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# A New Spherical Bessel Function Result Related to Quantum Mechanical Scattering Theory

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The authors present a derivative formula for the square of a spherical Bessel function in terms of the spherical Bessel function of twice the argument. This derivative formula is then applied in an inversion problem for the partial-wave Born approximation in quantum mechanical scattering theory. Several other closely related results and derivative formulas are also considered.

**KEY WORDS:** Bessel and spherical Bessel functions; derivative formulas; inverse scattering problem; partial-wave Born approximation; generalized hypergeometric functions; Hankel transforms.

For the Bessel function $J_\nu(z)$ of the first kind of order $\nu$, defined by

$$J_\nu(z) := \sum_{k=0}^{\infty} \frac{(-1)^k \left(\frac{1}{2}z\right)^{\nu+2k}}{k!\,\Gamma(\nu+k+1)} \tag{1}$$

$$(|\arg(z)| \leqq \pi - \varepsilon \ (0 < \varepsilon < \pi);\ \nu \in \mathbb{C})$$

or, equivalently, by

$$J_\nu(z) := \frac{\left(\frac{1}{2}z\right)^{\nu}}{\Gamma(\nu+1)}\, {}_0F_1\left(-;\nu+1;-\frac{1}{4}z^2\right) \tag{2}$$

$$(|\arg(z)| \leqq \pi - \varepsilon \ (0 < \varepsilon < \pi);\ \nu \in \mathbb{C}),$$

where ${}_pF_q$ denotes a generalized hypergeometric function with $p$ numerator and $q$ denominator parameters, each of the following derivative formulas is well-known

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(rather classical) (Watson, 1994, p. 46, Equations 3.2 (5) and 3.2 (6)):

$$\left(\frac{1}{z}\frac{d}{dz}\right)^m \{z^\nu J_\nu(z)\} = z^{\nu-m} J_{\nu-m}(z) \tag{3}$$

and

$$\left(\frac{1}{z}\ \frac{d}{dz}\right)^m \{z^{-\nu} J_\nu(z)\} = (-1)^m z^{-\nu-m} J_{\nu+m}(z), \tag{4}$$

where

$$m \in \mathbb{N}_0 := \mathbb{N} \cup \{0\} \qquad \mathbb{N} := \{1, 2, 3, \ldots\}.$$

Motivated essentially by its application in an inversion problem for the partial-wave Born approximation in quantum mechanical scattering theory, we aim here at presenting a (presumably new) derivative formula involving the *spherical* Bessel function $j_n(z)$ of the first kind, defined by Abramowitz and Stegun (p. 437)

$$j_n(z) := \sqrt{\frac{\pi}{2z}} J_{n+\frac{1}{2}}(z) \qquad n \in \mathbb{Z} := \{0, \pm 1, \pm 2, \ldots\} \tag{5}$$

with the following derivative representation (Abramowitz and Stegun, p. 439, Entry 10.1.25):

$$j_l(z) = z^l \left(-\frac{1}{z}\ \frac{d}{dz}\right)^l \left\{\frac{\sin z}{z}\right\} \qquad l \in \mathbb{N}_0. \tag{6}$$

We begin by recalling the familiar expansion formula (Watson, p. 147, Equation 5.4 (5)) (see also Gradshteyn and Ryzhik, p. 960, Entry 8.442.1):

$$J_\mu(z) J_\nu(z) = \sum_{k=0}^{\infty} \frac{(-1)^k \left(\frac{1}{2}z\right)^{\mu+\nu+2k} \Gamma(\mu+\nu+2k+1)}{k!\, \Gamma(\mu+k+1)\, \Gamma(\nu+k+1)\, \Gamma(\mu+\nu+k+1)}. \tag{7}$$

Upon multiplying each member of (7) by $z^\lambda$, if we differentiate both sides of the resulting equation, first $l$ times with respect to $z^2$ and then once with respect to $z$, we find from (7) that

$$\begin{aligned} &\frac{d}{dz}\left(\frac{d}{dz^2}\right)^l \{z^\lambda J_\mu(z) J_\nu(z)\} \\ &= \frac{z^{\lambda+\mu+\nu-2l-1}\Gamma\left[\frac{1}{2}(\lambda+\mu+\nu)+1\right]}{2^{\mu+\nu-1}\Gamma(\mu+1)\,\Gamma(\nu+1)\,\Gamma\left[\frac{1}{2}(\lambda+\mu+\nu)-l\right]} \\ &\quad \cdot {}_3F_4\left[\begin{matrix} \frac{1}{2}(\mu+\nu+1),\ \frac{1}{2}(\mu+\nu)+1,\ \frac{1}{2}(\lambda+\mu+\nu)+1; \\ \mu+1,\ \nu+1,\ \mu+\nu+1,\ \frac{1}{2}(\lambda+\mu+\nu)-l; \end{matrix} \ -z^2\right], \end{aligned} \tag{8}$$

which, for $\lambda = \mu + \nu$, immediately yields

$$\frac{d}{dz}\left(\frac{d}{dz^2}\right)^l \{z^{\mu+\nu} J_\mu(z) J_\nu(z)\}$$

$$= \frac{z^{2(\mu+\nu-l)}}{2^{\mu+\nu-1}\Gamma(\mu+1)\,\Gamma(\nu+1)\,\Gamma(\mu+\nu-l)}$$

$$\cdot\, {}_2F_3 \left[\begin{matrix} \frac{1}{2}(\mu+\nu+1),\, \frac{1}{2}(\mu+\nu)+1; & \\ & -z^2 \\ \mu+1,\, \nu+1,\, \mu+\nu-l; & \end{matrix}\right], \tag{9}$$

it being understood *throughout the present investigation* that

$$\frac{d}{dz^2} = \frac{1}{2z}\,\frac{d}{dz}.$$

In its *further* special case when $\mu = \nu$, the derivative formula (9) would reduce to the form:

$$\frac{d}{dz}\left(\frac{d}{dz^2}\right)^l \{z^{2\nu}[J_\nu(z)]^2\}$$

$$= \frac{2z^{2(2\nu-l)-1}\Gamma\left(\nu+\frac{1}{2}\right)}{\sqrt{\pi}\,\Gamma(\nu+1)\Gamma(2\nu-l)}\, {}_1F_2\left(\nu+\frac{1}{2};\nu+1,\, 2\nu-l; -z^2\right). \tag{10}$$

Finally, in terms of the spherical Bessel function defined by (5), we find from (10) *with* $\nu = l + \frac{1}{2} (l \in \mathbb{N}_0)$ that

$$\frac{d}{dz}\left(\frac{d}{dz^2}\right)^l \left\{z^{2l+1}\left[J_{l+\frac{1}{2}}(z)\right]^2\right\} = \frac{2z^{l+\frac{1}{2}}}{\sqrt{\pi}}\, J_{l+\frac{1}{2}}(2z), \tag{11}$$

that is, that

$$\frac{d}{dz}\left(\frac{d}{dz^2}\right)^l \{[z^{l+1} j_l(z)]^2\} = 2z^{l+1} j_l(2z). \tag{12}$$

By appealing to the classical results (3) and (4) in their *equivalent* forms:

$$\left(\frac{1}{z}\,\frac{d}{dz}\right)^m \{z^{n+1} j_n(z)\} = z^{n-m+1} j_{n-m}(z) \tag{13}$$

and

$$(-1)^m \left(\frac{1}{z}\,\frac{d}{dz}\right)^m \{z^{-n} j_n(z)\} = z^{-n-m} j_{n+m}(z), \tag{14}$$

respectively, (12) would yield the following additional derivative formulas:

$$j_{l-m}(2z) = \frac{1}{2z^{l-m+1}} \left(\frac{d}{dz^2}\right)^m \frac{d}{dz} \left(\frac{d}{dz^2}\right)^l \{[z^{l+1} j_l(z)]^2\} \tag{15}$$

and

$$j_{l+m}(2z) = (-1)^m \frac{z^{l+m}}{2} \left(\frac{d}{dz^2}\right)^m \frac{1}{z^{2l+1}} \frac{d}{dz} \left(\frac{d}{dz^2}\right)^l \{[z^{l+1} j_l(z)]^2\}. \tag{16}$$

In their special case when $m = l$, these last results (14) and (15) reduce to the forms:

$$j_0(2z) = \frac{1}{2z} \left(\frac{d}{dz^2}\right)^l \frac{d}{dz^2} \left(\frac{d}{dz^2}\right)^l \{[z^{l+1} j_l(z)]^2\} \tag{17}$$

and

$$j_{2l}(2z) = (-1)^l \frac{z^{2l}}{2} \left(\frac{d}{dz^2}\right)^l \frac{1}{z^{2l+1}} \frac{d}{dz} \left(\frac{d}{dz^2}\right) \{[z^{l+1} j_l(z)]^2\}, \tag{18}$$

respectively.

In view of the case $l = 0$ of the derivative representation in (6), (17) is the same as the known result (cf. Mavromatis and Al-Jalal, 1990, p. 1182, Equation (5); see also Al-Ruwaili and Mavromatis, 1996, p. 2207, Equation (3)):

$$\sin 2z = \left(\frac{d}{dz^2}\right)^l \frac{d}{dz} \left(\frac{d}{dz^2}\right)^l \{[z^{l+1} j_l(z)]^2\}. \tag{19}$$

Next, for the *spherical* Bessel function $y_n(z)$ of the *second* kind, defined by (Abramowitz and Stegun (1968, p. 437)

$$y_n(z) := \sqrt{\frac{\pi}{2z}} Y_{n+\frac{1}{2}}(z) \qquad n \in \mathbb{Z} \tag{20}$$

in terms of the Bessel function $Y_\nu(z)$ of the second kind:

$$Y_\nu(z) := \frac{J_\nu(z) \cos(\nu\pi) - J_{-\nu}(z)}{\sin(\pi\nu)}, \tag{21}$$

it is not difficult to observe that (Abramowitz and Stegun, 1968, p. 439, Entry 10.1.39)

$$y_n(z) = (-1)^{n+1} \sqrt{\frac{\pi}{2z}} J_{-n-\frac{1}{2}}(z) = (-1)^{n+1}\, j_{-n-1}(z) \qquad n \in \mathbb{Z} \tag{22}$$

and that (Abramowitz and Stegun, 1968, p. 439, Entry 10.1.26)

$$y_l(z) = -z^l \left(-\frac{1}{z} \frac{d}{dz}\right)^l \left\{\frac{\cos z}{z}\right\} \qquad l \in \mathbb{N}_0. \tag{23}$$

Thus, by making use of the limit formula (Srivastava and Manocha, 1984, p. 326, Equation 6.5 (13)):

$$\lim_{r\to -1}\left\{\frac{1}{\Gamma(\gamma)}\,{}_pF_{q+1}\left[\begin{matrix}\alpha_1,\ldots,\alpha_p;\\ \gamma,\beta_1,\ldots,\beta_q;\end{matrix}\; z\right]\right\}$$

$$=\frac{\prod_{j=1}^{p}(\alpha_j)_{l+1}}{\prod_{j=1}^{q}(\beta_j)_{l+1}}\frac{z^{l+1}}{(l+1)!}$$

$$\cdot\,{}_pF_{q+1}\left[\begin{matrix}\alpha_1+l+1,\ldots,\alpha_q+l+1;\\ l+2,\beta_1+l+1,\ldots,\beta_q+l+1;\end{matrix}\; z\right]\qquad l\in\mathbb{N}_0, \tag{24}$$

we can first deduce the following special case of the derivative formula (8) when $\lambda=-\mu-\nu$:

$$\frac{d}{dz}\left(\frac{d}{dz^2}\right)^l\{z^{-\mu-\nu}J_\mu(z)J_\nu(z)\}$$

$$=\frac{2(-1)^{l+1}z\Gamma\left[\frac{1}{2}(\mu+\nu+1)+l+1\right]\Gamma\left[\frac{1}{2}(\mu+\nu)+l+2\right]}{\sqrt{\pi}\Gamma(\mu+l+2)\Gamma(\nu+l+2)\Gamma(\mu+\nu+l+2)}$$

$$\cdot\,{}_2F_3\left[\begin{matrix}\frac{1}{2}(\mu+\nu+1)+l+1,\ \frac{1}{2}(\mu+\nu)+l+2;\\ \mu+l+2,\ \nu+l+2,\ \mu+\nu+l+2;\end{matrix}\; -z^2\right], \tag{25}$$

which, for $\mu=\nu$, yields

$$\frac{d}{dz}\left(\frac{d}{dz^2}\right)^l\{z^{-2\nu}[J_\nu(z)]^2\}$$

$$=\frac{2(-1)^{l+1}z\Gamma\left(\nu+l+\frac{3}{2}\right)}{\sqrt{\pi}\Gamma(\nu+l+2)\Gamma(2\nu+l+2)}$$

$$\cdot\,{}_1F_2\left(\nu+l+\frac{3}{2};\nu+l+2,2\nu+l+2;-z^2\right). \tag{26}$$

In light of the limit formula (24) once again, we find from (26) with $\nu=-l-\frac{1}{2}(l\in\mathbb{N}_0)$ that

$$\frac{d}{dz}\left(\frac{d}{dz^2}\right)^l\left\{z^{2l+1}\left[J_{-l-\frac{1}{2}}(z)\right]^2\right\}=-\frac{2z^{l+\frac{1}{2}}}{\sqrt{\pi}}J_{l+\frac{1}{2}}(2z), \tag{27}$$

which leads us at once to the following counterpart of the derivative formula (12) for the spherical Bessel function $y_n(z)$ of the second kind:

$$\frac{d}{dz}\left(\frac{d}{dz^2}\right)^l \{[z^{l+1}y_l(z)]^2\} = -2z^{l+1}j_l(2z). \tag{28}$$

By combining the derivative formulas (12) and (28), we have the fascinating differential equation:

$$\frac{d}{dz}\left(\frac{d}{dz^2}\right)^l \{[z^{l+1}j_l(z)]^2 + [z^{l+1}y_l(z)]^2\} = 0, \tag{29}$$

that is,

$$\left(\frac{d}{dz^2}\right)^l \{[z^{l+1}j_l(z)]^2 + [z^{l+1}y_l(z)]^2\} = C, \tag{30}$$

where $C$ is a constant of integration.

Yet another remarkable derivative formula involving the spherical Bessel function of the first as well as the second kind would follow readily from (8) when we set

$$\lambda = 2l+1 \quad \text{and} \quad \mu = -\nu = l + \frac{1}{2} \qquad l \in \mathbb{N}_0.$$

We thus obtain

$$\frac{d}{dz}\left(\frac{d}{dz^2}\right)^l \left\{z^{2l+1}J_{l+\frac{1}{2}}(z)J_{-l-\frac{1}{2}}(z)\right\} = \frac{2z^{l+\frac{1}{2}}}{\sqrt{\pi}}J_{-l-\frac{1}{2}}(z) \tag{31}$$

or, equivalently,

$$\frac{d}{dz}\left(\frac{d}{dz^2}\right)^l \{z^{2l+2}j_l(z)y_l(z)\} = 2z^{l+1}y_l(2z). \tag{32}$$

We now show that our derivative formula (12) has an interesting application in an inversion problem occurring in quantum mechanical scattering theory. Indeed we consider the partial-wave Born approximation (Merzbacher, 1970, p. 244):

$$\tan[\delta_l(\kappa)] = -\frac{2M\kappa}{\hbar^2}\int_0^\infty V_l(r)[j_l(\kappa r)]^2 r^2\, dr \tag{33}$$

associated with the scattering energy

$$E = \frac{\kappa^2\hbar^2}{2M}, \tag{34}$$

where $M$ denotes the mass of the scattered particle, $V_l(r)$ is the scattering potential in the channel $l$, and $\delta_l(k)$ is the resulting phase shift. Now, with the help of the derivative formula (12), we can rewrite (33) as follows:

$$-\frac{\hbar^2}{4M\kappa^{l+1}}\frac{d}{d\kappa}\left(\frac{d}{d\kappa^2}\right)^l\{\kappa^{2l+1}\tan[\delta_l(\kappa)]\} = \int_0^\infty r^{l+2}V_l(r)\,j_l(2\kappa r)\,dr, \tag{35}$$

which, in view of the Hankel inversion theorem (see, for example, Sneddon, 1972, p. 299 et seq.), yields the following explicit evaluation of the scattering potential $V_l(r)$:

$$r^l V_l(r) = -\frac{4\hbar^2}{M\pi}\int_0^\infty \frac{1}{\kappa^{l-1}}\left[\frac{d}{d\kappa}\left(\frac{d}{d\kappa^2}\right)^l\{\kappa^{2l+1}\tan[\delta_l(\kappa)]\}\right] j_l(2\kappa r)\,d\kappa. \tag{36}$$

Alternatively, the inversion problem in (35) can be solved by appealing to the Hankel transform result (Jackson, 1975, p. 110, Equation (3.112)):

$$\frac{2}{\pi}\int_0^\infty (ax)^2 j_l(ax)\,j_l(bx)\,dx = \delta(a-b), \tag{37}$$

which is a limit case of the relatively more familiar integral formula (cf. Sneddon, 1972, p. 314, Equation (5-5-3); see also Abramowitz and Stegun, 1968, p. 487, Entry 11.4.41):

$$\int_0^\infty x^{1-\mu+\nu}J_\mu(ax)J_\nu(bx)\,dx = \frac{b^\nu}{a^\mu\Gamma(\mu-\nu)}\left(\frac{a^2-b^2}{2}\right)^{\mu-\nu-1}H(a-b) \tag{38}$$

$$(a > 0; b > 0; \mathbb{R}(\mu) > \mathbb{R}(\nu) > -1)$$

when $\mu \to \nu$, $\delta(t)$ and $H(t)$ being the Dirac delta function and the Heaviside unit function, respectively.

In particular, for $l = 1$, (36) yields

$$r V_1(r) = -\frac{4\hbar^2}{M\pi}\int_0^\infty \left[\frac{d}{d\kappa}\left(\frac{d}{d\kappa^2}\right)\{\kappa^3\tan[\delta_1(\kappa)]\}\right] j_1(2\kappa r)\,d\kappa, \tag{39}$$

and so on.

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