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Quadratic Spherical Bessel Functions and the Inverse Scattering Problem

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In the course of inverting the partial-wave Born approximation, a new expression for the inverse function of $j_l^2(\rho)$ was obtained. Using this result, one can also derive two expressions involving the binomial coefficients. Finally, a particular differential operator whose effect on $j_l^2(\rho)$ was previously investigated by Mavromatis and Jalal is shown to have similar effects on $n_l^2(\rho)$ and $n_l(\rho)j_l(\rho)$.

1. INTRODUCTION

In order to obtain approximate solutions for the inverse problem in quantum mechanical scattering theory, we recently used the partial wave Born approximation (Merzbacher, 1970)

$$-\frac{\hbar^2}{2mk}\tan[\delta_l(k)] \simeq \int_0^\infty j_l^2(kr)V_l(r)r^2\,dr \tag{1}$$

Our aim was to obtain the scattering potential $V_l(r)$ as a function of the phase shifts $\delta_l(k)$ it produces. Two inversion techniques were used in this context (Mavromatis and Jalal, 1991). The first involved the following useful differential operator:

$$\hat{\theta}_l(\rho) \equiv \left(\frac{d}{d\rho^2}\right)^l \frac{d}{d\rho}\left(\frac{d}{d\rho^2}\right)^l \tag{2}$$

which has the property

$$\hat{\theta}_l(\rho)[\rho^{2l+2}j_l^2(\rho)] = \sin(2\rho) \tag{3}$$

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where

$$\frac{d}{d\rho^2} \equiv \frac{1}{2\rho}\frac{d}{d\rho}$$

and $j_l(\rho)$ is the spherical Bessel function (Schiff, 1968).

The second involved using the inverse function of $j_l^2(\rho)$, namely $g_l(\rho')$, which for $r, r' > 0$ satisfies the relation (Mavromatis and Jalal, 1991; Mavromatis and Schilcher, 1968)

$$\int_0^\infty \frac{g_l(kr')}{k^2 r'^2}\left(k^2 r^2 j_l^2(kr) - \frac{1}{2}\right) dk = \delta(r - r') \tag{4}$$

Using either expression (2) or the inverse function $g_l(\rho)$ enables one to invert equation (1). The former operator reduces equation (1) to a Fourier sine transform of $r^{2l+1}V_l(r)$, while operating on equation (1) minus its limit for large k with $g_l(kr')/(kr')^2$ and integrating over $k^2\,dk$ reduces the RHS of equation (1) to $r'^2 V_l(r')$.

2. INVERSE FUNCTIONS OF $j_l^2(\rho)$

In Mavromatis and Schilcher (1968) two expressions were given for the $g_l(\rho)$, namely

$$g_l(\rho) = -\frac{8\rho^2}{\pi(2l + 1)}\,{}_1F_2\left(\frac{3}{2}; \frac{1}{2} - l, l + \frac{3}{2}; -\rho^2\right) \tag{5}$$

and

$$g_l(\rho) = \frac{(-1)^l 16\rho^{3+l}\Gamma(\frac{1}{2} - l)}{\pi^{3/2}(l + \frac{1}{2})\, B(\frac{3}{2}, l)} \int_0^1 y^{l+3}(1 - y^2)^{l-1} n_l(2\rho y)\, dy, \qquad l > 0 \tag{6}$$

where ${}_1F_2$ is a particular generalized hypergeometric series and $n_l(\xi)$ is the spherical Neumann function (Schiff, 1968). Moreover, recently (Mavromatis and Jalal, 1991) another general expression was obtained for $g_l(\rho)$, namely

$$g_l(\rho) = -\frac{4}{\pi}\rho^{2l+2}\left(\frac{d}{d\rho}\frac{1}{2\rho}\right)^l \frac{d}{d\rho}\left(\frac{d}{d\rho}\frac{1}{2\rho}\right)^l \sin(2\rho)$$

$$= -\frac{4}{\pi}\rho^{2l+2}\hat{\theta}_l^\dagger(\rho)\sin(2\rho) \tag{7}$$

and the following property of the $g_l(\rho)$ was pointed out:

$$\int_0^\infty \left[\frac{g_l(\rho)}{\rho^2} - \frac{8(-1)^{l+1}}{\pi}\cos(2\rho)\right] d\rho = 0 \tag{8}$$

A fourth expression can also be obtained for these inverse functions, namely

$$g_l(\rho) = -(-1)^l \frac{8}{\pi} \rho^2 \cos(2\rho) + \frac{(-1)^l 16 l(l+1)}{\pi} \rho^2 \sum_{k=0}^{l} \frac{(-1)^k 2^k (l+k)!}{(k+1)!(l-k)!} \frac{j_k(2\rho)}{(2\rho)^k} \qquad (9)$$

i.e., the inverse function can also be expressed as a finite sum over Bessel functions. The new result, expression (9), is the most convenient of these expressions for programming-oriented applications since the j_k are standard functions.

Thus, for instance, for $l = 3$, from equation (9) one immediately obtains

$$g_3(\rho) = \frac{8}{\pi} \rho^2 \cos 2\rho - \frac{192}{\pi} \rho^2 \left\{ j_0(2\rho) - \frac{6 j_1(2\rho)}{\rho} + \frac{20 j_2(2\rho)}{\rho^2} - \frac{30 j_3(2\rho)}{\rho^3} \right\}$$

Expression (9) can be obtained by making a careful comparison between the $g_l(\rho)$ and the $j_l(\rho)$ functions. The values of these functions for $l = 0, 1, 2$ are listed in Table I. One notes that for large ρ, the leading term in the $g_l(\rho)$ is always $[(-1)^{l+1}(8/\pi)\rho^2 \cos(2\rho)]$. The remaining terms in $g_l(\rho)$ are polynomials times $\cos(2\rho)$ and $\sin(2\rho)$ and can be related to the $j_l(2\rho)$. For instance, $g_0(\rho)$ involves only the leading term $[-(8/\pi)\rho^2 \cos(2\rho)]$, while $g_1(\rho)$ additionally has polynomials involving $\sin(2\rho)$ and $\cos(2\rho)$. By comparing these expressions and the Bessel functions, one notes that the simplest two $g_l(\rho)$ can also be written as

$$g_0(\rho) = -\frac{8}{\pi} \rho^2 \cos(2\rho) + \underbrace{l(l+1)}_{l=0} \frac{16}{\pi} \{\rho^2 j_0(2\rho)\}$$

$$g_1(\rho) = \frac{8}{\pi} \rho^2 \cos(2\rho) + \underbrace{l(l+1)}_{l=1} \frac{16}{\pi} \left\{ -\rho^2 j_0(2\rho) + 2\rho^2 \frac{j_1(2\rho)}{(2\rho)} \right\}$$

Table I. Spherical Bessel Functions $j_l(\rho)$ and $g_l(\rho)$ for $l = 0, 1$, and 2

	$l = 0$	$l = 1$	$l = 2$
$j_l(\rho)$	$\frac{\sin(\rho)}{\rho}$	$\frac{\sin(\rho)}{\rho^2} - \frac{\cos(\rho)}{\rho}$	$\left(\frac{3}{\rho^3} - \frac{1}{\rho}\right)\sin(\rho) - \frac{3}{\rho^2}\cos(\rho)$
$g_l(\rho)$	$-\frac{8\rho^2}{\pi}\cos(2\rho)$	$\frac{8}{\pi}\left\{(\rho^2 - 2)\cos(2\rho) + \left(\frac{1}{\rho} - 2\rho\right)\sin(2\rho)\right\}$	$-\frac{8}{\pi}\left\{\left(\rho^2 - 18 + \frac{36}{\rho^2}\right)\cos(2\rho) + \left(-6\rho + \frac{33}{\rho} - \frac{18}{\rho^3}\right)\sin(2\rho)\right\}$

Similarly, for larger l, the terms in $g_l(\rho)$ other than the leading term can be related to a summation over $j_k(2\rho)$ where k ranges from 0 to l. The exact factors can be deduced by writing the first few l cases ($l = 0, 1, 2, 3, 4$) in a form similar to the example above ($l = 0, 1$) and then surmizing the behavior for general l. This leads to equation (9).

If equation (9) is used in conjunction with some of the other expressions mentioned above involving the $g_l(\rho)$, this leads to some interesting mathematical relations involving binomial coefficients. Thus, if one inserts equation (9) into equation (8), one has

$$\frac{(-1)^l 16l(l+1)}{\pi} \sum_{k=0}^{l} \frac{(-1)^k 2^k (l+k)!}{(k+1)!(l-k)!} \int_0^\infty \frac{j_k(2\rho)}{(2\rho)^k}\, d\rho = 0$$

But (Gradshteyn and Ryzhik, 1980, p. 672)

$$\int_0^\infty \frac{j_k(2\rho)}{(2\rho)^k}\, d\rho = \frac{\pi}{k!\,(2)^{k+2}}$$

Hence

$$\sum_{k=0}^{l} (-1)^k \binom{l}{k} \binom{l+k}{k+1} = 0 \tag{10}$$

where $\binom{0}{1} \equiv 0$ and $l = 0, 1, 2, 3, \ldots$.

To the authors' knowledge, equation (10) is not listed among the standard expressions involving binomial coefficients; see, for instance, Gradshteyn and Ryzhik (1980, p. 3).

Further, examining equation (9) for small ρ gives

$$\lim_{\rho \to 0} g_l(\rho) = \frac{(-1)^{l+1} 8\rho^2}{\pi} + \frac{(-1)^l 16l(l+1)}{\pi} \times \rho^2 \sum_{k=0}^{l} \frac{(-1)^k 2^k (l+k)!}{(k+1)!\,(l-k)!\,(2k+1)!!} \tag{11}$$

On the other hand for small ρ, equation (6) reduces to

$$\lim_{\rho \to 0} g_l(\rho) = \frac{(-1)^l 16 \rho^{3+l} \Gamma(\frac{1}{2} - l)}{\pi^{3/2} (l + \frac{1}{2}) B(\frac{3}{2}, l)} \times \int_0^1 y^{l+3} (1 - y^2)^{l-1} \left\{ \frac{-2(2l-1)!!}{(2\rho y)^{l+1}} \right\} dy$$

$$= -\frac{8\rho^2}{\pi(2l+1)} \tag{12}$$

Since equations (11) and (12) are equal, we have

$$\sum_{k=0}^{l} \frac{(-1)^k 2^{2k}}{(2k+1)(k+1)} \binom{l+k}{l-k} = \frac{2l+1-(-1)^l}{2l(l+1)(2l+1)}$$

$$= \begin{cases} \dfrac{1}{(l+1)(2l+1)}, & l = \text{even} \\ \dfrac{1}{l(2l+1)}, & l = \text{odd} \end{cases} \tag{13}$$

where $l = 0, 1, 2, 3, \ldots$.

To the authors' knowledge, equation (13) is also not given among the standard expressions for the binomial coefficients.

If one inserts equation (3) into equation (7), then one obtains

$$g_l(\rho) = -\frac{4}{\pi}\, \rho^{2l+2} \hat{\theta}_l^{\dagger}(\rho) \hat{\theta}_l(\rho) \rho^{2l+2} j_l^2(\rho) \tag{14}$$

Equation (14) relates $g_l(\rho)$ directly to $j_l^2(\rho)$ through a set of differential operations.

3. OPERATOR EXPRESSIONS INVOLVING $n_l(\rho) j_l(\rho)$ AND $n_l^2(\rho)$

When the differential operator $\hat{\theta}_l(\rho)$ given by equation (2) operates on $\rho^{2l+2} n_l^2(\rho)$ or $\rho^{2l+2} n_l(\rho) j_l(\rho)$, which also arise in mathematical physics, one obtains results similar to equation (3), namely

$$\hat{\theta}_l(\rho)[\rho^{2l+2} n_l^2(\rho)] = -\sin(2\rho) \tag{15}$$

and

$$\hat{\theta}_l(\rho)[\rho^{2l+2} n_l(\rho) j_l(\rho)] = -\cos(2\rho) \tag{16}$$

These simple results can easily be verified for $l = 0, 1, 2$. These new relations are not surprising, since the Neumann and Bessel functions are related. An interesting aspect of these expressions is that the RHS is simple and independent of l, though $n_l(\rho)$, $j_l(\rho)$, and $\hat{\theta}_l(\rho)$ are l-dependent. From equations (3), (15), and (16), it can easily be seen that

$$\hat{\theta}_l(\rho)[\rho^{l+1} h_l^{(1)}(\rho)]^2 = -2ie^{+2i\rho} \tag{17}$$

$$\hat{\theta}_l(\rho)[\rho^{l+1} h_l^{(2)}(\rho)]^2 = 2ie^{-2i\rho} \tag{18}$$

and

$$\hat{\theta}_l(\rho)[\rho^{2l+2} h_l^{(1)}(\rho) h_l^{(2)}(\rho)] = 0 \tag{19}$$

where $h_l^{(1)}(\rho)$ and $h_l^{(2)}(\rho)$ are the spherical Hankel functions of the first and second kind, respectively (Schiff, 1968).

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