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ADDENDUM

Orthogonal polynomials in neutron transport theory

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Abstract. The asymptotic average properties of zeros of the polynomials $g_k^m(x)$, which play a fundamental role in neutron transport and radiative transfer theories, are investigated analytically in terms of the angular expansion coefficients $\bar{w}_k$ of the scattering kernel for three wide classes of scattering models. In particular it is found that the scattering models of Eccleston–McCormick, Shultis *et al* and Henyey–Greenstein belong in one of the above-mentioned classes, and their associated polynomials $g_k^m(x)$ have the same asymptotic density of zeros.

In the transport theory of neutrons through an isotropic or anisotropic scattering medium, a special set of orthogonal polynomials $g_k^m(x)$ plays a fundamental role for the solution of direct and inverse problems (see e.g. Davison 1957, McCormick and Kuscer 1966, 1973, McCormick and Veeder 1978 and references therein). These polynomials were introduced long ago (Chandrasekhar 1950) for the $m = 0$ and azimuth-independent case and defined later (Mullikin 1964, McCormick and Kuscer 1966, 1973, McCormick and Veeder 1978) for the general case $m \neq 0$ and azimuthal dependence. The orthogonality properties of these polynomials and other of their important properties which are of particular interest in neutron transport theory have been analysed in detail (Inönü 1970, Veeder 1977).

The zeros of the polynomials g form an approximate representation for transport theory of the spectrum of discrete eigenvalues and the continuum from $-1 \leqslant x \leqslant +1$. In the method of spherical harmonics for solving transport problems, the zeros of $g_{L+1}(x) = 0$ are the eigenvalues for the P_L method. Several other properties of these zeros (Inönü 1970), and their connections with the exact eigenvalue spectra reproduced with a method such as the singular eigenfunction expansion technique (McCormick and Kuscer 1973), are known.

Recently (Dehesa 1981) the asymptotic distribution of the zeros $\rho(x)$ of the polynomials $g_k^m(x)$ has been examined in terms of the angular expansion coefficients $\bar{w}_k$ of the scattering kernel. As is well known, these parameters $\bar{w}_k$ describe the anisotropy of scattering of the medium. Here the general results relative to the distribution density $\rho(x)$ are applied to different scattering models, each of which is characterised by its corresponding set of parameters $\bar{w}_k$.

The polynomials $g_k^m(x)$ are uniquely defined by the recursion relation

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

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or (Dehesa 1981)

$$g_k^m(x) = x g_{k-1}^m(x) - \frac{(k-1)^2 - m^2}{h_{k-2} h_{k-1}} g_{k-2}^m(x) \tag{1a}$$

with the initial conditions

$$g_m^m(x) = \prod_{n=0}^{m-1} (2n+1) = (2m-1)!!, \qquad g_{m-1}^m(x) = 0. \tag{1b}$$

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

$$h_k = 2k + 1 - \bar{w}_k \qquad \text{where } \bar{w}_k = (2k+1) c f_k, \tag{2}$$

c and f_k being real parameters which physically represent the mean number of secondary particles per collision and the expansion coefficients of the scattering (or phase) function respectively. The polynomials $g_k^m(x)$ defined by equations ($1a$, b) are of order $k - m$, alternately even or odd. They are a generalisation of a modified version of the associated Legendre polynomials, and reduce to these in the limit of $\bar{w}_k \to 0$ for all k, i.e. when the medium becomes purely absorbing.

The main result of this note is the following theorem.

Theorem 1. Let us consider the three wide classes of scattering models defined by the following three sets of parameters $\bar{w}_k$:

(A) $\bar{w}_k = \mathrm{o}(k)$,

(B) $\bar{w}_k \sim k$, i.e. $\bar{w}_k = \alpha k + \mathrm{O}(1)$, α being a real parameter,

(C) $\bar{w}_k \sim k^{1+\varepsilon}$, $\varepsilon > 0$,

as $k \to \infty$. The moments of even order $\{\mu'_{2j}; j = 0, 1, 2, \ldots\}$ of the asymptotic density of zeros $\rho(x)$ of the polynomials $g_k^m(x)$ associated with each of these three scattering classes are given by

$$\text{(A)} \quad \mu'_{2j} = (2j-1)!!/j!2^j, \tag{3}$$

$$\text{(B)} \quad \mu'_{2j} = (2j-1)!!2^j/j!(2+\alpha)^{2j}, \tag{4}$$

$$\text{(C)} \quad \mu'_{2j} = 0. \tag{5}$$

The moments of odd order $\{\mu'_{2j+1}; j = 0, 1, 2, \ldots\}$ are all equal to zero for the three classes of scattering.

Here we have used the symbols 'o' and '$\sim$' with the conventional interpretation, e.g. $\bar{w}_k = \mathrm{o}(k)$ means that $\bar{w}_k$ grows more slowly than k as $k \to \infty$, and $\bar{w}_k \sim k^{1+\varepsilon}$ means that $\bar{w}_k$ and $k^{1+\varepsilon}$ grow at the same rate as $k \to \infty$. Also the double factorial notation is used in the following sense: $(2j-1)!! = 1 \times 3 \times 5 \ldots (2j-1) = \pi^{-1/2} 2^j \Gamma(j + \frac{1}{2})$.

The proof of theorem 1 is based on the following result (Dehesa 1981). If the non-negativity condition

$$\lim_{k \to \infty} \frac{[(k-1)^2 + m^2]^{1/2}}{h_{k-1}} = \frac{b}{2} \geqslant 0 \tag{6}$$

is fulfilled, then the moments of the asymptotic density of zeros $\rho(x)$ of the polynomials $g_k^m(x)$ are:

$$\left.\begin{aligned} \mu'_{2j} &= (b/2)^{2j}\binom{2j}{j} \\ \mu'_{2j+1} &= 0 \end{aligned}\right\} \qquad \text{for } j = 0, 1, 2, \ldots. \tag{7}$$

Now, taking into account that

$$\binom{2j}{j} = \frac{2^j(2j-1)!!}{j!}$$

and, according to (2) and (6), that

$$\bar{w}_k = \mathrm{o}(k) \Rightarrow h_k = 2k + \mathrm{O}(1) \Rightarrow b = 1,$$

$$\bar{w}_k = \alpha k + \mathrm{O}(1) \Rightarrow h_k = (2+\alpha)k + \mathrm{O}(1) \Rightarrow b = 2/(2+\alpha),$$

$$\bar{w}_k \sim k^{1+\varepsilon},\ \varepsilon > 0 \Rightarrow h_k \sim k^{1+\varepsilon} \Rightarrow b = 0,$$

one has only to put these values of b into the equation (7) to obtain the expressions (3), (4) and (5) which we were looking for.

In practice many precise neutron scattering models have been considered which belong in the three wide classes studied in theorem 1. Here we will take into account, for the sake of illustration, three scattering models frequently used in the literature (Eccleston and McCormick 1970, McCormick and Sanchez 1981). The binomial model (Kaper *et al* 1970, Shultis and Hill 1976) with predominantly forward (+) or backward (−) scattering is characterised by a set of coefficients $\bar{w}_k(\alpha\pm)$ given recurrently by

$$\bar{w}_k(\alpha\pm) = \pm\frac{(2k+1)(\alpha+1-k)}{(2k-1)(\alpha+1+k)}\bar{w}_{k-1}(\alpha\pm), \qquad k \geqslant 1,$$

once w_0 is specified. A second scattering model (Henyey and Greenstein 1941) has the following expansion coefficients:

$$\bar{w}_k(1) = (2k+1)l^k\bar{w}_0, \qquad -1 < l < 1.$$

A third scattering model used for one-speed neutron transport (Eccleston and McCormick 1970) is defined by the coefficients

$$\bar{w}_{2k} = (-1)^{k+1}\frac{(4k+1)(2k-3)!!}{2^k(k+1)!}, \qquad k \geqslant 2,$$

$$\bar{w}_{2k+1} = 2\bar{w}_0\delta_{k,0}, \qquad k \geqslant 0.$$

For all these three particular scattering models one easily notices that $\bar{w}_k$ grows more slowly than k as $k \to \infty$ and therefore each of the models is a member of the class A. As a consequence of this, it arises in a natural way that, according to our theorem, the different systems of orthogonal polynomials $g_k^m(x)$ associated with the scattering models just mentioned have the same asymptotic density of zeros.

There are many other scattering models which might belong in classes A, B or C, such as the scattering of visible light in fog (Spencer 1960, Pahor and Gross 1970, McCormick and Sanchez 1981) and the scattering in the speed-independent neutron transport of Murray, Siewert and Harrington (Murray *et al* 1967).

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