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Orthogonal polynomials in transport theories

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Abstract. The asymptotical ($k \to \infty$) behaviour of zeros of the polynomials $g_k^m(\nu)$ encountered in the treatment of direct and inverse problems of scattering in neutron transport as well as radiative transfer theories is investigated in terms of the amplitude $\bar{w}_k$ of the kth Legendre polynomial needed in the expansion of the scattering function. The parameters $\bar{w}_k$ describe the anisotropy of scattering of the medium considered. In particular, it is shown that the asymptotical density of zeros of the polynomials $g_k^m(\nu)$ is an inverted semicircle for the anisotropic non-multiplying scattering medium.

1. Introduction

The polynomials $g_k^m(\nu)$ were introduced long ago (Chandrasekhar 1950, Davison 1957) in the treatment of the fundamental transfer equation which governs the variation in energy intensity of a pencil of radiation traversing a medium. These polynomials have been shown to play a fundamental role for the solution of both direct (see, e.g., Davison 1957, Boffi and Trombetti 1967, Mullikin 1964, Cacuci and Goldstein 1977) and inverse problems (see, e.g., Case 1973, Kanal and Moses 1978a, b) in neutron transport theory. In particular the polynomials $g_k^m(\nu)$ have been extensively used to solve the transport technique (Davison 1957) in both cases of isotropic scattering medium and anisotropic scattering medium.

In the last case people always assume that the scattering function is of finite order N and can be expanded in terms of the first N Legendre polynomials. Recently (McCormick and Veeder 1978) in studying the infinite-medium inverse transport problem it has been shown that the polynomials $g_k^m(\nu)$ are very useful for the calculation of the integral moments of the neutron flux over all space and angles, in terms of which the scattering coefficients of the medium can be determined.

The orthogonality properties of these polynomials and other of their important properties which are of interest for neutron transport and radiative transfer theories have been considered in detail (Inönü 1970) in the case of $m = 0$ and azimuthal independence. For the general case, i.e. $m \neq 0$ and azimuthal dependence, these properties have been examined (Veeder 1977) and the relationship between these polynomials and the associated Legendre polynomials have been given.

The zeros of the polynomials g form an approximate representation for transport theory of the spectrum of discrete eigenvalues and the continuum from $-1 \leq \nu \leq +1$. These zeros are tabulated (see, e.g., Davison 1957, pp 119–21). In the method of spherical harmonics for solving transport problems, the zeros of $g_{L+1}(\nu) = 0$ are the eigenvalues for the P_L method. The largest eigenvalue tends to approximate the

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discrete eigenvalue, while others tend to fill in the continuum between -1 and $+1$ as L increases. It is known (McCormick and Kuščer 1973) that as the number of terms L in the P_L method becomes large, the results tend to be exact eigenvalue spectra reproduced with a method such as the singular eigenfunction expansion technique.

The purpose of the present paper is to investigate the asymptotical distribution of the zeros of the polynomials g in terms of the amplitude $\bar{w}_k$ of the kth Legendre polynomial needed in the above mentioned expansion of the scattering function. The parameters $\bar{w}_k$ describe (Case and Zweifel 1967) the anisotropy of scattering of the medium. The structure of the paper is as follows. Section 2 contains the definition of the polynomials and theorem A which play a predominant role later on. In § 3 the average asymptotic properties of the zeros obtained are included. First the results are written in the form of theorems and then the proofs of them are given. In particular, it is shown that in the case of anisotropic scattering the asymptotical density of zeros of the polynomials g for a non-multiplying medium is an inverted semicircular distribution.

2. Definition and tools

Let us consider the polynomials $g_k^m(\nu)$ defined by the following recurrence relation:

$$g_k^m(\nu)=\frac{h_{k-1}}{k-m}\nu g_{k-1}^m(\nu)-\frac{k+m-1}{k-m}g_{k-2}^m(\nu) \qquad k\geqslant m \tag{1}$$

with the initial conditions

$$g_m^m(\nu)=\prod_{n=0}^{m-1}(2n+1) \qquad g_{m-1}^m(\nu)=0.$$

Here m can be any non-negative integer and h_k is given by

$$h_k=2k+1-\bar{w}_k \tag{2}$$

with

$$\bar{w}_k=(2k+1)cf_k. \tag{3}$$

Here c and f_k are real parameters. From a physical point of view c is the mean number of secondary particles per collision and the values f_k are the expansion coefficients of the scattering or phase function. In particular, $f_0=1$ and f_1 is equal to the mean cosine of the scattering angle in the laboratory coordinate system.

The polynomials $g_k^m(\nu)$ are of order $k-m$, alternatively even and odd. They are a generalisation (Chandrasekhar 1950, McCormick and Veeder 1978) of a modified version of the associated Legendre polynomials, and reduce to these in the limit that $\bar{w}_k\to 0$ for all k, i.e. when the medium becomes purely absorbing.

To end this section we shall write a theorem from the general theory of orthogonal polynomials found recently (Nevai and Dehesa 1979) which is the main tool used to obtain the results of this paper.

Theorem A. Let $\mathbb{R}$ and $\mathbb{R}^+$ be the set of real numbers and the set of positive real numbers respectively. Let $\phi:\mathbb{R}^+\to\mathbb{R}^+$ be a non-decreasing function such that for every fixed $t\in\mathbb{R}$

$$\lim_{x\to\infty}\frac{\phi(x+t)}{\phi(x)}=1. \tag{4}$$

Let us consider the set of orthogonal polynomials $\{P_k(x);\ k=0,1,2,\ldots\}$ defined by the following three-term recursion relation:

$$\begin{aligned} &P_k(x)=(x-a_k)P_{k-1}(x)-b_k^2P_{k-2}(x)\\ &P_{-1}(x)=0 \qquad P_0(x)\equiv 1 \qquad k=1,2,3,\ldots. \end{aligned} \tag{5}$$

Furthermore, assume that there exist two numbers a and $b\geqslant 0$ such that the coefficients a_k and b_k satisfy

$$\lim_{k\to\infty}\frac{a_k}{\phi(k)}=a \qquad \text{and} \qquad \lim_{k\to\infty}\frac{b_k}{\phi(k)}=\tfrac{1}{2}b. \tag{6}$$

Then for every non-negative integer r

$$\lim_{k\to\infty}\frac{\sum_{l=1}^{k}x_{lk}^{r}}{\int_0^k[\phi(t)]^r\,\mathrm{d}t}=\sum_{j=0}^{[r/2]}b^{2j}a^{r-2j}2^{-2j}\binom{2j}{j}\binom{r}{2j} \tag{7}$$

where x_{lk} are the zeros of $P_k(x)$ and $[r/2]$ is equal to $\frac{1}{2}r$ or $\frac{1}{2}(r-1)$when r is even or odd respectively.

3. Results

The main results are written in the form of the following four theorems.

Theorem 1. Let ϕ be a function defined as in theorem A. If the h_k defined by (2) satisfy the condition

$$\lim_{k\to\infty}\left(\frac{(k-1)^2-m^2}{h_{k-1}h_{k-2}}\right)^{1/2}\frac{1}{\phi(k)}=\tfrac{1}{2}b\geqslant 0 \tag{8}$$

then for every non-negative integer r,

$$\lim_{n\to\infty}\frac{\sum_{l=1}^{n}[x_{ln}^{(m)}]^r}{\int_0^n[\phi(t)]^r\,\mathrm{d}t}=\begin{cases}0 & \text{if } r \text{ is odd}\\ (\frac{1}{2}b)^r\binom{r}{r/2} & \text{if } r \text{ is even}\end{cases} \tag{9}$$

where $\{x_{ln}^{(m)};\ l=1,2,\ldots,n\}$ are the zeros of the polynomial $g_n^m(x)$.

Notice that when the h_k's are either constant (i.e. not dependent on k) or continuous functions of the subscript k, then $h_{k-1}h_{k-2}\approx h_{k-1}^2$ for large k. This assumption is made from here onwards. Consequently

$$\lim_{k\to\infty}\left(\frac{(k-1)^2-m^2}{h_{k-1}h_{k-2}}\right)^{1/2}\frac{1}{\phi(k)}=\lim_{k\to\infty}\frac{[(k-1)^2-m^2]^{1/2}}{h_{k-1}\phi(k)}. \tag{10}$$

Theorem 2. Let us assume that there exists $B\geqslant 0$ such that

$$\lim_{k\to\infty}\frac{[(k-1)^2-m^2]^{1/2}}{k^Bh_{k-1}}=\tfrac{1}{2}b\geqslant 0. \tag{11}$$

Then for $r = 0, 1, 2, , \ldots$

$$\lim_{n\to\infty} \frac{1}{n} \sum_{l=1}^{n} \left(\frac{x_{ln}^{(m)}}{n^B}\right)^r = \begin{cases} 0 & \text{if } r \text{ is odd} \\ \dfrac{1}{rB+1} (\tfrac{1}{2}b)^r \dbinom{r}{r/2} & \text{if } r \text{ is even.} \end{cases} \tag{12}$$

Theorem 3. If the non-negativity condition

$$\lim_{k\to\infty} \frac{[(k-1)^2 - m^2]^{1/2}}{h_{k-1}} = \tfrac{1}{2}b \geqslant 0 \tag{13}$$

is fulfilled, then

$$\begin{cases} \mu'_{2s} = (\tfrac{1}{2}b)^{2s} \dbinom{2s}{s} \\ \mu'_{2s-1} = 0 \end{cases} \qquad s = 1, 2, 3, \ldots \tag{14}$$

where $\{\mu'_r; r = 1, 2, \ldots\}$ are the moments of the asymptotical distribution density of zeros of the polynomials $\{g_k^m(\nu)\}$.

Theorem 4. The asymptotical distribution density of zeros of the polynomials $g_k^m(x)$ which arise in transport theories (e.g. neutron or radiative for the cases of both an isotropic medium and an anisotropic non-multiplying medium is given by

$$\rho(\nu) = \begin{cases} (1-x^2)^{-1/2}/\pi & \text{for} -1 < x < 1 \\ 0 & \text{otherwise.} \end{cases} \tag{15}$$

In the rest of the paper we shall prove these theorems.

Proof of theorem 1. Any set of orthogonal polynomials $\{P_n(x); n = 1, 2, \ldots\}$ fulfils (Szegö 1978) a three-term recurrence relation of the form

$$\begin{aligned} &P_n(x) = (A_n x + B_n) P_{n-1}(x) - C_n P_{n-2}(x) \\ &P_{-1}(x) = 0 \qquad P_0(x) = 1 \qquad n = 1, 2, 3, \ldots \end{aligned} \tag{16}$$

with $A_n \neq 0$ and $C_n \neq 0$. It is easy to show that the polynomials $Q_n(x) = P_n(x)/A_1 A_2 \ldots A_n$ satisfy the recurrence relation

$$\begin{aligned} &Q_n(x) = (x - a_n) Q_{n-1}(x) - b_n^2 Q_{n-2}(x) \\ &Q_{-1}(x) \equiv 0 \qquad Q_0(x) \equiv 1 \qquad n = 1, 2, 3, \ldots \end{aligned} \tag{17}$$

with

$$a_n = -B_n/A_n \qquad \text{and} \qquad b_n^2 = C_n/A_n A_{n-1}.$$

Notice that the zeros of $Q_n(x)$ coincide with those of $P_n(x)$. Therefore the polynomials $g_k^m(\nu)$ defined by the relation (1) have the same zeros as the polynomials $Q_k(x)$ defined by (17) with the coefficients a_k and b_k as follows:

$$a_k = 0 \qquad \text{and} \qquad b_k^2 = [(k-1)^2 - m^2]/h_{k-2} h_{k-1}.$$

The application of theorem A to the polynomials $Q_k(x)$ first produces the values $a = 0$ and the expression (8) for the parameter b. Replacing these two values into (7) gives rise to equation (10). Then theorem 1 is proved.

Proof of theorem 2. Choosing $\phi(k)=k^B$, $B\geqslant 0$ and taking into account (10) it turns out that the inequality (8) of theorem 1 transforms into inequality (11). Since in this case

$$\int_0^n [\phi(t)]^r\,\mathrm{d}t = n^{Br+1}/(rB+1)$$

the equation (9) reduces to the simpler equation (12). Theorem 2 is also proved.

Proof of theorem 3. For $B=0$, equations (11) and (12) reduce in a straightforward manner to the simpler equations (13) and (14) of theorem 3, where we have used the definition of moments μ'_r of the asymptotical density of zeros $\rho(\nu)$ of the polynomials $\{g_k^m(\nu)\}$, i.e.

$$\mu'_r=\lim_{n\to\infty}\frac{1}{n}\sum_{l=1}^{n}[x_{ln}^{(m)}]^r.$$

To understand this, one should remember that

$$\rho(\nu)=\lim_{n\to\infty}\rho^{(n)}(\nu)$$

where $\rho^{(n)}(\nu)$ is the discrete distribution density of zeros of the polynomial $g_n^m(\nu)$. This proves theorem 3.

Proof of theorem 4. For an isotropic medium, $f_k=\delta_{k0}$. Therefore relations (2) and (3) show that

$$h_k=(2k+1)(1-c\delta_{k0}).$$

Then the value of b according to (13) is

$$b=2\lim_{k\to\infty}\frac{[(k-1)^2-m^2]^{1/2}}{(2k-1)(1-c\delta_{k-1,0})}=1,$$

with which the expressions (14) reduce to

$$\left.\begin{aligned}\mu'_{2s}&=2^{-2s}\binom{2s}{s}\\ \mu'_{2s-1}&=0\end{aligned}\right\}\qquad s=1,2,3,\ldots.$$

These quantities are the moments of the inverted semicircular distribution density given by (15).

In the case of an anisotropic non-multiplying medium, i.e. when $c<1$, it turns out that $|\bar{w}_k|<1$ and then according to (13) one gets

$$b=2\lim_{k\to\infty}\frac{[(k-1)^2-m^2]^{1/2}}{2k-1-\bar{w}_{k-1}}=1.$$

Therefore one again obtains the function defined by (15). Theorem 4 is therefore proved.

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