i r)+\frac{n+1}{\nu_i r}k_{n+1}(\nu_i r)\right] + (n+2)r^{n+1}k_{n+1}(\nu_i r)\\ &= \nu_i r^{n+2}\left[-k_{n+2}(\nu_i r)+\frac{2n+3}{\nu_i r}k_{n+1}(\nu_i r)\right]\\ &= -\nu_i r^{n+2}k_n(\nu_i r).\end{aligned} \quad \text{(A10)}$$

The result of the integration becomes

$$\int r^{n+2}k_n(\nu_i r)dr=-\frac{r^{n+2}}{\nu_i}k_{n+1}(\nu_i r). \quad \text{(A11)}$$

Thus, the varied constant is

$$C(r)=\frac{r^{n+2}}{4\pi}\sum_{i=1}^{\frac{N+1}{2}}\frac{\nu_i A_i}{n+1} \times\left[\frac{2n+1}{\nu_i}\mu_{an}H_n(\nu_i)-nH_{n-1}(\nu_i)\right]k_{n+1}(\nu_i r). \quad \text{(A12)}$$

Finally, the Legendre moment is obtained as

$$\phi_{n+1}(r)=\frac{C(r)}{r^{n+2}}=\frac{1}{4\pi}\sum_{i=1}^{\frac{N+1}{2}}\nu_i A_i H_{n+1}(\nu_i)k_{n+1}(\nu_i r), \quad \text{(A13)}$$

delivering Eq. (11). By applying the assumed formula to obtain the moment $\phi_{n+1}(r)$ we get the same result.

2. Legendre moments of the spherically symmetric SP_N equations

This Appendix contains the derivation of the Legendre moments in the SP_N theory, see Eq. (19). In the SP_N theory, normally the composite moments φ_i are used instead of the Legendre moments [7]. In our recent publication, analytical solutions of the composite moments of the SP_N equations were derived [8]. The composite moments are, in principle, given by a linear combination of two even-order Legendre moments for $i = 1,\ldots,(N+1)/2$

$$\varphi_i(r)=(2i-1)\phi_{2i-2}(r)+2i\phi_{2i}(r). \quad \text{(A14)}$$

More details about these moments can be obtained in Ref. [7]. All composite moments can be expanded in a sum of diffusion-like Green's functions. Thus, the even-order Legendre moments are also diffusion-like Green's functions, see Eq. (A14). Recently we showed that the zeroth-order Legendre moment, which equals the fluence of the planar-geometric P_N equations, is obtained as [5]

$$\phi_0(x)=\sum_{i=1}^{\frac{N+1}{2}}\frac{A_i}{2}\frac{e^{-\nu_i|x|}}{\nu_i}. \quad \text{(A15)}$$

Therefore, the ansatz for the even-order moments is

$$\phi_n(x)=\sum_{i=1}^{\frac{N+1}{2}}\frac{A_i}{2\nu_i}H_n(\nu_i)e^{-\nu_i|x|}. \quad \text{(A16)}$$

In the SP_N theory, the odd-order Legendre moments for the planar-geometric case are given by the derivative of the even-order Legendre moments for $n = 1,3,\ldots,N$ [7]

$$\phi_n(x) = -\frac{1}{\mu_{an}}\frac{d}{dx}\left[\frac{n+1}{2n+1}\phi_{n+1}(x) + \frac{n}{2n+1}\phi_{n-1}(x)\right]. \tag{A17}$$

Thus, the following ansatz

$$\phi_n(x) = -\sum_{i=1}^{\frac{N+1}{2}} \frac{A_i}{2\nu_i^2} H_n(\nu_i)\frac{d}{dx}e^{-\nu_i|x|} = \sum_{i=1}^{\frac{N+1}{2}} \frac{A_i}{2\nu_i} H_n(\nu_i)\mathrm{sgn}(x)e^{-\nu_i|x|}, \tag{A18}$$

for the odd-order Legendre moments is used. Substituting Eqs. (A16) and (A18) in the planar-geometric P_N equations [7]

$$\frac{n+1}{2n+1}\frac{d}{dx}\phi_{n+1}(x) + \frac{n}{2n+1}\frac{d}{dx}\phi_{n-1}(x) + \mu_{an}\phi_n(x) = S(x)\delta_{n,0}. \tag{A19}$$

leads to the condition

$$H_{n+1}(\nu_i) = \frac{1}{n+1}\left[\frac{2n+1}{\nu_i}\mu_{an}H_n(\nu_i) - nH_{n-1}(\nu_i)\right]. \tag{A20}$$

The special form of the ansatz in Eq. (A18) is used for getting the same recursion formula for even- and odd-order Legendre moments. The spherically symmetric results can be obtained by using the relation

$$\phi_n(r) = -\frac{1}{2\pi r}\frac{d}{dx}\phi_n(x)\bigg|_{x=r}, \tag{A21}$$

and by replacing the d/dx by the derivative d/dr along the radius vector [17]. The even-order moments become

$$\phi_n(r) = \sum_{i=1}^{\frac{N+1}{2}} A_i H_n(\nu_i)\frac{e^{-\nu_i r}}{4\pi r} = \frac{1}{4\pi}\sum_{i=1}^{\frac{N+1}{2}} \nu_i A_i H_n(\nu_i)k_0(\nu_i r). \tag{A22}$$

For obtaining the odd-order moments using Eq. (A21) the following calculation step

$$\frac{d}{dx}e^{-\nu_i|x|} \Rightarrow \frac{d}{dr}\left[\frac{-1}{2\pi r}\frac{d}{dr}e^{-\nu_i r}\right] = \frac{\nu_i^2}{2\pi}\frac{d}{dr}k_0(\nu_i r) = -\frac{\nu_i^3}{2\pi}k_1(\nu_i r), \tag{A23}$$

is used. The final result for odd n is given by

$$\phi_n(r) = \frac{1}{4\pi}\sum_{i=1}^{\frac{N+1}{2}} \nu_i A_i H_n(\nu_i)k_1(\nu_i r). \tag{A24}$$

3. Scaling principle within the P_N theory

In our earlier publication [5] it was shown that the one-dimensional P_N equations in the transformed space can be rewritten as

$$\mathbf{T}\,[\phi_0(k),\phi_1(k),\ldots,\phi_N(k)]^T = [1,0,\ldots,0]^T, \tag{A25}$$

with a symmetric tridiagonal system matrix

$$\mathbf{T} = \begin{pmatrix} \mu_a & jk & 0 & 0 & \cdots & 0 \\ jk & 3\mu_{a1} & j2k & 0 & \cdots & \vdots \\ 0 & j2k & \ddots & \ddots & \cdots & 0 \\ 0 & 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \cdots & \cdots & \ddots & \ddots & jNk \\ 0 & \cdots & 0 & 0 & jNk & (2N+1)\mu_{aN} \end{pmatrix}. \tag{A26}$$

The fluence that is the base for our derivation of the three-dimensional radiance can be extracted by using Cramer's rule as

$$\phi_0(k) = \frac{\det(\mathbf{T}_0)}{\det(\mathbf{T})} = \frac{\mathcal{P}(k)}{\mathcal{Q}(k)}, \tag{A27}$$

where $\mathbf{T}_0$ is a symmetric tridiagonal matrix obtained by replacing the first column of $\mathbf{T}$ by the vector $[1,0,\ldots,0]^T$. By scaling the absorption and scattering coefficients with $\sigma \in \mathbb{R}$ the nth-order absorption moments become $\tilde{\mu}_{an} = \sigma\mu_{an}$. Note that the diagonal elements of the given matrix contain these moments. The use of determinant rules gives the scaled fluence in the transformed space as

$$\tilde{\phi}_o(k) = \frac{\sigma^N\mathcal{P}\left(\frac{k}{\sigma}\right)}{\sigma^{N+1}\mathcal{Q}\left(\frac{k}{\sigma}\right)} = \frac{1}{\sigma}\phi_o\left(\frac{k}{\sigma}\right). \tag{A28}$$

The spherically symmetric fluence in the steady-state domain can be obtained from the Fourier-transformed fluence of the planar symmetric pendant as [8]

$$\phi_0(r) = \frac{1}{2\pi^2 r}\int_0^\infty k\phi_0(k)\sin(kr)\,dk. \tag{A29}$$

Inverting the scaled fluence gives

$$\tilde{\phi}_0(r) = \frac{1}{2\pi^2 r}\int_0^\infty k\frac{1}{\sigma}\phi_0\left(\frac{k}{\sigma}\right)\sin(kr)\,dk. \tag{A30}$$

The substitution of $k = \sigma\xi$ leads to

$$\tilde{\phi}_0(r) = \frac{\sigma^2}{2\pi^2\sigma r}\int_0^\infty \xi\phi_0(\xi)\sin(\sigma r\xi)d\xi = \sigma^2\phi_0(\sigma r). \tag{A31}$$

Using the scaled fluence for the derivation of the radiance Eq. (16) is obtained.

In addition the scaled radiance in the frequency domain becomes

$$\tilde{\psi}(r,\tau_r,\omega) = \sigma^2\psi(\sigma r,\tau_r,\omega/\sigma). \tag{A32}$$

Again the scaling rule of the Fourier transform leads to the scaled radiance

$$\tilde{\psi}(r,\tau_r,t) = \sigma^3\psi(\sigma r,\tau_r,\sigma t), \tag{A33}$$

in the time domain.

[1] A. Ishimaru, *Wave Propagation and Scattering in Random Media* (Academic Press, New York, 1978).
[2] F. Martelli, S. Del Bianco, A. Ismaelli, and G. Zaccanti, *Light Propagation Through Biological Tissue* (SPIE Press, Bellingham, WA, 2010).
[3] V. A. Markel, Waves Random Complex Media **14**, L13 (2004).
[4] M. Machida, G. Y. Panasyuk, J. C. Schotland, and V. A. Markel, J. Phys. A **43**, 065402 (2010).
[5] A. Liemert and A. Kienle, Phys. Rev. A **83**, 015804 (2011).
[6] P. S. Brantley and E. W. Larsen, Nucl. Sci. Eng. **134**, 1 (2000).
[7] A. D. Klose and E. W. Larsen, J. Comput. Phys. **220**, 441 (2006).
[8] A. Liemert and A. Kienle, Opt. Lett. **35**, 3507 (2010).
[9] T. Khan and A. Thomas, Opt. Commun. **255**, 130 (2005).
[10] A. Kienle, F. Foster, and R. Hibst, Opt. Lett. **26**, 1571 (2001).
[11] A. Kienle and M. S. Patterson, Physics in Medicine and Biology **41**, 2221 (1996).
[12] T. J. Farrell, M. S. Patterson, and B. Wilson, Med. Phys. **19**, 879 (1992).
[13] F. Martelli, M. Bassani, L. Alianelli, L. Zangheri, and G. Zaccanti, Physics in Medicine and Biology **45**, 1359 (2000).
[14] A. Kienle, PhD-thesis (University of Ulm, 1995).
[15] L. C. L. Chin, A. E. Worthington, W. M. Whelan, and I. A. Vitkin, J Biomed. Opt. **12**, 064027 (2007).
[16] L. C. L. Chin, B. Lloyd, W. M. Whelan, and I. A. Vitkin, J. Appl. Phys. **105**, 102025 (2009).
[17] E. L. Hull and T. H. Forster, J. Opt. Soc. Am. A **18**, 584 (2001).