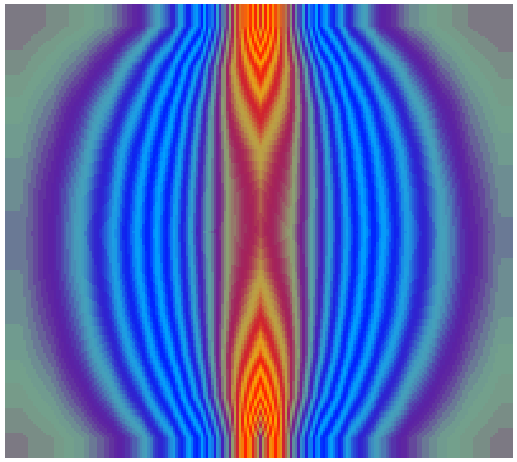

The Boltzmann transport equation and the diffusion equation

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Modeling light propagation in scattering media with transport theory

The Boltzmann transport equation (BTE) is a balance relationship that describes the flow of particles in scattering and absorbing media. The propagation of light in optically turbid media can be modeled by the transport equation, where the photons are treated as the transported particles. If we denote the angular photon density with $u(\mathbf{r},\hat{\Omega},t)$, which is defined as the number of photons per unit volume per unit solid angle traveling in direction $\hat{\Omega}$ at position **r** and time *t*, we can write the BTE as follows (Duderstadt and Hamilton, 1976):

$$\frac{\partial u(\mathbf{r},\hat{\Omega},t)}{\partial t} = -v\hat{\Omega}\cdot\nabla u(\mathbf{r},\hat{\Omega},t) - v(\mu_a+\mu_s)u(\mathbf{r},\hat{\Omega},t) + v\mu_s\int_{4\pi} u(\mathbf{r},\hat{\Omega}',t)\,f(\hat{\Omega}',\hat{\Omega})\,d\hat{\Omega}' + q(\mathbf{r},\hat{\Omega},t)\,, \quad (1)$$

where *v* is the speed of light in the medium, μ_a is the absorption coefficient (units of cm^{-1}), μ_s is the scattering coefficient (units of cm^{-1}), $f(\hat{\Omega}',\hat{\Omega})$ is the phase function or the probability density of scattering a photon that travels along direction $\hat{\Omega}'$ into direction $\hat{\Omega}$, and $q(\mathbf{r},\hat{\Omega},t)$ is the source term. $q(\mathbf{r},\hat{\Omega},t)$ has units of $s^{-1}m^{-3}sr^{-1}$ and represents the number of photons injected by the light source per unit volume, per unit time, per unit solid angle at position **r**, time *t*, and direction $\hat{\Omega}$. The left hand side of Eq. (1) represents the temporal variation of the angular photon density. Each one of the terms on the right hand side represents a specific contribution to this variation. The first term is the net gain of photons at position **r** and direction $\hat{\Omega}$ due to the flow of photons. The second term is the loss of photons at **r** and $\hat{\Omega}$ as a result of collisions (absorption and scattering). The third term is the gain of photons at **r** and $\hat{\Omega}$ due to scattering. Finally, the fourth term is the gain of photons due to the light sources. Let us now define some of the quantities used to describe photon transport.

Angular photon density: $u(\mathbf{r},\hat{\Omega},t)$

$u(\mathbf{r},\hat{\Omega},t)$ is defined such that $u(\mathbf{r},\hat{\Omega},t)d\mathbf{r}d\hat{\Omega}$ represents the number of photons in $d\mathbf{r}$ that travel in a direction within $d\hat{\Omega}$ around $\hat{\Omega}$. The units of $u(\mathbf{r},\hat{\Omega},t)$ are $m^{-3}sr^{-1}$.

Photon radiance: $L(\mathbf{r},\hat{\Omega},t)$

$L(\mathbf{r},\hat{\Omega},t) = vu(\mathbf{r},\hat{\Omega},t)$. $L(\mathbf{r},\hat{\Omega},t)d\hat{\Omega}$ represents the number of photons traveling per unit time per unit area (perpendicular to $\hat{\Omega}$) in a range of directions within $d\hat{\Omega}$ around $\hat{\Omega}$. The units of $L(\mathbf{r},\hat{\Omega},t)$ are $s^{-1}m^{-2}sr^{-1}$.

Photon density: $U(\mathbf{r},t)$

$U(\mathbf{r},t) = \int_{4\pi} u(\mathbf{r},\hat{\Omega},t)d\hat{\Omega}$. The photon density is the number of photons per unit volume. The units are m^{-3}.

Photon fluence rate: $E_0(\mathbf{r},t)$

$E_0(\mathbf{r},t) = vU(\mathbf{r},t) = \int_{4\pi} L(\mathbf{r},\hat{\Omega},t)d\hat{\Omega}$. The photon fluence rate is defined as the number of photons traveling per unit time per unit area (perpendicular to the direction of propagation) over all directions. The units are $s^{-1}m^{-2}$.

Photon current density, or photon flux: $\mathbf{J}(\mathbf{r},t)$

$\mathbf{J}(\mathbf{r},t) = \int_{4\pi} L(\mathbf{r},\hat{\Omega},t)\hat{\Omega}d\hat{\Omega}$. The photon flux is a vector that represents the net flow of photons. Its direction points in the direction of the net flux, while its amplitude gives the net number of photons transmitted per unit time per unit area in that direction. The units of $\mathbf{J}(\mathbf{r},t)$ are $s^{-1}m^{-2}$.

The above definitions can be extended to describe radiant energy (instead of photon number) by replacing the word "photon" with "energy," and by introducing a factor $h\nu$ in all definitions ($h\nu$ is the energy per photon, where h is Planck's constant and ν is the light frequency). A complete nomenclature for quantities used in medical optics can be found in (Hetzel *et al.*, 1993).

Expansion of the Boltzmann equation in spherical harmonics

To model light propagation in highly scattering media, as are most biological tissues, it is useful to expand the angular photon density $u(\mathbf{r},\hat{\Omega},t)$, the source term $q(\mathbf{r},\hat{\Omega},t)$, and the phase function $f(\hat{\Omega}',\hat{\Omega})$ into spherical harmonics $Y_l^m(\hat{\Omega})$ (Kaltenbach and Kaschke, 1993; Boas 1993; Arridge 1999). The so-called P_N approximation to the Boltzmann equation (see Section 3.3) is based on such an expansion. As a result of the completeness property of the spherical harmonics, any function $h(\theta,\varphi)$ (with sufficient continuity properties) can be expanded in the Laplace series (Wyld 1994):

$$h(\theta,\varphi) = \sum_{l=0}^{\infty}\sum_{m=-l}^{l} h_{lm} Y_l^m(\hat{\Omega}), \qquad (2)$$

where h_{lm} are coefficients independent of θ and φ, and the relationship among θ, φ, and $\hat{\Omega}$ is $\hat{\Omega} = \sin\theta\cos\varphi\hat{\mathbf{x}} + \sin\theta\sin\varphi\hat{\mathbf{y}} + \cos\theta\hat{\mathbf{z}}$. Accordingly, we expand $u(\mathbf{r},\hat{\Omega},t)$ and $q(\mathbf{r},\hat{\Omega},t)$ into spherical harmonics as follows:

$$u(\mathbf{r},\hat{\Omega},t) = \sum_{l=0}^{\infty}\sum_{m=-l}^{l} u_{lm}(\mathbf{r},t)Y_l^m(\hat{\Omega}), \tag{3}$$

$$q(\mathbf{r},\hat{\Omega},t) = \sum_{l=0}^{\infty}\sum_{m=-l}^{l} q_{lm}(\mathbf{r},t)Y_l^m(\hat{\Omega}). \tag{4}$$

We assume that the phase function $f(\hat{\Omega}',\hat{\Omega})$ only depends on $\hat{\Omega}'\cdot\hat{\Omega}$ (i.e. on the cosine of the scattering angle γ). We can thus expand $f(\hat{\Omega}',\hat{\Omega})$ in Legendre polynomials, by recalling that a function $H(x)$ (which is sectionally continuous together with its derivative in the interval [-1,1]) has the general Legendre series representation (Wyld 1994):

$$H(x) = \sum_{l=0}^{\infty}\frac{2l+1}{2}H_l P_l(x). \tag{5}$$

where $P_l(x)$ is the Legendre polynomial of order l, and $H_l = \int_{-1}^{1}H(x')P_l(x')dx'$. We then write:

$$\begin{aligned} f(\hat{\Omega}'\cdot\hat{\Omega}) &= \sum_{l=0}^{\infty}\frac{2l+1}{4\pi}f_l P_l(\hat{\Omega}'\cdot\hat{\Omega}) \\ &= \sum_{l=0}^{\infty}\sum_{m=-l}^{l} f_l Y_l^{m*}(\hat{\Omega}')Y_l^m(\hat{\Omega}), \end{aligned} \tag{6}$$

where the last expression follows from the addition theorem for spherical harmonics (Wyld 1994), namely $P_l(\hat{\Omega}'\cdot\hat{\Omega}) = 4\pi/(2l+1)\sum_{m=-l}^{l}Y_l^{m*}(\hat{\Omega}')Y_l^m(\hat{\Omega})$. Here, $f_l = 2\pi\int_{-1}^{1}f(\cos\gamma)P_l(\cos\gamma)d(\cos\gamma)$.

By substituting these expressions into Eq. (1), we obtain:

$$\begin{aligned} \sum_{l=0}^{\infty}\sum_{m=-l}^{l}\Bigg\{&\left[\frac{\partial}{\partial t} + v\hat{\Omega}\cdot\nabla + v(\mu_a + \mu_s)\right]u_{lm}(\mathbf{r},t)Y_l^m(\hat{\Omega}) - q_{lm}(\mathbf{r},t)Y_l^m(\hat{\Omega}) \\ &- v\mu_s\int_{4\pi}u_{lm}(\mathbf{r},t)Y_l^m(\hat{\Omega}')\sum_{l'=0}^{\infty}\sum_{m'=-l'}^{l'}f_{l'}Y_{l'}^{m'*}(\hat{\Omega}')Y_{l'}^{m'}(\hat{\Omega})d\hat{\Omega}'\Bigg\} = 0. \end{aligned} \tag{7}$$

The integral in $d\hat{\Omega}'$ can be calculated using the orthogonality property of the spherical harmonics: $\int_{4\pi}Y_l^{m*}(\hat{\Omega})Y_{l'}^{m'}(\hat{\Omega})d\hat{\Omega} = \delta_{ll'}\delta_{mm'}$. The BTE thus becomes:

$$\sum_{l=0}^{\infty}\sum_{m=-l}^{l}\left\{\left[\frac{\partial}{\partial t} + v\hat{\Omega}\cdot\nabla + v[\mu_s(1-f_l) + \mu_a]\right]u_{lm}(\mathbf{r},t) - q_{lm}(\mathbf{r},t)\right\}Y_l^m(\hat{\Omega}) = 0. \tag{8}$$

We then multiply this equation by $Y_L^{M*}(\hat{\Omega})$ and integrate over $\hat{\Omega}$ to obtain the relationship between the specific coefficients u_{LM} and q_{LM}, and all the coefficients of the spherical harmonic expansion of u, u_{lm}:

$$\frac{\partial}{\partial t}u_{LM}(\mathbf{r},t)+v[\mu_s(1-f_l)+\mu_a]u_{LM}(\mathbf{r},t)$$
$$+v\sum_{l=0}^{\infty}\sum_{m=-l}^{l}\int_{4\pi}\hat{\Omega}\cdot\nabla u_{lm}(\mathbf{r},t)Y_l^m(\hat{\Omega})Y_L^{M*}(\hat{\Omega})d\hat{\Omega}=q_{LM}(\mathbf{r},t)\,. \tag{9}$$

The integral over $\hat{\Omega}$ can be evaluated by writing the *x*, *y*, and *z* components of the vector $Y_L^M(\hat{\Omega})\hat{\Omega}$ in terms of spherical harmonics. This can be done by using the recurrence relations for the associated Legendre functions $P_l^m(x)$. The result is the following:

$$\begin{aligned}
Y_L^M(\hat{\Omega})\Omega_x &= Y_L^M(\hat{\Omega})\sin\theta\cos\varphi \\
&= -\frac{1}{2}\left[\frac{(L+M+1)(L+M+2)}{(2L+1)(2L+3)}\right]^{1/2} Y_{L+1}^{M+1}(\hat{\Omega}) \\
&\quad + \frac{1}{2}\left[\frac{(L-M)(L-M-1)}{(2L-1)(2L+1)}\right]^{1/2} Y_{L-1}^{M+1}(\hat{\Omega}) \\
&\quad + \frac{1}{2}\left[\frac{(L-M+1)(L-M+2)}{(2L+1)(2L+3)}\right]^{1/2} Y_{L+1}^{M-1}(\hat{\Omega}) \\
&\quad - \frac{1}{2}\left[\frac{(L+M)(L+M-1)}{(2L-1)(2L+1)}\right]^{1/2} Y_{L-1}^{M-1}(\hat{\Omega})\,,
\end{aligned} \tag{10}$$

$$\begin{aligned}
Y_L^M(\hat{\Omega})\Omega_y &= Y_L^M(\hat{\Omega})\sin\theta\sin\varphi \\
&= -\frac{1}{2i}\left[\frac{(L+M+1)(L+M+2)}{(2L+1)(2L+3)}\right]^{1/2} Y_{L+1}^{M+1}(\hat{\Omega}) \\
&\quad + \frac{1}{2i}\left[\frac{(L-M)(L-M-1)}{(2L-1)(2L+1)}\right]^{1/2} Y_{L-1}^{M+1}(\hat{\Omega}) \\
&\quad - \frac{1}{2i}\left[\frac{(L-M+1)(L-M+2)}{(2L+1)(2L+3)}\right]^{1/2} Y_{L+1}^{M-1}(\hat{\Omega}) \\
&\quad + \frac{1}{2i}\left[\frac{(L+M)(L+M-1)}{(2L-1)(2L+1)}\right]^{1/2} Y_{L-1}^{M-1}(\hat{\Omega})\,,
\end{aligned} \tag{11}$$

$$\begin{aligned}
Y_L^M(\hat{\Omega})\Omega_z &= Y_L^M(\hat{\Omega})\cos\theta \\
&= \left[\frac{(L-M+1)(L+M+1)}{(2L+1)(2L+3)}\right]^{1/2} Y_{L+1}^{M}(\hat{\Omega}) \\
&\quad + \left[\frac{(L-M)(L+M)}{(2L-1)(2L+1)}\right]^{1/2} Y_{L-1}^{M}(\hat{\Omega})\,.
\end{aligned} \tag{12}$$

Using these expressions for the *x*, *y*, and *z* components of $Y_L^M(\hat{\Omega})\hat{\Omega}$, it is possible to calculate the integral using the orthogonality relations for spherical harmonics. We find that the relationship between the specific coefficients u_{LM} and q_{LM} does not involve all the coefficients of the spherical harmonic expansion of *u*, u_{lm}, but it only contains u_{lm} with indices *l* ranging from *L*-1 to *L*+1, and *m* ranging from *M*-1 to *M*+1:

$$
\begin{aligned}
&\frac{\partial}{\partial t}u_{LM}(\mathbf{r},t)+v\left[\mu_s\left(1-f_L\right)+\mu_a\right]u_{LM}(\mathbf{r},t)\\
&+\frac{1}{2}\left[\frac{(L-M+1)(L-M+2)}{(2L+1)(2L+3)}\right]^{1/2}\left(\frac{\partial}{\partial x}-i\frac{\partial}{\partial y}\right)vu_{L+1}^{M-1}(\mathbf{r},t)\\
&-\frac{1}{2}\left[\frac{(L+M)(L+M-1)}{(2L+1)(2L-1)}\right]^{1/2}\left(\frac{\partial}{\partial x}-i\frac{\partial}{\partial y}\right)vu_{L-1}^{M-1}(\mathbf{r},t)\\
&-\frac{1}{2}\left[\frac{(L+M+2)(L+M+1)}{(2L+1)(2L+3)}\right]^{1/2}\left(\frac{\partial}{\partial x}+i\frac{\partial}{\partial y}\right)vu_{L+1}^{M+1}(\mathbf{r},t)\\
&+\frac{1}{2}\left[\frac{(L-M-1)(L-M)}{(2L+1)(2L-1)}\right]^{1/2}\left(\frac{\partial}{\partial x}+i\frac{\partial}{\partial y}\right)vu_{L-1}^{M+1}(\mathbf{r},t)\\
&+\left[\frac{(L+M+1)(L-M+1)}{(2L+1)(2L+3)}\right]^{1/2}\frac{\partial}{\partial z}vu_{L+1}^{M}(\mathbf{r},t)\\
&+\left[\frac{(L-M)(L+M)}{(2L-1)(2L+1)}\right]^{1/2}\frac{\partial}{\partial z}vu_{L-1}^{M}(\mathbf{r},t)=q_{LM}(\mathbf{r},t).
\end{aligned}
\tag{13}
$$

The P_N approximation

The expansion of the BTE into spherical harmonics has led to an infinite set of equations with indices L (ranging from 0 to ∞) and M (ranging from $-L$ to L). Truncation of the Laplace series at $L = N$, leads to the so-called P_N approximation. The reason for this name is that the last term in the truncated Laplace series contains $Y_N^M(\hat{\Omega})$ which can be written in terms of the associated Legendre functions $P_N^M(x)$, which in turn can be written in terms of the Legendre polynomial $P_N(x)$. The relationships are the following:

$$
Y_N^M(\hat{\Omega})=(-1)^M\left[\frac{(2N+1)}{4\pi}\frac{(N-M)!}{(N+M)!}\right]^{1/2}P_N^M(\cos\theta)e^{iM\varphi}\,, \tag{14}
$$

$$
P_N^M(x)=\left(1-x^2\right)^{M/2}\frac{d^M}{dx^M}P_N(x)\,. \tag{15}
$$

The P_1 approximation

We now consider the P_1 approximation, which is often used to describe photon migration in tissues. In the P_1 approximation $u_{LM}(\mathbf{r},t)$ is set to 0 for $L>1$. In the P_1 approximation, Eq. (13) is a set of 4 equations. The first, for L=0, M=0:

$$\begin{aligned}&\frac{\partial}{\partial t}u_{0,0}(\mathbf{r},t)+v[\mu_s(1-f_0)+\mu_a]u_{0,0}(\mathbf{r},t)\\&+\frac{1}{2}\sqrt{\frac{2}{3}}\left(\frac{\partial}{\partial x}-i\frac{\partial}{\partial y}\right)vu_{1,-1}(\mathbf{r},t)\\&-\frac{1}{2}\sqrt{\frac{2}{3}}\left(\frac{\partial}{\partial x}+i\frac{\partial}{\partial y}\right)vu_{1,1}(\mathbf{r},t)+\sqrt{\frac{1}{3}}\frac{\partial}{\partial z}vu_{1,0}(\mathbf{r},t)=q_{0,0}(\mathbf{r},t)\,,\end{aligned}\tag{16}$$

the second, for L=1, M=-1:

$$\begin{aligned}&\frac{\partial}{\partial t}u_{1,-1}(\mathbf{r},t)+v[\mu_s(1-f_1)+\mu_a]u_{1,-1}(\mathbf{r},t)\\&+\frac{1}{2}\sqrt{\frac{2}{3}}\left(\frac{\partial}{\partial x}+i\frac{\partial}{\partial y}\right)vu_{0,0}(\mathbf{r},t)=q_{1,-1}(\mathbf{r},t)\,,\end{aligned}\tag{17}$$

the third, for L=1, M=0:

$$\begin{aligned}&\frac{\partial}{\partial t}u_{1,0}(\mathbf{r},t)+v[\mu_s(1-f_1)+\mu_a]u_{1,0}(\mathbf{r},t)\\&+\sqrt{\frac{1}{3}}\frac{\partial}{\partial z}vu_{0,0}(\mathbf{r},t)=q_{1,0}(\mathbf{r},t)\,,\end{aligned}\tag{18}$$

and the fourth, for L=1, M=1:

$$\begin{aligned}&\frac{\partial}{\partial t}u_{1,1}(\mathbf{r},t)+v[\mu_s(1-f_1)+\mu_a]u_{1,1}(\mathbf{r},t)\\&-\frac{1}{2}\sqrt{\frac{2}{3}}\left(\frac{\partial}{\partial x}-i\frac{\partial}{\partial y}\right)vu_{0,0}(\mathbf{r},t)=q_{1,1}(\mathbf{r},t)\,.\end{aligned}\tag{19}$$

The coefficients $u_{0,0}(\mathbf{r},t)$ and $u_{1,M}(\mathbf{r},t)$ are related to the photon density $U(\mathbf{r},t)$ and to the photon flux $\mathbf{J}(\mathbf{r},t)$, respectively. In fact:

$$\begin{aligned}U(\mathbf{r},t)&=\int_{4\pi}u(\mathbf{r},\hat{\Omega},t)d\hat{\Omega}\\&=\sum_{l=0}^{\infty}\sum_{m=-l}^{l}u_{lm}(\mathbf{r},t)\int_{4\pi}Y_l^m(\hat{\Omega})d\hat{\Omega}=\sqrt{4\pi}u_{0,0}(\mathbf{r},t)\,,\end{aligned}\tag{20}$$

(since $\int_{4\pi}Y_l^m(\hat{\Omega})d\hat{\Omega}=0$ for $m\neq 0$ and $Y_0^0(\hat{\Omega})=1/\sqrt{4\pi}$), and:

$$
\begin{aligned}
\mathbf{J}(\mathbf{r},t) &= \int_{4\pi} v u(\mathbf{r},\hat{\Omega},t)\hat{\Omega}d\hat{\Omega} \\
&= \sum_{l=0}^{\infty}\sum_{m=-l}^{l} v u_{lm}(\mathbf{r},t)\int_{4\pi}\left(\sin\theta\cos\varphi\hat{\mathbf{x}} + \sin\theta\sin\varphi\hat{\mathbf{y}} + \cos\theta\hat{\mathbf{z}}\right)Y_l^m(\hat{\Omega})d\hat{\Omega} \\
&= \sum_{l=0}^{\infty}\sum_{m=-l}^{l} v u_{lm}(\mathbf{r},t)\int_{4\pi}\sqrt{\frac{4\pi}{3}}\left\{\begin{array}{l}\sqrt{\frac{1}{2}}\left[-Y_1^{1*}(\hat{\Omega}) + Y_1^{-1*}(\hat{\Omega})\right]\hat{\mathbf{x}} \\ + \sqrt{\frac{1}{2}}\frac{1}{i}\left[Y_1^{1*}(\hat{\Omega}) + Y_1^{-1*}(\hat{\Omega})\right]\hat{\mathbf{y}} + Y_1^{0}(\hat{\Omega})\hat{\mathbf{z}}\end{array}\right\}Y_l^m(\hat{\Omega})d\hat{\Omega} \\
&= \sqrt{\frac{4\pi}{3}}v\left[\sqrt{\frac{1}{2}}\left(-u_{1,1}(\mathbf{r},t) + u_{1,-1}(\mathbf{r},t)\right)\hat{\mathbf{x}} - i\sqrt{\frac{1}{2}}\left(u_{1,1}(\mathbf{r},t) + u_{1,-1}(\mathbf{r},t)\right)\hat{\mathbf{y}} + u_{1,0}(\mathbf{r},t)\hat{\mathbf{z}}\right].
\end{aligned} \tag{21}
$$

The set of four equations (16)-(19) of the P_1 approximation are thus equivalent to the following two equations (one scalar and one vectorial):

$$
\frac{\partial}{\partial t}U(\mathbf{r},t) + v\left[\mu_s\left(1 - f_0\right) + \mu_a\right]U(\mathbf{r},t) + \nabla\cdot\mathbf{J}(\mathbf{r},t) = \sqrt{4\pi}q_{0,0}(\mathbf{r},t), \tag{22}
$$

$$
\begin{aligned}
&\frac{1}{v}\frac{\partial}{\partial t}\mathbf{J}(\mathbf{r},t) + \left[\mu_s\left(1 - f_1\right) + \mu_a\right]\mathbf{J}(\mathbf{r},t) + \frac{1}{3}v\nabla U(\mathbf{r},t) = \\
&= \sqrt{\frac{4\pi}{3}}\left[\sqrt{\frac{1}{2}}\left(q_{1,-1}(\mathbf{r},t) - q_{1,1}(\mathbf{r},t)\right)\hat{\mathbf{x}} - i\sqrt{\frac{1}{2}}\left(q_{1,-1}(\mathbf{r},t) + q_{1,1}(\mathbf{r},t)\right)\hat{\mathbf{y}} + q_{1,0}(\mathbf{r},t)\hat{\mathbf{z}}\right].
\end{aligned} \tag{23}
$$

The vectorial equation is obtained by combining Eqs. (17), (18), (19) according to the following formal relationship: $\sqrt{2\pi/3}[(7.17) - (7.19)]\hat{\mathbf{x}} - i\sqrt{2\pi/3}[(7.17) + (7.19)]\hat{\mathbf{y}} + \sqrt{4\pi/3}(7.18)\hat{\mathbf{z}}$. From the general definition of the coefficients f_l, we find that f_0 and f_1 are given by:

$$
f_0 = 2\pi\int_{-1}^{1} f(\cos\gamma)P_0(\cos\gamma)d(\cos\gamma) = 2\pi\int_{-1}^{1} f(\cos\gamma)d(\cos\gamma) = 1, \tag{24}
$$

$$
f_1 = 2\pi\int_{-1}^{1} f(\cos\gamma)P_1(\cos\gamma)d(\cos\gamma) = 2\pi\int_{-1}^{1} f(\cos\gamma)\cos\gamma\, d(\cos\gamma) = <\cos\gamma>, \tag{25}
$$

where in Eq. (24) we have used the fact that the scattering probability is normalized according to the condition $\int_{4\pi} f(\hat{\Omega}'\cdot\hat{\Omega})d\hat{\Omega}' = 1$, which is equivalent to $2\pi\int_{-1}^{1} f(\cos\gamma)d(\cos\gamma) = 1$. Therefore f_0 is 1, whereas f_1 is the average cosine of the scattering angle γ ($<\cos\gamma>$). The source terms in Eqs. (22) and (23) are formally a monopole term (spherically symmetric) and a dipole term, respectively. We will indicate them with the symbols $S_0(\mathbf{r},t)$ and $\mathbf{S}_1(\mathbf{r},t)$, respectively. The final expressions for the P_1 equations are:

$$
\frac{\partial}{\partial t}U(\mathbf{r},t) + v\mu_a U(\mathbf{r},t) + \nabla\cdot\mathbf{J}(\mathbf{r},t) = S_0(\mathbf{r},t), \tag{26}
$$

$$
\frac{1}{v}\frac{\partial}{\partial t}\mathbf{J}(\mathbf{r},t) + \left[\mu_s\left(1 - <\cos\gamma>\right) + \mu_a\right]\mathbf{J}(\mathbf{r},t) + \frac{1}{3}v\nabla U(\mathbf{r},t) = \mathbf{S}_1(\mathbf{r},t). \tag{27}
$$

The reduced scattering coefficient

Equations (26) and (27) show that, in the P_1 approximation, μ_s and $\cos\gamma$ only appear in the term $\mu_s(1-<\cos\gamma>)$. In this section, we give a physical meaning to this term on the basis of an analysis reported by (Zaccanti *et al*., 1994). Suppose that a photon is emitted at the point $P_0 \equiv (0,0,0)$ in direction $\hat{\mathbf{z}}$. This photon will first be scattered at a point $P_1 \equiv (x_1, y_1, z_1)$ after having traveled a distance r_1. Then it will be scattered at point $P_2 \equiv (x_2, y_2, z_2)$ after having traveled a distance r_2, and so on. In general, we refer to the scattering at point P_n as the *n*-th order scattering. We want to define the reduced scattering coefficient, μ_s', as the inverse of the average distance projected along the *z* axis that the photon has to travel to lose memory of the initial direction of propagation. In other words, $1/\mu_s'$ represents the average distance between what are effectively isotropic scattering events. In the derivation of μ_s', we neglect the absorption of the medium, since we are only interested in its scattering properties. The probability density, $g(r)$, of traveling a distance r without suffering a scattering event is defined as $g(r) = \mu_s e^{-\mu_s r}$. The first order scattering occurs at $P_1 \equiv (0,0,r_1)$, whose average coordinates are (Zaccanti *et al;*., 1994):

$$
\begin{aligned}
&< x_1 >=< y_1 >= 0\,, \\
&< z_1 >= \int_0^\infty r_1 g(r_1) dr_1 = \frac{1}{\mu_s}\,.
\end{aligned}
\tag{28}
$$

The second order scattering occurs at $P_2 \equiv (r_2 \sin\theta_2 \cos\varphi_2, r_2 \sin\theta_2 \sin\varphi_2, z_1 + r_2 \cos\theta_2)$. Since r_1, r_2, θ_2, φ_2 are not statistically correlated, the average values of the coordinates of P_2 are (Zaccanti *et al;*., 1994):

$$
\begin{aligned}
&< x_2 >=< r_2 >< \sin\theta_2 >< \cos\varphi_2 >= 0\,, \\
&< y_2 >=< r_2 >< \sin\theta_2 >< \sin\varphi_2 >= 0\,, \\
&< z_2 >=< r_1 > + < r_2 >< \cos\theta_2 >= \frac{1}{\mu_s}(1 + < \cos\gamma >).
\end{aligned}
\tag{29}
$$

The third order scattering occurs at $P_3 \equiv (x_3, y_3, z_3)$ where:

$$
\begin{aligned}
x_3 &= x_2 + r_3(\sin\theta_3 \cos\varphi_3 \cos\theta_2 \cos\varphi_2 - \sin\theta_3 \sin\varphi_3 \sin\varphi_2 + \cos\theta_3 \sin\theta_2 \cos\varphi_2), \\
y_3 &= y_2 + r_3(\sin\theta_3 \cos\varphi_3 \cos\theta_2 \sin\varphi_2 + \sin\theta_3 \sin\varphi_3 \cos\varphi_2 + \cos\theta_3 \sin\theta_2 \sin\varphi_2), \\
z_3 &= z_2 + r_3(-\sin\theta_3 \cos\varphi_3 \sin\theta_2 + \cos\theta_3 \cos\theta_2).
\end{aligned}
\tag{30}
$$

The average values of the coordinates of P_3 are (Zaccanti *et al;*., 1994):

$$
\begin{aligned}
&< x_3 >=< y_3 >= 0\,, \\
&< z_3 >= \frac{1}{\mu_s}(1 + < \cos\theta > + < \cos\theta >^2).
\end{aligned}
\tag{31}
$$

In general, at the *n*-th order of scattering, the average values of the coordinates of the scattering point P_n are (Zaccanti *et al;*., 1994):

$$
\begin{aligned}
&< x_n >=< y_n >= 0\,, \\
&< z_n >= \frac{1}{\mu_s} \sum_{k=0}^{n-1} < \cos\gamma >^k = \frac{1 - < \cos\gamma >^n}{\mu_s (1 - < \cos\gamma >)}\,,
\end{aligned}
\tag{32}
$$

where we have used the result for the geometric series $\sum_{k=0}^{n-1} a^k = \frac{1-a^n}{1-a}$, with $a<1$. In the limit of a high number of scattering events $(n \to \infty)$, $<x_\infty> = <y_\infty> = 0$ and $<z_\infty> = 1/[\mu_s(1-<\cos\gamma>)]$ give the coordinates of the center of symmetry of the statistical photon distribution. In particular, the coordinate $<z_\infty>$ can be interpreted as the average distance between consecutive, effectively isotropic scattering events, and its inverse is defined as the reduced scattering coefficient μ_s':

$$\mu_s' = \mu_s\left(1-<\cos\gamma>\right). \tag{33}$$

In the case of isotropic scattering, $<\cos\gamma> = 0$ and $\mu_s' = \mu_s$. In the case of forward scattering, $<\cos\gamma> = 1$ and $\mu_s' = 0$.

The P$_1$ equation and the standard diffusion equation (SDE)

We now reduce the P_1 approximation to a single equation for the photon density $U(\mathbf{r},t)$. From Eq. (27) we obtain $\mathbf{J}(\mathbf{r},t)$:

$$\begin{aligned}\mathbf{J}(\mathbf{r},t) &= -\frac{1}{v\left(\mu_s'+\mu_a\right)}\frac{\partial}{\partial t}\mathbf{J}(\mathbf{r},t) - \frac{v}{3\left(\mu_s'+\mu_a\right)}\nabla U(\mathbf{r},t) + \frac{1}{\left(\mu_s'+\mu_a\right)}\mathbf{S}_1(\mathbf{r},t) \\ &= -\frac{3D}{v^2}\frac{\partial}{\partial t}\mathbf{J}(\mathbf{r},t) - D\nabla U(\mathbf{r},t) + \frac{3D}{v}\mathbf{S}_1(\mathbf{r},t),\end{aligned} \tag{34}$$

where we have defined the diffusion coefficient $D = v/[3(\mu_s'+\mu_a)]$. By substituting this expression for $\mathbf{J}(\mathbf{r},t)$ in Eq. (26), we get:

$$\frac{\partial}{\partial t}U(\mathbf{r},t) + v\mu_a U(\mathbf{r},t) - \frac{3D}{v^2}\frac{\partial}{\partial t}\nabla\cdot\mathbf{J}(\mathbf{r},t) - D\nabla^2 U(\mathbf{r},t) + \frac{3D}{v}\nabla\cdot\mathbf{S}_1(\mathbf{r},t) = S_0(\mathbf{r},t). \tag{35}$$

From Eq. (26), $\nabla\cdot\mathbf{J}(\mathbf{r},t) = S_0(\mathbf{r},t) - \frac{\partial}{\partial t}U(\mathbf{r},t) - v\mu_a U(\mathbf{r},t)$. By substituting this expression and by rearranging the terms, we finally get the P_1 equation for the photon density:

$$\begin{aligned}\nabla^2 U(\mathbf{r},t) &= \frac{3}{v^2}\frac{\partial^2 U(\mathbf{r},t)}{\partial t^2} + \frac{1}{D}\left(1+\frac{3D}{v}\mu_a\right)\frac{\partial U(\mathbf{r},t)}{\partial t} + \frac{v\mu_a}{D}U(\mathbf{r},t) \\ &\quad - \frac{3}{v^2}\frac{\partial S_0(\mathbf{r},t)}{\partial t} - \frac{1}{D}S_0(\mathbf{r},t) + \frac{3}{v}\nabla\cdot\mathbf{S}_1(\mathbf{r},t).\end{aligned} \tag{36}$$

By making a few assumptions, which are often satisfied in the case of light propagation in biological tissue, Eq. (36) reduces to the standard diffusion equation (SDE). The assumptions are the following:

(1) Strongly scattering regime, or $\mu_a << \mu_s'$. This condition means that a photon, on the average, will undergo many effectively isotropic scattering events before being absorbed. In this case, $3D\mu_a/v \equiv \mu_a/(\mu_a+\mu_s') << 1$, and the second term on the right hand side of Eq. (36) reduces to $(1/D)\,\partial U(\mathbf{r},t)/\partial t$.

(2) Time scale of the variations of $U(\mathbf{r},t)$ and $S_0(\mathbf{r},t)$ are much greater than the average time between collisions $1/[v(\mu_a + \mu_s')]$. This condition can be expressed by the formal inequality: $\partial/\partial t << v(\mu_a + \mu_s') \equiv v^2/(3D)$. Consequently:

$$\frac{3}{v^2}\frac{\partial^2 U(\mathbf{r},t)}{\partial t^2} << \frac{1}{D}\frac{\partial U(\mathbf{r},t)}{\partial t}, \tag{37}$$

$$\frac{3}{v^2}\frac{\partial S_0(\mathbf{r},t)}{\partial t} << \frac{1}{D}S_0(\mathbf{r},t). \tag{38}$$

In the frequency-domain, where the harmonic time dependence is given by a factor exp(-$i\omega t$), the time derivative operator becomes a multiplication by -$i\omega$. Here, ω is the angular modulation frequency of the intensity modulation (which should not be confused with the frequency of light). Consequently, this condition poses an upper limit to the modulation frequency given by $\omega << v^2/(3D)$. In the case of biological tissues, the SDE usually breaks down at modulation frequencies on the order of 1 GHz (Fishkin *et al.*, 1996).

(3) The source term is isotropic, i.e. $\mathbf{S}_1(\mathbf{r},t) = 0$.

With these assumptions, the P_1 equation (Eq. 36) reduces to the standard diffusion equation:

$$\frac{\partial U(\mathbf{r},t)}{\partial t} = D\nabla^2 U(\mathbf{r},t) - v\mu_a U(\mathbf{r},t) + S_0(\mathbf{r},t), \tag{39}$$

and the photon flux $\mathbf{J}(\mathbf{r},t)$ is related to the photon density $U(\mathbf{r},t)$ by Fick's law:

$$\mathbf{J}(\mathbf{r},t) = -D\nabla U(\mathbf{r},t). \tag{40}$$

In the frequency-domain, $\partial/\partial\mathrm{t} \to -i\omega$ and the diffusion equation takes the form of the Helmholtz equation:

$$\left(\nabla^2 + k^2\right)U(\mathbf{r}) = -\frac{S_0(\mathbf{r})}{D}, \tag{41}$$

where $k^2 = (i\omega - v\mu_a)/D$.

Solution of the standard diffusion equation in the frequency-domain

The solution to the diffusion equation for a homogeneous, infinite medium containing a harmonically modulated point source of power $P(\omega)$ at $\mathbf{r} = 0$ is given by (Boas *et al.*, 1994):

$$U(r,\omega) = \frac{P(\omega)}{4\pi D}\frac{e^{ikr}}{r}. \tag{42}$$

The explicit expressions for the average photon density (U_{DC}), and for the amplitude (U_{AC}) and phase (Φ) of the photon-density wave are (Fishkin and Gratton, 1993; Haskell *et al.*, 1994; Fantini *et al.*, 1994):

$$U_{\mathrm{DC}}(r) = \frac{P_{\mathrm{DC}}}{4\pi D}\frac{e^{-r(v\mu_a/D)^{1/2}}}{r}, \tag{43}$$

$$U_{\mathrm{AC}}(r,\omega)=\frac{P(\omega)}{4\pi D}\frac{e^{-r(v\mu_a/2D)^{1/2}\left[\left(1+\frac{\omega^2}{v^2\mu_a^2}\right)^{1/2}+1\right]^{1/2}}}{r}, \quad (44)$$

$$\Phi(r,\omega)=r(v\mu_a/2D)^{1/2}\left[\left(1+\frac{\omega^2}{v^2\mu_a^2}\right)^{1/2}-1\right]^{1/2}+\Phi_s, \quad (45)$$

where Φ_s is the source phase in radians. Analytical solutions in the frequency-domain have also been reported for a semi-infinite medium (Patterson *et al.*, 1991; Haskell *et al.*, 1994; Fantini *et al.*, 1994), infinite slab (Arridge *et al.*, 1992), cylindrical and spherical geometries (Arridge *et al.*, 1992). Equations (39) and (41) refer to homogeneous media. For quantitative tissue spectroscopy and oximetry, one typically assumes that tissues are macroscopically homogeneous, so that Eqs. (39) and (41) are applicable. By contrast, optical imaging of tissues aims at measuring the spatial distribution of the tissue optical properties, and Eq. (39) must be generalized to account for the spatial dependence of μ_a and D.

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