Multipole moments for Coulomb and oscillator wavefunctions and the Heun equation

1999 J. Phys. A: Math. Gen. 32 1773

(http://iopscience.iop.org/0305-4470/32/9/019)

J. Phys. A: Math. Gen. **32** (1999) 1773–1778. Printed in the UK PII: S0305-4470(99)95976-0

Multipole moments for Coulomb and oscillator wavefunctions and the Heun equation

Sergei Yu Slavyanov†
Institut für Theoretische und Angewandte Physik, Universität Stuttgart, Germany

Received 17 July 1998, in final form 7 December 1998

Abstract. A new method for calculating multipole moments with eigenfunctions related to Sturm–Liouville problems is proposed. The method is based on an auxiliary third-order equation and its Laplace transform. The multipole moments for Coulomb and oscillator problems in quantum mechanics are calculated as an application of this method. The relation between the multipole moments for these problems and equations of Heun type is observed.

1. Introduction

There are two purposes of this paper. The first is to present a new, practical and efficient method for calculating multipole moments with eigenfunctions related to boundary problems for the one-dimensional Schrödinger-type equation. The other purpose is to show that multipole moments arising from Coulomb and oscillator potentials are expressed in terms of solutions of the Heun equation and the biconfluent Heun equation [1].

Consider $\psi_n(z)$, and λ_n to be eigenfunctions and eigenvalues, respectively, of the boundary problem

$$\begin{gathered}(-L+\lambda)\psi = \frac{\mathrm{d}}{\mathrm{d}z}\left(r(z)\frac{\mathrm{d}}{\mathrm{d}z}\psi(z)\right) + (\lambda - q(z))\psi(z) = 0 \\ |\psi(z_1)| < \infty \qquad |\psi(z_2)| < \infty\end{gathered} \tag{1}$$

where z_1, z_2 are the endpoints of the interval of consideration (finite or infinite). Suppose that the following orthogonality condition is satisfied:

$$\int_{z_1}^{z_2} \psi_n(z)\,\psi_m(z)\,\mathrm{d}z = \delta_{nm}$$

where δ_{nm} is the Kronecker symbol. It is assumed that the function $r(z)$ is a polynomial and $q(z)$ is a rational function, and also that z_1, z_2 are singularities of equation (1)‡. By multipole moments we mean the integrals

$$V_{nn}^{(k)} = \int_{z_1}^{z_2} z^k\,\psi_n(z)\,\psi_n(z)\,\mathrm{d}z \tag{2}$$

† On leave from: State University of St Petersburg Department of Computational Physics. E-mail address: slav@slav.usr.pu.ru

‡ If we multiply the equation by the denominator of $r(z)$ we find that it has polynomial coefficients. Moreover, the eigenvalue parameter λ should be one of the so-called accessory parameters of the equation. This obstacle induces further limitations on the properties of singularities of the equation.

where k is a positive integer. They might also be called diagonal matrix elements for multipole perturbation. Two conventional methods are used for the explicit evaluation of $V_{nn}^{(k)}$ in the simplest cases of $r(z)$ and $q(z)$. The first method is to use the integral

$$\int_{z_1}^{z_2} z^k \, \psi_n(z)(-L+\lambda)\, \psi_n(z)\, \mathrm{d}z$$

substituting a simple representation of ψ_n and integrating by parts. The other method is to use the group-theory approach. Here, another method is proposed, based on the transform to an auxiliary third-order equation and its Laplace transform.

2. General theory

The first step in the general method is based on the following well known lemma.

Lemma 1. *The square $w_n(z) = (\psi_n(z))^2$ of the eigenfunction in (1) satisfies the third-order equation*

$$r w''' + 3r' w'' + \left(r'' + \frac{(r')^2}{r} + 4(\lambda - q) \right) w' + \left(2(\lambda - q)\frac{r'}{r} - 2q' \right) w = 0. \tag{3}$$

For the sake of completeness we give here the draft of computations leading to the proof of the lemma. The derivatives of the function $w_n(z)$ are

$$w' = 2\psi\psi' \qquad w'' = 2(\psi\psi'' + (\psi')^2) \qquad w''' = 2(\psi\psi''' + 3\psi'\psi'').$$

As a result of differentiating equation (1) the third-order equation

$$r y''' + 2r' y'' + r'' y' + (\lambda - q) y' - q' y = 0$$

holds. Multiplying this formula by y and also using equation (1) we obtain equation (3).

In [2] the notion of the s-rank for the singularity of a second-order linear ordinary differential equation (ODE) with rational coefficients was introduced. Here, the definition of the s-rank is extended to an equation of arbitrary order. Suppose that the nth-order linear ODE is written as

$$v^{(n)}(z) + Q_1(z) v^{(n-1)}(z) + Q_2(z) v^{(n-2)}(z) + \cdots + Q_n(z)\, v(z) = 0 \tag{4}$$

with rational functions $Q_n(z)$. Let $z = z^*$ be a singularity of equation (4). Then in a neighbourhood of z^* the functions $Q_m, m = 1, \ldots, n$ are either regular or have poles of order K_m.

Definition. *The s-rank $R(z^*)$ is a quantitative characteristic feature of the singularity z^* which for an irregular singularity is defined by the formula*

$$R(z^*) = \max(K_1, K_2/2, \ldots, K_n/n). \tag{5}$$

The s-rank of the regular singularity is by definition equal to unity.

The s-rank of an irregular singularity is either a positive integer larger than unity or a fraction, the denominator of which is not larger than the order of the equation. The singularity at infinity is studied with the help of a Möbius transformation to a finite point.

In terms of this definition another lemma might be proven.

Lemma 2. *The singularities of equations (1) and (3) and their s-ranks coincide.*

Proof. The only singularities for both equations (1) and (3) are zeros of the function $r(z)$, poles of the function $q(z)$ and, possibly, the point at infinity. Suppose that the singularity z^* is the pole of order k of the function $q(z)$ and is not a zero of $r(z)$. Then, it is a pole of order $k+1$ of the function $q'(z)$. In this case the lemma holds. Suppose now that the singularity z^* is the zero of order k of the function $r(z)$ and is a regular point of $q(z)$. Then, the s-rank of z^* in equation (1) is equal to $\max(1, k/2)$, whereas the s-rank of the same singularity in (3) is equal to $\max(1, k/2, (k+1)/3)$. Since $k/2 \geqslant (k+1)/3$ for $k \geqslant 2$, lemma 2 holds once again. The case in which z^* is simultaneously the zero of $r(z)$ and the pole of $q(z)$ is studied in the same way. The singularity at infinity may be transposed to a finite point by a Möbius transform. □

Multiplying equation (3) by the greater common divisor of the coefficients we can obtain an equation with purely polynomial coefficients $P_j(z),\ j = 0, 1, 2, 3,$

$$P_0(z)\, w'''(z) + P_1(z)\, w''(z) + P_2(z)\, w'(z) + P_3(z)\, w(z) = 0. \tag{6}$$

In other terms equation (6) might be written as

$$T(z, D)\, w(z) = 0 \qquad D = \frac{\mathrm{d}}{\mathrm{d}z} \tag{7}$$

where $T(z, D)$ is a polynomial in both variables z and D.

The next step is to apply an analogue of the Laplace transform to $w_n(z)$.

$$w_n(z) \mapsto u_n(p) \qquad u_n(p) = \int_{z_1}^{z_2} \exp(-pz)\, w_n(z)\, \mathrm{d}z. \tag{8}$$

Convergence of the integral is verified by the behaviour of $\psi_n(z)$ at the endpoints. In fact, we need convergence only in the neighbourhood of $p = 0$.

The expansion of the function $u_n(p)$ in the neighbourhood of the origin is expressed in terms of multipole moments

$$u_n(p) = \sum_0^\infty V_{nn}^{(k)} (-p)^k / k! := \sum_0^\infty g_k p^k. \tag{9}$$

On the other hand, according to easily modified properties of the Laplace transform, the function $u_n(p)$ is a solution of the linear ordinary differential equation

$$T(-D_p, p) u_n(p) = 0. \tag{10}$$

To obtain equation (10) it is only necessary to prove the following lemma.

Lemma 3. *In the course of the transform from equation (7) to equation (10) the nonintegral terms vanish.*

Proof. Suppose that the singularity $z = z_1$ is an irregular one. Then the eigensolution $\psi_n(z)$ due to self-adjointness of the equation decreases exponentially, while z tends to z_1. As a result the nonintegral terms arising on integration by parts vanish. Suppose that $z = z_1$ is a finite regular singularity. Two different cases should be studied:

(a) the function $q(z)$ is regular at $z = z_1$;
(b) the function $q(z)$ has a simple pole at $z = z_1$.

Otherwise, if $q(z)$ has a pole of higher order we obtain once again the irregular singularity. The first case, (a), is a more difficult one. The function $r(z)$ has a simple zero at $z = z_1$ (otherwise the point $z = z_1$ would be an ordinary point of equation (1)). As a result, the polynomials $P_0(z)$, $P_1(z)$, and $P_2(z)$ will be characterized by the following behaviour in the neighbourhood of $z = z_1$:

$$\begin{aligned} P_0(z) &= (r'(z_1))^2(z-z_1)^2(1+\mathrm{o}(z-z_1)) \\ P_1(z) &= 3(r'(z_1))^2(z-z_1)(1+\mathrm{o}(z-z_1)) \\ P_0(z) &= (r'(z_1))^2(1+\mathrm{o}(z-z_1)). \end{aligned} \tag{11}$$

Without loss of generality it might be assumed that z_1 lies at the origin. Keeping only those terms in the Laplace transform which are 'leading' from the point of view of local behaviour at the origin we obtain, for equation (10)

$$\begin{aligned} &(r'(0))^2[D_p^2(t^3u(p) - w(0)p^2 - w'(0)p - w''(0)) \\ &\qquad -3D_p(t^2u(p) - w(0)p - w'(0)) + (tu(p) - w(0))] + \cdots = 0 \end{aligned} \tag{12}$$

where terms containing higher differentiation and denoted by ... are omitted. It is seen from (12) that the terms arising from integration by parts are either 'killed' by differentiation or cancel out. The terms in which a higher order of differentiation stands in front of the function are 'killed' as well.

In case (b) higher orders of differentiation appear in each term and, moreover, the function $\psi_n(z)$ becomes zero at $z = z_1$. Both obstacles make the proof easier. The regular point at infinity might be studied by a Möbius transform to a finite point. The second endpoint of the interval is studied as the first one. This completes the proof. □

Now we formulate the main result of the paper.

Theorem. *The multipole moments $V_{nn}^{(k)}$ related to a Sturm–Liouville problem (1) are, up to a multiple $(-1)^k k!$, equal to the coefficients of the Taylor series of the regular solution of equation (10), which resembles the Laplace transform of the auxiliary third-order equation (3) for the square of the eigenfunction.*

The proof is given above.

3. Examples

First the following boundary problem is studied:

$$\begin{gathered} \frac{\mathrm{d}}{\mathrm{d}z}\left(z\frac{\mathrm{d}}{\mathrm{d}z}\psi(z)\right) + \left(\lambda - \frac{z}{4} - \frac{(l+\frac{1}{2})^2}{z^2}\right)\psi(z) = 0 \\ |\psi(0)| < \infty \qquad |\psi(\infty)| < \infty. \end{gathered} \tag{13}$$

Here, the integer l is related to the orbital momentum. Eigenfunctions $\psi_n(z)$ comprise the so-called Sturmian basis in the quantum Coulomb problem and eigenvalues are known to be

$$\lambda_n = n + l + 1. \tag{14}$$

For simplicity we introduce new parameters $N = n + l + 1$, $L = l(l+1)$. Then, the auxiliary third-order equation in the form (6) becomes

$$z^2w''' + 3zw'' + (-z^2 + 4Nz - 4L)w' + (-z + 2N)w = 0. \tag{15}$$

After a Laplace transform we obtain

$$p(p^2-1)u''(p) + (3p^2 - 4Np - 1)u'(p) - (4Lp + 2N)u(p) = 0. \tag{16}$$

Equation (16) is a special case of the Heun equation [1]

$$p(p-1)(p-t)v''(p) + (c(p-1)(p-t) + dp(p-t) \\ +(a+b+1-c-d)p(p-1))v'(p) + (abp-\mu)v(p) = 0. \tag{17}$$

The coefficients g_k of the expansion of the regular in the vicinity of the zero solution $v(z)$ of equation (17) satisfy the following three-term recurrence relation:

$$t(k+1)(k+t)g_{k+1} - ((t+1)(k+1)(k+c+d) + (a+b+1-c)(k+1) - \mu)g_k \\ +(k(k+a+b)+ab)g_{k-1} = 0 \qquad g_0 = 1. \tag{18}$$

Comparing equation (17) with (16) it is easy to obtain that equation (16) is derived from equation (17) using the following parameter values:

$$t=-1 \qquad c=1 \qquad d=1-2N \qquad a=2(l+1) \qquad b=-2l.$$

For these values of the parameters, equation (18) yields

$$(1-k^2)g_{k+1} - (2(k+1)-2N)g_k + (k(k+2)-4L)g_{k-1} = 0. \tag{19}$$

If the coefficients g_k are substituted for multipole moments $V_{nn}^{(k)}$ equation (19) converts to the recurrence relation

$$(1-k)V_{nn}^{(k+1)} + (2(k+1)-2N)V_{nn}^{(k)} + k(k(k+2)-4L)V_{nn}^{(k-1)} = 0. \tag{20}$$

Another physical example is the quantum oscillator for which the boundary problem is posed on the whole axis $-\infty, \infty$,

$$\psi''(z) + (\lambda - z^2)\psi(z) = 0 \\ |\psi(-\infty)| < \infty \qquad |\psi(\infty)| < \infty. \tag{21}$$

The eigenfunctions ψ_n and the eigenvalues λ_n are known to be

$$\lambda_n = 2n+1.$$

The auxiliary third-order equation reads

$$w'''(z) + 4(\lambda - z^2)w'(z) - 4zw(z) = 0 \tag{22}$$

whereas after a Laplace transform we obtain

$$pu''(p) + u'(p) - (\lambda p + \tfrac{1}{4}p^3)u(p) = 0. \tag{23}$$

Equation (23) is a special case of the biconfluent Heun equation. It is invariant under the inversion transform $p \mapsto -p$. As a consequence of this property, equation (23) may be transformed into a simpler equation, namely to a confluent hypergeometric equation. For this purpose the transform of the independent variable

$$p^2 = x$$

is needed. The resulting equation reads

$$4xu''(x) + 4u'(x) - (\lambda + x/4)u(x) = 0. \tag{24}$$

However, for our purpose equation (23) is sufficient. The regular at $z = 0$ solution of equation (23) is sought in the form of a power series

$$u_n(p) = \sum_0^\infty g_k p^{2k}. \tag{25}$$

The coefficients g_k satisfy the three-term recurrence relation

$$16(k+1)^2 g_{k+1} - 4(2n+1)g_k - g_{k-1} = 0. \tag{26}$$

For the multipole moments $V_{nn}^{(2k)}$ equation (19) converts to the recurrence relation

$$\frac{k+1}{k+\frac{1}{2}}V_{nn}^{(2k+2)} - (2n+1)V_{nn}^{(2k)} - k(k-\tfrac{1}{2})V_{nn}^{(2k-2)} = 0. \tag{27}$$

Formulae (20) and (27) are the only examples (at least known to the author) of multipole moments closely related to equations of Heun class. Of course, they might be found in many other publications but in another context.

4. Conclusions

The third simple example which could be exposed in this paper is the example with one more type of classical orthogonal polynomial—Jacoby polynomials (taking Gegenbauer and Legendre polynomials as specialized cases). We do not present this example here, since it does not fit our second goal—the corresponding equation after Laplace transform does not belong to the Heun class.

These examples, taken together in general, include all those cases for which the proposed method delivers explicit results. The reason for this is that in these cases we have an explicit expression for the eigenvalues in the starting boundary conditions. All other calculations with more sophisticated starting equations (with polynomial coefficients!) require knowledge of eigenvalues. The latter can be obtained numerically or asymptotically if some parameter is assumed to be small. Briefly, we can list the problems where such techniques may be applied: the two Coulomb centres problem, the anharmonic oscillator, the Stark effect in hydrogen, etc. Exposing these examples requires a comparison with numerical results. A possible extension of the proposed method is to take functions other than exponents as weight functions. It is only required that the auxiliary third-order equation has polynomial coefficients. However, it seems rather complicated to construct a general theory for this case, although special cases can be treated.

Acknowledgments

The research was sponsored by RFFR grants 96-01-00-618 98-01-01-075 and by a DFG grant. The author is pleased to thank Dr W Lay for a critical reading of the article and the Institute for Theoretical and Applied Physics at Stuttgart University for hospitality.

References

[1] Ronveaux A 1995 *Heun's Differential Equations* (Oxford: Oxford University Press)
[2] Seeger A, Lay W and Slavyanov S 1995 *Theor. Math. Phys.* **104** 950–60