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A New Application of the Discrete Laguerre Polynomials in the Numerical Evaluation of the Hankel Transform of a Strongly Decreasing Even Function

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Starting from a scattering problem of intermediate-energy nuclear particles, a new numerical method for the evaluation of the Hankel transform of an even function has been performed. The main feature of our method is the expansion of the even function in series of discrete Laguerre polynomials. It was found that the use of discrete Laguerre polynomials decreases the computer time without any loss of the advantages found in the use of classical polynomials.

1. INTRODUCTION

The Glauber theory [4] is known to be one of the most successful approximation methods for describing the scattering of high-energy interacting particles. In this theory, the complicated interactions of a projectile with a nucleus are reduced to a simple additivity of phase shifts due to the particle–nucleon interactions. The forward differential cross-section for elastic scattering of a nuclear particle, neglecting the spin–orbit and Coulomb potential, can be related to the two-dimensional Fourier transform of a suitable phase shift in the impact parameter representation.

We have (see [2])

$$\frac{d\sigma}{d\Omega} = | F_e(\mathbf{q}_\perp)|$$

with

$$F_e(\mathbf{q}_\perp) = \frac{ik}{2\pi} \int d^2\mathbf{b} e^{i\mathbf{q}_\perp \cdot \mathbf{b}} \varphi(\mathbf{b}),$$

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where

$$\varphi(\mathbf{b}) = 1 - \exp\left[-\frac{im}{\hbar^2 k}\int_{-\infty}^{+\infty} V(\mathbf{b}, z)\, dz\right].$$

In the above expression k is the wave number of the incident particle of mass m scattered by the potential $V(\mathbf{r}) = V(\mathbf{b}, z)$, $\mathbf{b}$ is the transverse component of the vector $\mathbf{r}$ and $q_\perp$ is the perpendicular component of the momentum transfer. If the problem is spherically symmetric, as appears in the majority of the cases, the function $\varphi(\mathbf{b})$ depends only on $|\mathbf{b}|^2 \equiv b^2$ and for physical reasons it is exponentially decreasing as $b \to \infty$.

In this case we can write

$$\varphi(b) = e^{-\alpha b^2} g(b^2),$$

where α is a suitable constant, and the evaluation of $F_e(\mathbf{q}_\perp)$ leads now to the Hankel transform of a strongly decreasing even function.

By taking polar coordinates (b, φ) with the polar axis in the direction of $\mathbf{q}_\perp$, we have $d^2 b = b db \cos\varphi$, $\mathbf{q}_\perp \cdot \mathbf{b} = q_\perp \cdot b \cos\varphi$ and, after some calculations, we obtain

$$\begin{aligned} F_e &= \frac{ik}{2\pi}\int_0^\infty \varphi(b)\, b \cdot db \int_0^{2\pi} e^{iq_\perp b\cos\varphi}\, d\varphi \\ &= ik \int_0^\infty e^{-\alpha b^2} J_0(q_\perp b)\, g(b^2)\, b \cdot db. \end{aligned}$$

A little manipulation reduces our problem to the evaluation of integrals of the type

$$I(\omega) = \int_0^\infty e^{-x^2} J_0(\omega x) f(x^2)\, x\, dx, \tag{1}$$

where ω is proportional to the momentum transfer $q_\perp$ and $f(x^2) \equiv g(x^2/d^2)$. Since the Glauber approximation improves with higher energy, the values of ω used in practical comparison of experimental and theoretical results can be very large [9].

2. Method

In principle, one can seek to evaluate the integral (1) by some standard numerical quadrature methods but, as ω increases, the rapid oscillations of the integrand function may create serious numerical problems; the error due to the cancellation of nearly equal positive and negative terms can grow prohibitively. (See Table III.)

On the other hand, one can evaluate $I(\omega)$, for $\omega \to \infty$ by some asymptotic formulas. In recent years the asymptotic expansions of the Hankel transform have stirred up considerable attention [7, 10, 11, 13].

Unfortunately the asymptotic relations quoted in the above papers cannot be used in our case because $f(x^2)$ is an even function, the coefficients of the expansion being identically zero.

The last observation suggests the existence of an exponential term in a possible asymptotic expansion.

In order to take into account the exponential behaviour when ω is large, we propose, before term by term integration, to expand $f(x^2)$ in series of Laguerre polynomials. This follows from the consideration that the Hankel transform of $L_n(x^2)$ can be performed analytically and it is exponentially decreasing as $\omega \to \infty$. Let

$$f(x^2) = \sum_{n=0}^{\infty} b_n L_n(x^2) \tag{2}$$

with

$$b_n = \int_0^{\infty} e^{-y} L_n(y) f(y)\, dy, \tag{3}$$

where $y = x^2$.

Substitution of (2) in (1) gives

$$I(\omega) = \int_0^{\infty} e^{-x^2} J_0(\omega x) \sum_{n=0}^{\infty} b_n L_n(x^2)\, x\, dx = \sum_{n=0}^{\infty} b_n V_n, \tag{4}$$

where (Gradshteyn and Ryzhik [6])

$$V_n = \int_0^{\infty} e^{-x^2} J_0(\omega x)\, L_n(x^2)\, x\, dx = \frac{e^{-\omega^2/4}}{2(n!)} \left(\frac{\omega}{2}\right)^{2n}. \tag{5}$$

The computation of V_n may be carried out by the simple recurrence relations [3]

$$V_{n-1} = \frac{4n}{\omega^2} V_n, \qquad n = 0, 1, \ldots, n_\omega, \tag{6}$$

$$V_{n+1} = \frac{\omega^2}{4(n+1)} V_n, \qquad n = n_\omega, \quad n_\omega + 1, \ldots, \tag{7}$$

where

$$n_\omega = \left[\frac{\omega^2}{4}\right].$$

($[X]$ denotes the integer part of X.) When ω is "not too large," it is convenient to consider only forward recurrence relation (7) with $n_\omega = 0$ and

$$V_0 = \tfrac{1}{2} e^{-\omega^2/4},$$

whereas for ω "very large" the asymptotic estimate for V_n,

$$V_n \sim \frac{1}{(2\pi)^{1/2}} \left[\omega\left(1+\frac{1}{3\omega^2}+\frac{1}{18\omega^2}-\frac{139}{810\omega^6}-\frac{571}{9720\omega^8}\right)\right]^{-1},$$

is recommended.

3. The Evaluation of the Laguerre–Fourier Coefficients

Formula (4) requires the Laguerre–Fourier coefficients b_n.

From (6), (7) it is easy to see to see that the sequence $\{V_n\}$, $n = 0, 1, \ldots$, reaches the maximum value for $n = n_\omega$ and is strongly decreasing as $n > n_\omega$. The same behaviour can be expected for the sequence $\{|b_n V_n|\}$; thus the summation (4) converges rapidly for $n > n_\omega$.

In principle many standard methods are available for the calculation of b_n (for instance, the Gaussian integration formulas, trapezoidal rule, etc.), but in many practical situations the calculations are time consuming and are not manageable when n increases.

We will propose here a method, utilizing the Laguerre discrete orthogonal polynomials, which is particularly appropriate (see [1]) when the values of the function $f(y)$ are subjected to independent normally distributed errors (due, for example, to observational errors, rounding errors, etc.). Moreover the method turns out to be of easy application and suitable to compute a large number of b_n coefficients.

We begin with a standard procedure for the evaluation of b_n; the application of the modified trapezoidal rule (see [8, Chap. 15]), with integration step size $h > 0$, to (3), gives

$$\begin{aligned} b_n &= \int_0^\infty e^{-y} L_n(y)\, dy \\ &= h \sum_{k=0}^{\infty} e^{-(k+1/2)h} \cdot L_n\left(kh+\frac{h}{2}\right) f\left(kh+\frac{h}{2}\right) + G \end{aligned} \tag{8}$$

with

$$G = \sum_{k=1}^{\infty} \alpha_k h^{2k}, \tag{9}$$

where the α_k's are independent of h and the function $f(y)$ is supposed infinitely times differentiable. If $f(y)$ is only $2s$ ($s > 0$ integer) times differentiable the summation (9) ends after the sth term.

An explicit expression for α_k is given by Luke [8].

It is well known, when a formula of type (9) is applicable, that Romberg's extrapolation method is very efficient. Romberg's extrapolation and trapezoidal rule converge rapidly to the correct value; however, when n is large, the amount of calculation can grow prohibitively. The halving of h in Romberg's table, requires new values of L_n (computed by the standard three term recurrence relation) which must be evaluated starting from L_0. This procedure may require a large amount of computing time. The utilization of discrete orthogonal Laguerre polynomials avoids such an inconvenience without losing the advantages given by formula (9). The discrete othogonal Laguerre polynomials were developed by Gottlieb [5] but for our purpose it is convenient to redefine them in a more suitable form. In Appendix A some of the most important properties of such polynomials are displayed.

As an approximate value of b_n, we assume $b_n^{(h)}$ is given by

$$b_n^{(h)} = h \sum_{k=0}^{\infty} e^{-(k+1/2)h} l_n^{(h)} \left(h + \frac{1}{2}\right) f\left(kh + \frac{h}{2}\right), \tag{10}$$

where $l_n^{(h)}$, the Laguerre discrete polynomials defined by (A.1), are calculated by the three term recurrence relation

$$\begin{gathered}(k+1)\, l_n^{(h)}(k+\tfrac{3}{2}) = [n+k+1+e^h(k-n)]\, l_n^{(h)}(k+\tfrac{1}{2}) - ke^h l_n^{(h)}(k-\tfrac{1}{2}),\\ l_n^{(h)}(\tfrac{1}{2}) = e^{-hn/2}, \qquad l_n^{(h)}(-\tfrac{1}{2}) = 0; \qquad k = 0, 1, \ldots,\end{gathered} \tag{11}$$

which may be easily obtained by combining (A.5) with the symmetrical relation (A.4). The starting value $l_n^{(h)}(\frac{1}{2})$ ensues immediately from (A.3).

Finally we observe that

$$\begin{aligned} b_n - b_n^{(h)} = {} & \int_0^\infty e^{-y} \left[L_n(y) - l_n^{(h)}\left(\frac{y}{h}\right)\right] f(y)\, dy + \int_0^\infty e^{-y} l_n^{(h)}\left(\frac{y}{h}\right) f(y)\, dy \\ & - h \sum_{k=0}^{\infty} e^{-(k+1/2)h} l_n^{(h)} \left(k + \frac{1}{2}\right) f\left(kh + \frac{1}{2}\right). \end{aligned}$$

By using asymptotic relation (A.8) in the first integral and applying the trapezoidal rule (8), (9), to the second integral, the analogous formula of (8)

$$b_n = b_n^{(h)} + \sum_{k=0}^{\infty} \beta_k h^{2k} \tag{12}$$

(with β_k constants independent of h) can be proved.

We remark that the computation of $b_n^{(h)}$ given by (10) is much less expensive than (8). In fact stopping the summations in (8) and (10) after N terms, formula (10) requires, for the evaluation of $l_n^{(h)}$, only N iterations of (11), whereas formula (8) implies, for the computation of $L_n(kh + h/2)$, $n \cdot N$ iterations of the three term recurrence relation of the Laguerre polynomials without increasing the accuracv in the numerical results.

4. Numerical Examples

The complete evaluation of the integral (1) with $f(x^2) = \sin(x^2)$ is performed to test the global usefulness of our method.

Equation (4) used to evaluate the integral

$$I(\omega) = \int_0^\infty e^{-x^2} J_0(\omega x) \sin(x^2)\, x\, dx \tag{13}$$

can be expressed in the form

$$I(\omega) \sim I_N(\omega) = \sum_{k=1}^{N} C_k V_k.$$

The Laguerre coefficients

$$C_k = \int_0^\infty e^{-y} L_k(y) \sin y\, dy \tag{14}$$

were evaluated by the method outlined in Section 3; working with ≈ 15 significant digits we were able to compute about a hundred C_k coefficients, all correct at least up to 6 decimal digits. In Tables I and II the elements of Romberg's table relative, respectively, to the coefficients C_{74}, C_{75} are listed.

The exact values are: $C_{74} = 0$, $C_{75} = -0.3637978... \times 10^{-11}$.

In order to show the power of our method we performed the evaluation of (13) with two standard methods. Namely, we first evaluate the integral in the finite interval $0 \div 15$ by the repeated Simpson rule (a larger interval was not considered to avoid exponential underflow). Second, we use again the repeated Simpson rule after the subdivision of the interval $0 \div 15$ into subintervals where ends are zeros of $J_0(\omega x)$. The relative accuracies of the numerical results for increasing values of ω are listed in Table III. From the second column it appears that for a given $\omega \leqslant 12$ our

TABLE I

Romberg's Table for the 74th Laguerre's Coefficient.[a]

M	h					
340	0.50	0.3373×10^{-11}				
680	0.25	0.2261×10^{-11}	0.1890×10^{-11}			
1020	0.167	0.1140×10^{-11}	0.2428×10^{-12}	0.3696×10^{-13}		
1360	0.125	0.6675×10^{-12}	0.6036×10^{-13}	-0.4665×10^{-15}	-0.2961×10^{-14}	
2040	0.083	0.3050×10^{-12}	0.1499×10^{-13}	-0.1371×10^{-15}	-0.9595×10^{-16}	-0.1408×10^{-16}

Note. M = total number of integrand evaluation; h = stepsize of integration.
[a] The exact value is $C_{74} = 0$.

TABLE II

$C_{75} \times 10^{11}$; Romberg's Table for the 75th Laguerre's Coefficient.[a]

M	h						
340	0.500	−0.165542					
680	0.250	−0.163107	−0.272657				
1020	0.167	−0.271204	−0.357682	−0.368311			
1360	0.125	−0.311223	−0.362675	−0.364340	−0.364075		
2040	0.083	−0.340303	−0.363567	−0.363864	−0.363805	−0.363796	
2720	0.0625	−0.350560	−0.363747	−0.363807	−0.363797	−0.363797	−0.363797

Note. M = total number of integrand evaluation; h = stepsize of integration.
[a] The exact value is $C_{75} = -0.3637978... \times 10^{-11}$.

method can be used to compute $I(\omega)$ in (12). Indeed for $\omega > 12$ we notice a loss of accuracy in the computation of the coefficients (14) by means of the discrete polynomial method. The use of higher precision arithmetic could delay this stumbling block (but not remove it), and convergence of series (8) could be improved by applying linear or non-linear transformations. However, in this paper we do not consider these devices.

Finally we focus our attention on the efficiency of the discrete Laguerre polynomials method and we compare the numerical evaluation of the coefficients (14) obtained by means of (10) with the corresponding results given by compound

TABLE III

Relative Accuracies in the Evaluation of
$\int_0^\infty e^{-x^2} J_0(\omega x) \sin x^2 \cdot x\, dx$ Obtained via Different Numerical Methods

ω	Relative accuracy of formula (8)	Relative accuracy of repeated Simpson rule in subintervals	Relative accuracy in repeated Simpson rule
6	1.4×10^{-9}	2.9×10^{-7}	$1.6 = 10^{-7}$
7	6.0×10^{-9}	5.0×10^{-7}	5.3×10^{-7}
8	3.9×10^{-9}	3.9×10^{-6}	3.5×10^{-6}
9	2.1×10^{-8}	2.8×10^{-4}	2.8×10^{-4}
10	1.6×10^{-8}	2.7×10^{-4}	3.4×10^{-4}
11	1.5×10^{-7}	2.7×10^{-4}	3.6×10^{-3}
12	1.6×10^{-6}	5.7×10^{-3}	6.3×10^{-2}
13	2.2×10^{-3}	2.0×10^{-1}	1.4×10^{0}
14	7.1×10^{-5}	5.1×10^{0}	4.2×10^{1}
15	2.8×10^{-3}	6.2×10^{1}	1.9×10^{3}
16	5.8×10^{-1}	1.5×10^{3}	3.8×10^{5}
17	6.2×10^{1}	6.1×10^{5}	6.6×10^{6}
18	7.7×10^{3}	6.6×10^{7}	4.1×10^{8}

Gaussian quadrature formulas. To approximlate C_k by Gaussian quadrature we split the integral in the following way:

$$C_k = \int_0^a e^{-y} L_k(y) \sin y \, dy + \int_a^\infty e^{-y} L_k(y) \sin y \, dy = d_k + e_k.$$

If a is sufficiently large (in practice we found a ≈ 60 to be adequate) then e_k is negligible with respect to d_k. To evaluate the d_k's we utilize a compound 24th node Legendre quadrature formula. The computation of several coefficients C_k with eight significant exact decimal digits has been performed on an IBM 370/158 computer (system IAT) and the corresponding results are plotted in Fig. 1, where the CPU time (in seconds) is given for the first k coefficients C_k. We observe that the Gaussian quadrature is remarkably more efficient than the discrete polynomials method when k is small, however, our method becomes competitive when $k > 60$.

Another example is supplied with the numerical evaluation of the coefficients:

$$C_k = \int_0^\infty e^{-y} L_k(y) \, |y(y-20)| \, dy, \qquad k = 0, 1, \ldots.$$

Here the integrand function has a discontinuity in the first derivative.

Results analogous to those plotted in Fig. 1 are shown in Fig. 2. (In this case lowest degree formulas are usually preferred to higher degree ones, however, the use of repeated trapezoidal rule has led to poor results; indeed we are not able to evaluate more than about 25 coefficients C_k with the requested accuracy.)

From the above examples it would appear that the CPU time consumed by Gauss formulas increases (at a rough guess) exponentially, whereas the time consumed by

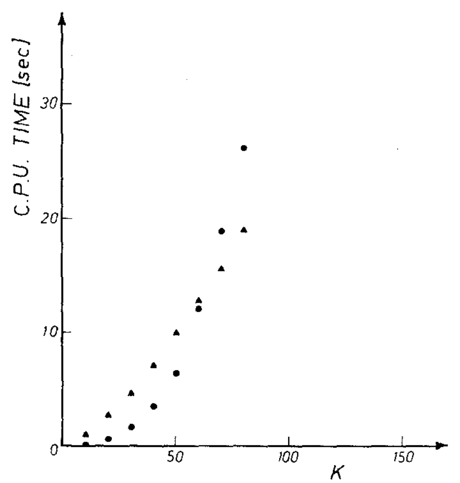

FIG. 1. CPU time (in seconds) needed to evaluate the first k Laguerre's coefficients of the function $f(y) = \sin y$: ●, with Gaussian quadrature method: ▲, with discrete Laguerre polynomial method.

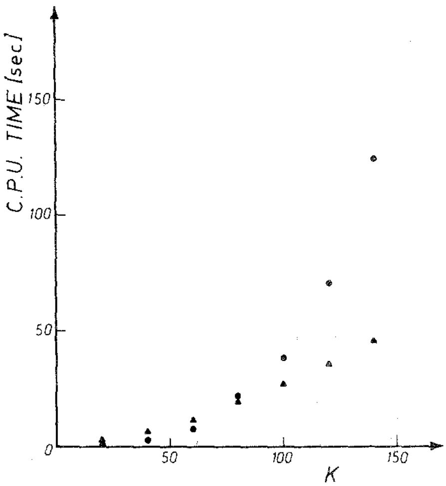

FIG. 2. The same as for Fig. 1 but for the function $|y \cdot (y-20)|$.

the discrete polynomial method grows approximately linearly when the number of coefficients becomes large. (This is not surprising: for the classical Laguerre polynomials we do not have a recurrence relation of type (11).) Thus our method is particularly recommended when a large number of Laguerre coefficients is required; in this sense it appears useful for the evaluation of the integral (1).

CONCLUSIONS

The reliability of the numerical evaluation of integral (1) using series (4) is considered. It appears that most of the computational effort will be expended in computing the coefficients (3). To solve this quadrature problem we suggest a method involving the Laguerre discrete polynomials which, taking into account the special features of the problem, shows some advantages with respect to other standard quadrature methods. An improvement could be attempted by using acceleration methods of series. These include: Euler's transformation, ε-Algorithm, Levin's transformation. Although here we do not consider these possibilities, we notice that in [3] an empirical acceleration method of the whole problem is suggested. The practical utilization of this will be considered in a future paper.

APPENDIX A

In [5] Gottlieb considers the discrete Laguerre polynomials $l_n^{(h)}(k)$ defined in the points $k = 0, 1, 2,...$ which are connected with the Laguerre polynomials $L_n(x)$ by the limit relation: $l_n^{(h)}(x/h) = L_n(x) + O(h)$, $h \to 0$. Here we modify the definition of $l_n^{(h)}$ given in [5] in order to get

$$l_n^{(h)}(x/h) = L_n(x) + O(h^2).$$

Let

$$l_n^{(h)}\left(m+\frac{1}{2}\right) = e^{mh}\delta^n\left\{e^{-mh}\binom{m+n/2}{n}\right\}, \tag{A.1}$$

where n, $m = 0, 1, 2, \ldots$, and δ denotes the standard central difference operator.

It is easy to prove, by Abel's transform, that $l_n^{(h)}$ satisfy the orthogonality relations

$$e^{-h/2}\sum_{m=0}^{\infty} e^{-mh} l_k^{(h)}\left(m+\frac{1}{2}\right)\cdot l_n^{(h)}\left(m+\frac{1}{2}\right) = \begin{cases} 0 & \text{if } k \neq n \\ \dfrac{1}{2\,\mathrm{sh}(h/2)} & \text{if } k = n. \end{cases} \tag{A.2}$$

Using a well known formula for δ^n, we obtain for $l_n^{(h)}$ the explicit expression

$$l_n^{(h)}\left(m+\frac{1}{2}\right) = e^{-nh/2}\cdot\sum_{j=0}^{n}(1-e^h)^j\binom{n}{j}\binom{m}{j}, \qquad m, n = 0, 1, 2, \ldots. \tag{A.3}$$

The symmetry property

$$e^{nh/2} l_n^{(h)}(m+\tfrac{1}{2}) = e^{mh/2} l_m^{(h)}(n+\tfrac{1}{2}), \qquad m, n = 0, 1, 2, \ldots, \tag{A.4}$$

immediately follows.

In the usual way, the three term recurrence relation

$$(n+1)\, l_n^{(h)}\left(m+\frac{1}{2}\right) = 2\left[\mathrm{sh}\left(\frac{h}{2}\right)\left(m+\frac{1}{2}\right) + \mathrm{ch}\left(\frac{h}{2}\right)\left(n+\frac{1}{2}\right)\right] \cdot l_n^{(h)}\left(m+\frac{1}{2}\right) - n l_{n-1}^{(h)}\left(m+\frac{1}{2}\right), \qquad m, n = 0, 1, 2, \ldots, \tag{A.5}$$

$$l_0^{(h)} = 1, \qquad l_{-1}^{(h)} = 0$$

may be proved.

The discrete polynomials defined by (A.1) are connected to the Laguerre polynomials by the relation

$$l_n^{(h)}\left(\frac{x}{h}\right) - L_n(x) = \sum_{k=1}^{\infty}\beta_k h^{2k} \qquad \text{as} \qquad h \to 0, \tag{A.6}$$

where $x = (m + \frac{1}{2})\,h$, $m = 0, 1, 2, \ldots$ and β_k are constants independent of h.

In order to prove (A.6) we write (A.1) in the form

$$l_n^{(h)}\left(\frac{x}{h}\right)=e^x\delta^n\left\{e^{-x}\frac{\Gamma(x/h+(n+1)/2)}{n!\,\Gamma(x/h-(n-1)/2)}\right\}. \tag{A.7}$$

Expanding the ratio of gamma functions through the Tricomi–Erdeli formula, (see [12])

$$\frac{\Gamma(x/h+(n+1)/2)}{\Gamma(x/h-(n-1)/2)}\sim\left(\frac{x}{h}\right)^n+\sum_{k=1}^{n/2}B_{2k}^{(n+1)}\left(\frac{n+1}{2}\right)\binom{n}{2k}\left(\frac{x}{2h}\right)^{-2k}$$

$$\text{as}\qquad \frac{x}{h}\to\infty, \tag{A.8}$$

where $B_{2k}^{(n+1)}((n+1)/2)$ denote the Bernoulli polynomials, and using the formula giving the central differences in terms of the derivatives, we obtain (A.6).

Finally, we notice the following generating function:

$$G(x,w)=\sum_{n=0}^{\infty}l_n^{(h)}(x)\,w^n=e^{hx}\frac{(w-e^{-h/2})^{x-1/2}}{(w-e^{h/2})^{x+1/2}},\qquad (|w|<1). \tag{A.9}$$

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