JOURNAL OF COMPUTATIONAL PHYSICS 85, 245–252 (1989)

Note

Closed Expressions for Some Useful Integrals Involving Legendre Functions and Sum Rules for Zeroes of Bessel Functions

1. Introduction

In Ref. [1] closed analytical expressions were obtained for a number of useful sums and integrals involving Legendre functions. The key point of the method was a comparison of magnetic vector-potential components for the toroidal solenoid derived by different methods (but for the same gauge and boundary conditions). Their coincidence stems from a well-known theorem (see, e.g., [2]) according to which a harmonic function (the difference of two solutions of the same Poisson equation is such a function) that is equal to zero at infinity (the vector-potentials of Ref. [1] satisfy this condition) is identically equal to zero. This trick (i.e., the construction of new relations between special functions by comparing the solutions of the same equations derived by different methods) is not new. Examples of this type may be found in a well-known treatice on Bessel functions [3].

The present treatment is similar to [1] and is organized as follows. In Section 2 we consider three different integral representations of the same function. By comparing them we obtain integrals involving Legendre functions in closed form. In Section 3 we study how eigenvalues of the Schrödinger equation change when the vector potential $\mathbf{A} \neq 0$ (but $\mathbf{H} = \operatorname{rot} \mathbf{A} = 0$) is switched on in a simply connected space region. According to the theory (see, e.g., [4]) in the simply connected region the eigenvalues for $\mathbf{A} \neq 0$ should be the same as those for $\mathbf{A} = 0$. Evaluating the second-order terms of the perturbation theory (PT) and equating them to zero we obtain the sum rules for zeroes of Bessel functions of integer and semi-integer orders. We have not found these expressions in mathematical handbooks, treatises, and original publications (see, e.g., [3, 5–7]).

2. Closed Expressions for Some Integrals Involving Legendre Functions

2.1. In Ref. [8] a functions α which connected the vector-potential of the toroidal solenoid in different gauges was used. It is defined by the double integral

$$\alpha(\rho, z) = \frac{1}{2} \iint \frac{dx_1\, dy_1}{|\mathbf{r} - \mathbf{r}_1|}. \tag{2.1}$$

0021-9991/89 $3.00

The integration in (2.1) is performed inside a circle of radius a lying in the $z=0$ plane: $0 \leqslant \rho_1 \leqslant a$, $0 < \varphi_1 < 2\pi$. For this function in [8], the three different integral representations

$$\alpha = \pi(\sqrt{z^2+a^2} - |z|) - \sqrt{a} \int_0^\rho \frac{dx}{\sqrt{x}} \cdot Q_{1/2}(t) \qquad \left(t = \frac{z^2+x^2+a^2}{2ax}\right) \tag{2.2}$$

$$\alpha = \frac{1}{\sqrt{\rho}} \int_0^a \sqrt{x}\, dx \cdot Q_{-1/2}(y) \qquad \left(y = \frac{z^2+x^2+\rho^2}{2\rho x}\right) \tag{2.3}$$

$$\alpha = \sqrt{\operatorname{ch}\mu - \cos\theta} \sum_{n=0}^{\infty} \alpha_n(\mu) \cdot \cos n\theta \tag{2.4}$$

were obtained. The variables μ, θ in (2.4) are toroidal coordinates connected with the cylindrical coordinates as follows:

$$\rho = a \frac{\operatorname{sh}\mu}{\operatorname{ch}\mu - \cos\theta}, \qquad z = a \frac{\sin\theta}{\operatorname{ch}\mu - \cos\theta} \qquad (0 < \mu < \infty,\ -\pi < \theta < \pi). \tag{2.5}$$

The function $\alpha_n(\mu)$ is equal to

$$\alpha_n(\mu) = \frac{2a}{1+\delta_{n,0}} \cdot (-1)^n \cdot \left[Q_{n-1/2}(\operatorname{ch}\mu) \int_1^{\operatorname{ch}\mu} \frac{dx}{(1+x)^{3/2}} \cdot P_{n-1/2}(x) + P_{n-1/2}(\operatorname{ch}\mu) \int_{\operatorname{ch}\mu}^{\infty} \frac{dx}{(1+x)^{3/2}} \cdot Q_{n-1/2}(x) \right]. \tag{2.6}$$

(P_ν and Q_ν are the Legendre functions of the first and second kind, respectively.)

2.2. Set $\mu=0$ in (2.4). In accordance with (2.5) we should take $\rho=0$ in (2.2). Equating (2.2) and (2.4) results in

$$\pi(\sqrt{z^2+a^2} - |z|) = \sqrt{1-\cos\theta} \sum_{n=0}^{\infty} \alpha_n(0) \cdot \cos n\theta. \tag{2.7}$$

Substitute $z = (a\sin\theta)/(1-\cos\theta)$ in (2.7), divide both sides by $\sqrt{1-\cos\theta}$, and integrate over θ to obtain

$$\int_1^\infty \frac{dx}{(1+x)^{3/2}} \cdot Q_{n-1/2}(x) = \frac{(-1)^n}{\sqrt{2}} \int_{-\pi/2}^{\pi/2} \frac{d\varphi}{1+\cos\varphi} \cdot \cos 2n\varphi \qquad \left(\varphi = \frac{1}{2}\theta\right). \tag{2.8}$$

The integral on the r.h.s. of (2.8) is easily evaluated. Thus,

$$\int_1^\infty \frac{dx}{(1+x)^{3/2}} Q_{n-1/2}(x) = \sqrt{2}\left[1 - \pi n \cdot (-1)^n - 4n \cdot (-1)^n \sum_{k=1}^{n} \frac{(-1)^k}{2k-1}\right]. \tag{2.9}$$

In particular cases,

$$\int_1^\infty \frac{dx}{(1+x)^{3/2}} Q_{-1/2}(x) = \sqrt{2},$$

$$\int_1^\infty \frac{dx}{(1+x)^{3/2}} Q_{1/2}(x) = \sqrt{2}\,(\pi - 3),$$

$$\int_1^\infty \frac{dx}{(1+x)^{3/2}} Q_{3/2}(x) = \sqrt{2}\left(\frac{19}{3} - 2\pi\right).$$

Using the Whipple relation between the Legendre functions, one may transform (2.9) to the form

$$\int_0^\mu d\mu \exp\left(-\frac{3}{2}\mu\right) \cdot P^n_{-1/2}(\operatorname{ch}\mu)$$
$$= \frac{2}{\sqrt{\pi}} \frac{1}{\Gamma(\frac{1}{2}-n)} \cdot \left[1 - (-1)^n \cdot \pi n - 4n \cdot (-1)^n \sum_{k=1}^{n} \frac{(-1)^k}{2k-1}\right]. \tag{2.10}$$

2.3. Equating (2.2) and (2.3) one obtains the following relation between the integrals involving Legendre functions:

$$\pi(\sqrt{z^2+a^2} - |z|) - \sqrt{a} \int_0^\rho \frac{dx}{\sqrt{x}} Q_{1/2}(t) = \frac{1}{\sqrt{\rho}} \int_0^a \sqrt{x}\, dx\, Q_{-1/2}(y). \tag{2.11}$$

Taking the limits $\rho \to \infty$ and $a \to \infty$ and differentiating the expressions obtained we get explicit expressions for the integrals

$$\int_0^\infty \frac{dx}{\sqrt{x}} Q_{1/2}(t) = \frac{\pi}{\sqrt{a}} (\sqrt{z^2+a^2} - |z|),$$

$$\int_0^\infty \sqrt{x}\, dx\, Q^1_{1/2}(t) = -\frac{\pi a^{5/2}}{|z|},$$

$$\int_0^\infty \frac{dx}{\sqrt{x}} \frac{1}{\sqrt{t^2-1}} Q^1_{-1/2}(t) = -\frac{\pi a^{3/2}}{|z|},$$

$$\int_0^\infty \frac{dx}{x^{3/2}} \frac{1}{\sqrt{t^2-1}} Q^1_{1/2}(t) = \pi\sqrt{a}\left(\frac{1}{\sqrt{z^2+a^2}} - \frac{1}{|z|}\right) \qquad \left(t = \frac{z^2+x^2+a^2}{2ax}\right).$$

A change of variables transforms these integrals into known integrals (see, e.g., [5]). Put $\rho = a$, $z = 0$ in (2.11). This gives

$$\pi = \int_0^1 dx \left[\frac{1}{\sqrt{2}} Q_{1/2}\left(\frac{1+x^2}{2x}\right) + \sqrt{x}\, Q_{-1/2}\left(\frac{1+x^2}{2x}\right)\right]. \tag{2.12}$$

We have not found epressions (2.9)–(2.12) in the mathematical literature.

3. Sum Rules for the Zeroes of the Bessel Functions

3.1. Consider an infinite cylinder C of radius R. Let its axis coincide with the z axis: $\rho=\sqrt{x^2+y^2}=R$, $-\infty<z<\infty$. We are interested in the eigenfunctions and eigenvalues of the free Schrödinger equation inside this cylinder. The following boundary condition is imposed on the eigenfunction: $\Psi=0$ for $\rho=R$. The eigenfunctions and eigenvalues are equal to (see any textbook on mathematical physics or quantum mechanics)

$$\Psi^0_{ms}=C_{ms}J_m\left(\Lambda_{ms}\frac{\rho}{R}\right)\cdot\exp(im\varphi),$$
$$E^0_{ms}=\frac{\hbar^2}{2\mu R^2}\Lambda^2_{ms}. \tag{3.1}$$

Here μ is the mass of a particle moving inside C, m is its angular momentum, Λ_{ms} is an sth nonzero root of the equations $J_m(x)=0$. Finally, C_{ms} is the normalizing constant: $C_{ms}=(1/R\sqrt{\pi})[-J_{m-1}(\Lambda_{ms})\,J_{m+1}(\Lambda_{ms})]^{1/2}$. For simplicity (and without loss of generality) we limited ourselves in (3.1) to motion in the $z=0$ plane.

Now install outside C an infinite cylindrical solenoid with magnetic flux Φ. Let its axis be parallel to the z axis and pass through the point $x=a$, $y=0$. Outside the solenoid the strength H of the magnetic field equals zero, while the vector-potential $\mathbf{A}$ ($\mathbf{H}=\operatorname{rot}\mathbf{A}$) differs from zero:

$$A_x=-\frac{\Phi}{2\pi}\frac{y}{y^2+(x-a)^2},\qquad A_y=\frac{\Phi}{2\pi}\frac{x-a}{y^2+(x-a)^2}. \tag{3.2}$$

Does the presence of a nonzero $\mathbf{A}$ inside C change the energy levels E^0_{ms}? We note that the space accessible for particles (the interior of C) is simply connected, there is no path along which $\oint A_l\,dl\neq 0$. The theory (see, e.g., [4] says that in such a situation there should be no observable effects. In particular, eigenvalues of the Schrödinger equation $-(\hbar^2/2\mu)(\nabla-(ie/\hbar c)\,\mathbf{A})^2\,\Psi=E\Psi$ with nonzero $\mathbf{A}$ given by (3.2) should coincide with E^0_{ms} defined by (3.1). This is true for any value of the dimensionless parameter $\gamma=e\Phi/\hbar c$. This means that in the particular perturbation expansion in γ ($H=H_0+H_1+H_2$, $\Psi_{ms}=\Psi^0_{ms}+\Psi^1_{ms}+\Psi^2_{ms}+\cdots$, $E_{ms}=E^0_{ms}+E^1_{ms}+E^2_{ms}+\cdots$) the corrections to E^0_{ms} should vanish separately for each order in γ. In the first-order PT one has $E^1_{ms}=\langle\Psi^0_{ms}|\,H_1\,|\Psi^0_{ms}\rangle$, $H_1=(2ie/\hbar c)\,A\nabla$. From the expansion in the angular variable γ,

$$A_\rho=-\frac{\Phi}{2\pi\rho}\sum_{n=1}^{\infty}\exp(-\mu n)\cdot\sin n\varphi,$$
$$A_\varphi=-\frac{\Phi}{2\pi\rho}\sum_{n=1}^{\infty}\exp(-\mu n)\cdot\cos n\varphi \qquad (\rho=\sqrt{x^2+y^2},\ \exp\mu=a/\rho), \tag{3.3}$$

it follows at once that the equation $E^1_{ms}=0$ is satisfied automatically. In the second-order PT one obtains for the eigenvalues

$$E^2_{ms}=\langle \Psi^0_{ms}|\, H_2\, |\Psi^0_{ms}\rangle+\sum_{ns'}\frac{|\langle \Psi^0_{ns'}|\, H_1\, |\Psi^0_{ms}\rangle|^2}{E^0_{ms}-E^0_{ns'}}. \qquad (3.4)$$

$$\left(H_2=\frac{e^2}{\hbar^2c^2}\mathbf{A}^2\right).$$

It follows from (3.4) that E^2_{ms} does not vanish trivially. The substitution of the unperturbed eigenfunctions (3.1) and vector-potentials (3.3) in (3.4) leads to cumbersome relations between the radial integrals. Fortunately, they are simplified for $R\ll a$ (i.e., when the radius of the available cylindrical cavity is small). Thus,

$$\frac{2\mu}{\hbar^2}\frac{\pi^2a^2}{4\gamma^2}E^2_{ms}=\frac{1}{4}-\Lambda^2_{ms}\sum_{s'}\left[\frac{\Lambda^2_{m+1,s'}}{(\Lambda^2_{m+1,s'}-\Lambda^2_{ms})^3}+\frac{\Lambda^2_{m-1,s'}}{(\Lambda^2_{m-1,s'}-\Lambda^2_{ms})^3}\right].$$

(It should be recalled that Λ_{ms} is an sth nonzero root of the equation $J_m(x)=0$). The requirement that E^2_{ms} vanish suggests the following sum rule for the zeroes of Bessel functions:

$$\frac{1}{4\Lambda^2_{ms}}=\sum_{s'}\frac{\Lambda^2_{m+1,s'}}{(\Lambda^2_{m+1,s'}-\Lambda^2_{ms})^3}+\sum_{s'}\frac{\Lambda^2_{m-1,s'}}{(\Lambda^2_{m-1,s'}-\Lambda^2_{ms})^3}. \qquad (3.5)$$

This expression is simplified for $m=0$,

$$\frac{1}{8\Lambda^2_{0s}}=\sum_{s'}\frac{\Lambda^2_{1s'}}{(\Lambda^2_{1s'}-\Lambda^2_{0s})^3}. \qquad (3.6)$$

3.2. Let the space available for particles be a sphere S of radius R (i.e., inside the sphere the eigenfunctions satisfy the free Schrödinger equation with boundary condition $\Psi(r=R)=0$). Installing outside the sphere a cylindrical solenoid we create inside S a magnetic field with $H=0$, but $\mathbf{A}\neq 0$. The space accessible for particles is simply connected. Thus the existence of a nonzero $\mathbf{A}$ inside S should not change the energy levels. Thus, we require the energy shift to vanish in each order of PT in the parameter $\gamma=e\Phi/\hbar c$. The corrections of the first order vanish automatically. In the second-order correction one obtains the two nontrivial sum rules

$$\frac{2l+3}{16\omega^2_{ls}}=-\sum_{s'}\frac{\omega^2_{l+1,s'}}{(\omega^2_{ls}-\omega^2_{l+1,s'})^3} \qquad (l\geqslant 0), \qquad (3.7)$$

$$\frac{2l-1}{16\omega^2_{ls}}=\sum_{s'}\frac{\omega^2_{l-1,s'}}{(\omega^2_{ls}-\omega^2_{l-1,s'})^3} \qquad (l\geqslant 1). \qquad (3.8)$$

Here ω_{ls} is an sth root of the equation $J_{l+1/2}(x)=0$. For $l=0, 1$, one finds

$$\frac{3}{16}\frac{1}{\omega_{0s}^2}=-\sum_{s'}\frac{\omega_{1s'}^2}{(\omega_{0s}^2-\omega_{1s'}^2)^3}, \qquad \frac{1}{16\omega_{1s}^2}=\sum_{s'}\frac{\omega_{0s'}^2}{(\omega_{1s}^2-\omega_{0s'}^2)^3}.$$

As mentioned earlier, we have not found these expressions in the mathematical literature.

4. Conclusion

It is astonishing how closely mathematical and physical aspects are intermixed in some problems. For example, a rather abstract quantum-mechanical principle (non-observability of certain physical effects in simply connected space regions) generates nontrivial relations between the zeroes of Bessel functions. There is no doubt that once these relations have been derived, they will be obtained later without reliance on the physical aspects. This is confirmed by consideration of the two integrals (as suggested by one of the referees)

$$\frac{1}{2\pi i}\int_{C_R}\frac{J_{\nu+1}(z)}{J_\nu(z)}\frac{P(z)}{Q(z)}\,dz, \qquad \frac{1}{2\pi i}\int_{C_R}\frac{J_{\nu-1}(z)}{J_\nu(z)}\frac{P'(z)}{Q'(z)}\,dz.$$

Here C_R is a circle of radius R; P, P', Q, and Q' are polynomials in z. If P/Q and P'/Q' go to zero, like $|z|^{-2}$ (or faster), then the integral over C_R vanishes as $R\to\infty$. According to Cauchy's residue theorem

$$\sum_s\frac{P(z_{\nu s})}{Q(z_{\nu s})}=\sum \text{Res}\,\frac{J_{\nu+1}}{J_\nu}\frac{P}{Q}, \qquad \sum_s\frac{P'(z_{\nu s})}{Q'(z_{\nu s})}=-\sum \text{Res}\,\frac{J_{\nu-1}}{J_\nu}\frac{P'}{Q'},$$

where the sums on the r.h.s. are taken over the zeroes of Q and Q' and $z_{\nu s}$ are non-zero roots of the equation $J_\nu(z)=0$. For $P=P'=z^2$, $Q=(z^2-z_{\nu-1,s}^2)^3$, $Q'=(z'-z_{\nu+1,s}^2)^3$, one obtains

$$\sum\frac{z_{\nu s'}^2}{(z_{\nu s'}^2-z_{\nu\pm 1,s}^2)^3}=\mp\frac{\nu}{8z_{\nu\pm 1,s}^2}.$$

In this equation and in the equations given below the sum is taken over the positive zeroes. For $\nu=m$ and $\nu=l+\frac{1}{2}$ these equations transform into those obtained in the previous section. Other choices of P and Q are also interesting. For example,

$$P=P'=1, \qquad Q=z^2-z_{\nu-1,s}^2, \qquad Q'=z^2-z_{\nu+1,s}^2$$

$$\sum\frac{1}{z_{\nu s'}^2-z_{\nu\pm 1,s}^2}=\mp\frac{\nu}{z_{\nu\pm 1,s}^2};$$

$$P = P' = z^2, \qquad Q = (z^2 - z^2_{\nu-1,s})^2, \qquad Q' = (z^2 - z^2_{\nu+1,s})^2$$

$$\sum \frac{z^2_{\nu s'}}{(z^2_{\nu s'} - z^2_{\nu\pm 1,s})^2} = \frac{1}{4};$$

$$P = P' = 1, \qquad Q = (z^2 - z^2_{\nu-1,s})^2, \qquad Q' = (z^2 - z^2_{\nu+1,s})^2$$

$$\sum \frac{1}{(z^2_{\nu s'} - z^2_{\nu+1,s})^2} = \frac{1}{z^2_{\nu\pm 1,s}}\left(\frac{1}{4} \pm \frac{\nu}{z^2_{\nu\pm 1,s}}\right);$$

$$P = P' = 1, \qquad Q = (z^2 - z^2_{\nu-1,s})^3, \qquad Q' = (z^2 - z^2_{\nu+1,s})^3$$

$$\sum \frac{1}{(z^2_{\nu s'} - z^2_{\nu\pm 1,s})^3} = -\frac{1}{z^4_{\nu\pm 1,c}}\left[\frac{1}{4} \pm \nu\left(\frac{1}{8} + \frac{1}{z^2_{\nu\pm 1,s}}\right)\right];$$

$$P = P' = z^4, \qquad Q = (z^2 - z^2_{\nu-1,s})^3, \qquad Q' = (z^2 - z^2_{\nu+1,s})^3$$

$$\sum \frac{z^4_{\nu s'}}{(z^2_{\nu s'} - z^2_{\nu\pm 1,s})^3} = \frac{2 \mp \nu}{8}.$$

An extensive use of residue calculus for deducing previously unknown sums may be found in a very interesting reference [9].

Addendum. Having been acquainted with a preprint version of this manuscript, Prof. Krupnikov E. D. (Novosibirsk State University) succeeded in deriving Eq. (2.12) without appeal to the physical considerations. In fact, he proved (private communication) that

$$\int_0^1 x^{-\nu} Q_\nu\left(\frac{1+x^2}{2x}\right) dx = \frac{\sqrt{\pi}\,\Gamma(\nu)}{\Gamma(\frac{1}{2}+\nu)} - \frac{1}{\nu}.$$

For $\nu = \pm\frac{1}{2}$ this gives:

$$\int_0^1 x^{-1/2} Q_{1/2}\, dx = \pi - 2, \qquad \int_0^1 x^{1/2} Q_{-1/2}\, dx = 2.$$

Their adding leads to Eq. (2.12).

Acknowledgment

The author thanks the referees for their efforts to improve the contents of this manuscript.

References

1. G. N. Afanasiev, *J. Comput. Phys.* **69**, 196 (1987).
2. R. Courant and D. Hilbert, *Methods of Mathematical Physics*, Vol. II (Interscience, New York, 1962), p. 254.
3. G. N. Watson, *A Treatise of the Theory of Bessel Functions*, Vol. I (Cambridge Univ. Press, Cambridge, 1958).

4. T. T. Wu and C. N. Yang, *Phys. Rev. D* **12**, 3845 (1975).
5. I. S. Gradshteyn and I. M. Ryzik, *Tables of Integrals, Series and Products* (Academic Press, New York, 1965).
6. A. P. Prudnikov, Yu. A. Brychkov, and O. I. Marichev, *Integrals and Series*, Vols. 1–3 (Nauka, Moscow, 1981–1986; W. Magnus, F. Oberhettinger, and R. P. Soni, *Formulas and Theorems for the Special Functions of Mathematical Physics* (Springer-Verlag, Berlin, 1966); E. R. Hansen, *A Table of Series and Products* (Prentice–Hall, Englewood Cliffs, NJ, 1975); H. Bateman and A. Erdely, *Higher Transcendental Functions*, Vols. 1, 2 (McGraw–Hill, New York/Toronto/London, 1953); L. Robin, *Fonctions Spherique de Legendre et Fonctions spheroidales*, Vols. 1–3 (Gauthier–Villars, Paris, 1957); A. D. Wheelon, *Tables of Summable Series and Integrals Involving Bessel Functions* (Holden–Day, San Francisco, 1968); M. Abramowitz and I. A. Stegun, *Handbook of Mathematical Physics* (Dover, New York, 1965); G. Petiau, *La Theorie des Fonctions de Bessel* (CNRS, Paris, 1955).
7. S. Ahmed, M. Bruschi, F. Calogero, M. A. Olshanetsky, and A. M. Perelomov, *Nuovo Cim. B* **49**, 173 (1979); P. J. Forrester and J. B. Rogers, *SIAM J. Math. Anal.* **17**, 461 (1986); R. G. Campos, *SIAM J. Math. Anal.* **18**, 1664 (1987).
8. G. N. Afanasiev, JINR P4-87-106, Dubna, 1987 (unpublished); shortened version, *J. Phys. A* **21**, 2095 (1988).
9. P. J. Forrester, *Rocky Mountain J. Math.* **13**, 557 (1983).

Received: March 14, 1988; revised: October 19, 1988

G. N. Afanasiev
Laboratory of Theoretical Physics
Joint Institute for Nuclear Research
Dubna, Moscow District, 141980, USSR