THE ANISOTROPIC APPROXIMATIONS OF THE HENYEY-GREENSTEIN PHASE FUNCTION FOR NEUTRON TRANSPORT EQUATION

by

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The effect of anisotropic scattering on the eigenvalues of a multiplying ($c > 1$) and non-multiplying ($c < 1$) slab in one-speed neutron transport equation is studied. We have made some calculations, not only for the cases $c < 1$ and $0 < g < 1$, but also the cases of $c > 1$ and $-1 < g < 0$ by using the linear and quadratic approximations of the Henyey-Greenstein scattering kernel. The asymmetry parameter g consists of isotropic, backward and forward bias. An extensive numerical survey is carried out for the eigenvalues in order to provide an accurate evaluation. The numerical results indicate that the discrete eigenvalue increases with forward scattering and decreases with backward scattering in expansions of linear and quadratic anisotropic scattering.

Key words: Henyey-Greenstein scattering, transport equation, eigenvalue problem, diffusion length

INTRODUCTION

There is an increasing need to take into account the anisotropic scattering in many branches of physics. The accurate evaluation of certain parameters needs to take into account the anisotropy of neutral particle scattering in the nuclear applications. The eigenvalue spectrum of the transport operator consists of two parts. They are the discrete spectrum ($\nu_j > 1$) and the continuous spectrum ($-1 < \nu < 1$). We present here an approximation method and corresponding computer code to compute all eigenvalues for linear and quadratic anisotropic expansion of the Henyey-Greenstein scattering kernel.

An important parameter in this analysis is the eigenvalue which has been the subject of many recent investigations [1-3]. The diffusion coefficient, or the diffusion length which is closely related to the discrete eigenvalues, can be inferred from the solution of the infinite medium transport problem with a given scattering kernel and absorption cross-section [4-7]. The diffusion coefficient is obtained either from the P_1 approximation or from the asymptotic diffusion approximation of the transport equation. The diffusion length is produced by using the high order approximation in transport equation. In the latter case one essentially solves eq. (4) to obtain the discrete eigenvalue from which the diffusion length and diffusion coefficient are inferred. Since ν_j determines the rate of decrease of the asymptotic flux with distance, as is apparent from eq. (7), it is here called the asymptotic diffusion length. The diffusion length L has already been defined and it has been shown that this can be easily calculated for any medium. While diffusing through a medium, a neutron follows a zig-zag path and migrates a certain distance from its origin before being absorbed. This is a standard practice in neutron transport studies [8].

There is a difference between the photon transport problem and the neutron transport. The scattering of near infrared photons in soft tissues is highly peaked in the forward directions. The scattering distribution for neutrons, in most of the applications, is isotropic or nearly linear anisotropic for almost all the materials of interest. For these purposes we consider the linear and quadratic scattering of Henyey-Greenstein kernel. The Henyey-Greenstein kernel is given as

$$f_{\mathrm{HG}}(\mu_0) = \frac{1}{4\pi} \frac{1-g^2}{\sqrt{(1-2g\mu_0 + g^2)^3}} \tag{1}$$

where μ_0 is equal to $\cos\theta_0$. The θ_0 describes the angle between the direction of the neutron before and after the collision. The asymmetry factor g is positive if the scattering anisotropy is biased in the forward direc-

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tions and g is negative if the bias is backward [1, 9, 10]. The asymmetry factor g is also equal to the average of cosine of the scattering angle. In many cases, g assumes a value that is close to unity in the light transport. But g is not close to unity in eq. (1) for neutron transport calculation. Either g should be limited or the Henyey-Greenstein scattering should be modified to obtain an agreement with a respect to the reference value.

In this study we want to use the linear and quadratic approximations of the Henyey-Greenstein scattering in neutron transport calculation. This study expands our earlier work [3] by using the negative asymmetry values, and proves that the eigenvalue exists for some values of the asymmetry parameters and some absorption ratios.

THE TRANSPORT EQUATION AND SOLUTION

The approximations of the Henyey-Greenstein scattering kernel

The scattering law of interaction between the radiation and the particle may be written as $f(\vec{\Omega},\vec{\Omega}')\mathrm{d}\Omega$ and quantitatively is the probability that a photon incident on the particle in the direction denoted by the unit vector $\vec{\Omega}'$ will be scattered into the solid angle $\mathrm{d}\Omega$ about the unit vector $\vec{\Omega}$. For many media of interest we can write $f(\vec{\Omega},\vec{\Omega}')\mathrm{d}\Omega = f(\cos\theta_0)$ where $\cos\theta_0 = \vec{\Omega}\cdot\vec{\Omega}'$, $f(\cos\theta_0)$ is predicted or measured experimentally by the Henyey-Greenstein, Rayleigh or Mie scattering theories.

There have been many attempts to find rational approximations to $f(\cos\theta_0)$ and the formulate approximate models which contain the essential features. Typical of the former approach is that of Henyey and Greenstein who propose eq. (1). This has the useful property in terms of Legendre polynomials that is

$$\frac{1}{4\pi}\frac{1-g^2}{\sqrt{(1-2g\mu_0+g^2)^3}} = \sum_{l=0}^{\infty}\frac{2l+1}{4\pi}g^l P_l(\mu_0) \quad (2)$$

This means that when eq. (1) is expanded in powers of g, the coefficient of $(2l + 1)g^l$ is Legendre polynomials, where the mean cosine of the scattering angle $\bar{\mu}_0$ is defined as $\bar{\mu}_0 = g$. Thus, as g varies from –1 to 1 we trace out the transition from pure back scattering through isotropy to purely forward scattering. It is known that the first three terms in eq. (2) are sufficient for neutron transport in nuclear reactor theory. For $l = 0$, eq. (1) corresponds isotropic; for $l = 1$, eq. (2) corresponds linear anisotropic scattering; for $l = 2$, eq. (2) corresponds quadratic anisotropic scattering [7, 11].

The Henyey-Greenstein scattering is considerably larger, and depends strongly on g. This scattering phase function is commonly used in studies of light propagation and radiative transfer. The g gets values between $-1 < g < 1$, such as, $0.65 < g < 0.95$ in biological tissues. The scattering is not strongly anisotropic for nuclear reactor calculation. The anisotropic order and anisotropy factor g should be chosen correctly.

We begin our analysis by considering the transport equation for a neutron population in multiplying ($c > 1$) and non-multiplying ($c < 1$) systems. For convenience we take the origin at the center of the slab so that the slab extends from $x = -d/2$ to $x = d/2$. The system is surrounded by a vacuum. Then, with the conventional notation, the starting linear transport equation for neutrons of one speed can be written as [4, 12-14]

$$\mu\frac{\partial\psi(x,\mu)}{\partial x} + \textstyle\sum_{\mathrm{t}}\psi(x,\mu) = \\ = \textstyle\sum_{\mathrm{s}}\displaystyle\int_{-1}^{1}\int_{0}^{2\pi} f(\mu,\mu')\psi(x,\mu')\,\mathrm{d}\mu'\,\mathrm{d}\varphi \quad (3)$$

Here, the $\psi(x, \mu)$ is the neutron flux density depending on x and μ (μ is the cosine of the angle between the positive x-axis, and $\vec{\Omega}$), with $\mathrm{d}\Omega = \mathrm{d}\mu'\mathrm{d}\varphi$. The θ and φ are the axial and azimuthal angles of $\vec{\Omega}$, respectively. All distances are measured in units of the neutron mean free path (*mfp*). The Σ_s and Σ_t denote the macroscopic scattering and total cross-sections in the time independent system. The neutron flux density may be assumed to decay exponentially with space for all $\vec{\Omega}$. The recalling of the addition theorem for Legendre polynomials in terms of spherical harmonics, and plugging this expansion into eq. (2) result in the following expression

$$\mu\frac{\partial\psi(x,\mu)}{\partial x} + \psi(x,\mu) = \\ = c\int_{-1}^{1}\sum_{l=0}^{\infty}\frac{2l+1}{2}g^l P_l(\mu)P_l(\mu')\psi(x,\mu')\,\mathrm{d}\mu' \quad (4)$$

Here, the criticality factor and a change of scale of the variable are considered as $c = (\sum_\mathrm{s} + \bar{\nu}\sum_\mathrm{f})/\Sigma_\mathrm{t}$ and $x\Sigma_\mathrm{t} \rightarrow x$.

The spherical harmonics method

The knowledge of neutron flux distributions is important in the design of experiments and to the utilization of the nuclear reactor. Knowing the neutron flux at different positions in the reactor allows researchers and reactor operators to determine how long and where in the core samples must be irradiated in order to achieve a desired activity.

According to the above section, it is sufficient to solve the corresponding integro-differential eq. (4). For the solution, the angular flux is expanded in a series of Legendre polynomials as

$$\psi(x,\mu) = \sum_{n=0}^{N}\left(\frac{2n+1}{2}\right)\phi_\mathrm{n}(x)P_\mathrm{n}(\mu) \quad (5)$$

This expansion and the scattering function given by eq. (1) can now be substituted into eq. (4) in order to obtain the function $\phi_n(x)$. By multiplying both sides of the resulting equation by $P_m(\mu)$, integrating over μ and utilizing the orthogonally properties and the recursion relations of Legendre polynomials [4, 8, 13], after some rearrangement we have

$$\frac{d\phi_1(x)}{dx} + \phi_0(x) = c\phi_0(x), \quad n = 0 \tag{6a}$$

$$n\frac{d\phi_{n-1}(x)}{dx} + (n+1)\frac{d\phi_{n+1}(x)}{dx} + (2n+1)\phi_n(x) = \\ = (2n+1)(cg\delta_{n1} + cg^2\delta_{n2})\phi_n \\ n = 1, 2, \ldots N \tag{6b}$$

with the requirement that $\phi_{-1}(x)$ is zero. The spherical harmonics approximation (P_N) may be defined by considering the first $N+1$of these equations and setting $d\phi_{N+1}(x)/dx = 0$. One may employ the well-known procedure of seeking a solution of the homogeneous eq. (6) in the form [4, 5]

$$\phi_n(x) = G_n(\nu)\exp\left(-\frac{x}{\nu}\right) \tag{7}$$

where the $G_n(\nu)$ are some constants. Each of the $\phi_n(x)$ defined in eq. (7) will satisfy eq. (6) provided that the characteristic P_N equations

$$G_1(\nu) - \nu(1-c)G_0(\nu) = 0, \quad n = 0 \tag{8a}$$

$$(n+1)G_{n+1}(\nu) + nG_{n-1}(\nu) - \\ -(2n+1)\nu[1 - cg\delta_{n1} - cg^2\delta_{n2}]G_n(\nu) = 0, \\ n = 1, 2, 3, \ldots N \tag{8b}$$

are satisfied. The essential idea of the P_N method is that $\phi_{N+1}(\nu) = 0$, *i. e.*, the permissible eigenvalue ν_j, is the j^{th} positive zero of $G_{N+1}(\nu)$ and $G_n(-\nu) = (-1)^n G_n(\nu)$. The determination of the roots is obtained using the Maple. All calculations are reported in tabs. 1-4.

A physical interpretation of the diffusion length

The flux solution derived in eq. (7) can be employed to develop a physical interpretation of the diffusion length L. The mean straight distance $\bar{x}$ travelled by the neutrons from their point of thermalization to their final absorption can be expressed mathematically as the neutron normalized distribution function

$$\bar{x} = \frac{1}{N}\sum_{i=1}^{N} x_i = \frac{\int_0^\infty x\phi(x)dx}{\int_0^\infty \phi(x)dx} \tag{9}$$

Substituting the relationship for the flux in eq. (7), eq. (9) becomes

$$\bar{x} = L \tag{10}$$

Therefore, the diffusion length can be interpreted as mean straight distance travelled by the thermal neutrons from their point of thermalization to the location where they are absorbed.

In similar way, the mean square straight distance can be determined as

$$L^2 = \frac{1}{2}\overline{x^2} \tag{11}$$

The square of the diffusion length can also be interpreted as twice the mean square straight distance in plane geometry.

For point sources

$$L = \frac{\bar{r}}{2} \tag{12}$$

and

$$L^2 = \frac{1}{6}\overline{r^2} \tag{13}$$

THE NUMERICAL RESULTS AND CONCLUSION

Many important problems in physics and practical applications in technology involve the motion of particles through an object or a medium. We compute the eigenvalue corresponding to the diffusion length of eq. (8b) by using the transport equation. We consider the linear and quadratic approximations of the Henyey-Greenstein scattering. In case of the linear anisotropy, the discrete and continuous solutions are given in tabs. 1-2. For the quadratic anisotropy, all eigenvalues are calculated and only discrete eigenvalues are given in tabs. 3-4. We discuss the numerical computation of the discrete eigenvalue ν_j, and other continuous eigenvalue ν, truncating these expansions after $N = 10$ terms.

The discrete eigenvalue $|\nu_j|$ (in units of mean free path) is the largest real root or purely imaginary root of eq. (8b). The discrete eigenvalue ν_j is 5.945745254 and others continuous eigenvalue ν are 0.17449, 0.50251, 0.76994, 0.94369 for $c = 0.99$ and $g = 0.05$ in tab. 1. For $c = 1.01$ and for $g = 0.05$, the discrete eigenvalue is 5.90147i. The absolute value of imaginary eigenvalue should be taken to obtain the diffusion length L. The discrete eigenvalue ν_j is known as diffusion length and characterizes the diffusive properties of the system. The diffusion coefficient D is then given by the expression [7, 8, 15]

$$D = \nu_j^2(1-c) \tag{14}$$

Tables 1 and 3 give eigenvalues of multiplying ($c > 1$) and non-multiplying medium ($c < 1$) for different free forward parameter g. Tables 2 and 4 give eigenvalues of multiplying and non-multiplying medium for backward scattering.

Table 1. Discrete and continuous eigenvalue for forward scattering $g \geq 0$, $N = 10$

c	$g = 0$	$g = 0.05$	$g = 0.1$	$g = 0.2$	$g = 0.3$	$g = 0.4$	$g = 0.5$
0.5	0.16083 0.46685 0.72734 0.91623 1.04374	0.16085 0.46715 0.72840 0.91791 1.05282	0.16086 0.46744 0.72942 0.91944 1.06256	0.16088 0.46802 0.73135 0.92213 1.08411	0.16091 0.46859 0.73314 0.92437 1.10860	0.16093 0.46914 0.73481 0.92626 1.13629	0.16096 0.46968 0.73637 0.92785 1.16756
0.99	0.17449 0.50251 0.76994 0.94369 5.79672	0.17449 0.50251 0.76994 0.94369 5.94574	0.17449 0.50251 0.76994 0.94369 6.10687	0.17449 0.50251 0.76994 0.94369 6.47281	0.17449 0.50251 0.76994 0.94369 6.91355	0.17449 0.50251 0.76995 0.94369 7.45863	0.17449 0.50252 0.76995 0.94369 8.15700
1.01	0.17508 0.50385 0.77109 0.94411 5.75053i	0.17508 0.50385 0.77109 0.94411 5.90147i	0.17508 0.50385 0.77109 0.94411 6.06495i	0.17508 0.50385 0.77109 0.94411 6.43731i	0.17508 0.50385 0.77109 0.94411 6.88792i	0.17508 0.50385 0.77109 0.94411 7.44869i	0.17508 0.50385 0.77110 0.94411 8.17333i
2.0	0.20673 0.54790 0.79775 0.95218 0.42923i	0.20715 0.55040 0.80023 0.95315 0.44763i	0.20758 0.55321 0.80319 0.95437 0.46904i	0.20850 0.56003 0.81129 0.95809 0.52530i	0.20948 0.56911 0.82442 0.96577 0.61516i	0.21054 0.58184 0.84824 0.98909 0.80349i	0.21168 0.60085 0.88861 1.26551 ....

Table 2. Discrete and continuous eigenvalue for backward scattering $g < 0$, $N = 10$

c	$g = -0.05$	$g = -0.1$	$g = -0.2$	$g = -0.3$	$g = -0.4$	$g = -0.5$
0.5	0.16082 0.46655 0.72625 0.91440 1.03531	0.16081 0.46624 0.72512 0.91241 1.02750	0.16078 0.46561 0.72273 0.90793 1.01369	0.16076 0.46497 0.72017 0.90277 1.00215	0.16073 0.46431 0.71744 0.89699 0.99269	0.16071 0.46364 0.71453 0.89074 0.98504
0.99	0.17449 0.50251 0.76994 0.94369 5.65838	0.17449 0.50251 0.76994 0.94369 5.52949	0.17449 0.50251 0.76994 0.94369 5.29611	0.17449 0.50251 0.76994 0.94369 5.08999	0.17449 0.50251 0.76994 0.943692124 4.906205566	0.17449 0.50251 0.76994 0.94369 4.74099
1.01	0.17508 0.50385 0.77109 0.94411 5.61062i	0.17508 0.50385 0.77109 0.94411 5.48045i	0.17508 0.50385 0.77109 0.94411 5.24516i	0.17508 0.50385 0.77109 0.94411 5.03779i	0.175087540 0.503851605 0.771091288 0.944111714 4.85322435i	0.17508 0.50385 0.77109 0.94411 4.68756i
2.0	0.20632 0.54565 0.79565 0.95139 0.41318i	0.20593 0.54363 0.79385 0.95074 0.39900i	0.20517 0.54012 0.79092 0.94973 0.37495i	0.20446 0.53718 0.78864 0.94898 0.35518i	0.203796810 0.534692699 0.786819615 0.948404243 0.33852787i	0.20316 0.53254 0.78532 0.94794 0.32423i

Table 3. Selected discrete eigenvalues with quadratic anisotropy for forward scattering $g \geq 0$, $N = 10$

c	$g = 0$	$g = 0.05$	$g = 0.1$	$g = 0.2$	$g = 0.3$	$g = 0.4$	$g = 0.5$
0.5	1.04374	1.05309	1.06367	1.08869	1.11928	1.15616	1.20043
0.99	5.79672	5.94580	6.10712	6.47388	6.91626	7.46425	8.16773
1.01	5.75053i	5.90141i	6.06470i	6.43623i	6.88517i	7.44296i	8.16229i
2.0	0.42923i	0.44720i	0.46707i	0.51445i	0.57713i	0.66687i	0.81306i

Table 4. Selected discrete eigenvalues with quadratic anisotropy for backward scattering $g < 0$, $N = 10$

c	$g = -0.05$	$g = -0.1$	$g = -0.2$	$g = -0.3$	$g = -0.4$	$g = -0.5$
0.5	1.03557	1.02854	1.01775	1.01105	1.01105	1.00924
0.99	5.65844	5.52971	5.29699	5.09200	4.90995	4.74734
1.01	5.61056i	5.48022i	5.24428i	5.03580i	4.84953i	4.68134i
2.0	0.41283i	0.39771i	0.37051i	0.34628i	0.32403i	0.30301i

A nuclear reactor is the complex system consisting of fuel, moderators, coolant, control rods, and environmental structures. Since the reactor parameters are important for nuclear reactor systems, the values of parameters g and c should be adjusted. The variation of correct eigenvalue is given in tables. In fact, the expected roots do not appear if the parameter g is larger as seen in tab. 1. The accurate numerical results are obtained for low values of parameter g.

It is interesting to note that v_j increases almost monotonically with the asymmetry parameter g. This is understandable. By increasing values of g, the particles direct in the forward directions. When the negative values of g increase, the variation of v_j starts to decrease. The asymmetry parameter g should be limited as given in tables for the neutron transport applications with the Henyey-Greenstein scattering. In this study, g should be ranged from –0.5 to 0.5. Our approximations are not good enough for cases $-1 < g < -0.5$ and $0.5 < g < 1$. If scattering is strongly asymmetric ($0.5 < g < 1$) in some applications, the approximations of the Henyey-Greenstein scatering need more terms than $l > 2$ in eq. (2).

Sahni, Dahl, and Sjostrand [7] have given representative values of the discrete eigenvalues and diffusion coefficient for some value of g and the case of $c < 1$. They used the Case method to solve the transport equation. In this study we use P_N method. We have made some calculations not only for the case $c < 1$ but also for the case $c > 1$ by using approximations of the Henyey-Greenstein. When obtained results are compared to the values of references [4, 8-10], they are quite similar.

We have proved the existence of the discrete eigenvalues, and hence the diffusion lengths for the linear and quadratic anisotropic scattering, given by the Henyey-Greenstein kernel. The P_N method is quite general and applicable to all non-negative scattering kernels. If one needs diffusion coefficient, it can be easily and accurately obtained from the diffusion length in eq. (8).

AUTHOR CONTRIBUTIONS

The theoretical analysis and literature research were carried out by K. Kacira and F. Yasa. The calculations were performed by K. Kacira. The computer programming was prepared by H. Bilgic. All authors discussed the result and participated in the writing of the manuscript.

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АНИЗОТРОПНЕ АПРОКСИМАЦИЈЕ ХЕНИ-ГРИНШТАЈНОВЕ ФАЗНЕ ФУНКЦИЈЕ У ТРАНСПОРТНОЈ ЈЕДНАЧИНИ НЕУТРОНА

Проучаван је утицај анизотропног расејања на својствене вредности једнобрзинске неутронске једначине за плочу са умножавајућим ($c > 1$) и апсорбујућим ($c < 1$) својствима. Коришћењем линеарне и квадратне апроксимације Хени-Гринштајновог кернела расејања, обављени су прорачуни не само за случајеве $c < 1$ и $0 < g < 1$, већ и за $c > 1$ и $-1 < g < 0$. Параметар асиметрије g усмерава расејање да буде изотропно, уназад, или унапред оријентисано. У циљу исправне процене тачности да је широк преглед својствених вредности. Нумерички резултати указују да се, при линеарној и квадратној апроксимацији анизотропног расејања, дискретне својствене вредности увећавају када је расејање унапред, а смањују за расејање уназад.

Кључне речи: Хени-Гринштајново расејање, транспортна једначина, својствена вредност, дифузиона дужина