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Integral relations for solutions of the confluent Heun equation

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ABSTRACT

Firstly, we construct kernels for integral relations among solutions of the confluent Heun equation (CHE). Additional kernels are systematically generated by applying substitutions of variables. Secondly, we establish integral relations between known solutions of the CHE that are power series and solutions that are series of special functions. Thirdly, by using one of the integral relations as an integral transformation we obtain a new series solution of the ordinary spheroidal wave equation (a particular CHE). From this solution we construct new series solutions of the general CHE, and show that these are suitable for solving the radial part of the two-center problem in quantum mechanics.

1. Introductory remarks

Recently we have found that the transformations of variables which preserve the form of the general Heun equation correspond to transformations which preserve the form of the equation for kernels of integral relations among solutions of the Heun equation [1]. In fact, by using the known transformations of the Heun equation [2,3] we have found prescriptions for transforming kernels and, in this manner, we have generated several new kernels for the equation.

The above correspondence can be extended to the confluent equations of the Heun family, that is, to the (single) confluent, double-confluent, biconfluent and triconfluent Heun equations [4,5], as well as to the reduced forms of such equations [6,7]. In the present study we investigate only the confluent Heun equation (CHE). Specifically:

- we deal with the construction and transformations of integral kernels for the CHE;
- from some of these kernels, we establish integral relations between known solutions of the CHE;
- from another kernel, we obtain new solutions in series of confluent hypergeometric functions for the CHE; we show that these solutions are suitable to solve the radial part of the two-centre problem in quantum mechanics [8].

We write the CHE as [9]

$$z(z-z_0)\frac{d^2U}{dz^2}+(B_1+B_2z)\frac{dU}{dz}+\left[B_3-2\omega\eta(z-z_0)+\omega^2z(z-z_0)\right]U=0,\qquad [\text{CHE}] \tag{1}$$

where z_0, B_i, η and ω are constants. This CHE is called *generalized spheroidal wave equation* by Leaver [9], but sometimes the last expression refers to a particular case of the CHE [5,10]. Excepting the Mathieu equation, the CHE is the most studied of the confluent Heun equations and includes the (ordinary) spheroidal equation [5] as a particular case. Its recent occurrence

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in several classes of quantum two-state systems [11], certainly will require new solutions for Eq. (1). On the other side, the reduced confluent Heun equation (RCHE) is written as

$$z(z-z_0)\frac{d^2U}{dz^2}+(B_1+B_2z)\frac{dU}{dz}+[B_3+q(z-z_0)]U=0, \qquad \text{[RCHE]} \tag{2}$$

where z_0, B_i and q $(q \neq 0)$ are constants. The RCHE describes the angular part of the Schrödinger equation for an electron in the field of a point electric dipole [12,13]. It appears as well in the study of two-level systems [14], polymer dynamics [15] and theory of gravitation [16]. The form (2) for the RCHE results from the CHE (1) by means of the limits

$$\omega \to 0, \quad \eta \to \infty \quad \text{such that} \quad 2\eta\omega = -q, \qquad \text{[Whittaker-Ince limit]}. \tag{3}$$

In both equations, $z = 0$ and $z = z_0$ are regular singular points with exponents $(0, 1 + B_1/z_0)$ and $(0, 1 - B_2 - B_1/z_0)$, respectively, that is, from ascending power series solutions we find

$$\lim_{z\to 0} U(z) \sim 1, \qquad \lim_{z\to 0} U(z) \sim z^{1+\frac{B_1}{z_0}}; \qquad \lim_{z\to z_0} U(z) \sim 1, \qquad \lim_{z\to z_0} U(z) \sim (z-z_0)^{1-B_2-\frac{B_1}{z_0}}: \quad \text{[CHE, RCHE]}. \tag{4}$$

In contrast, at the irregular singular point $z = \infty$ the behaviour of the solutions is different for each equation since

$$\lim_{z\to\infty} U(z) \sim e^{\pm i\omega z}\, z^{\mp i\eta-(B_2/2)} \text{for the CHE(1)}, \qquad \lim_{z\to\infty} U(z) \sim e^{\pm 2i\sqrt{qz}}\, z^{(1/4)-(B_2/2)} \text{for the RCHE(2)}, \tag{5}$$

as follow from the normal and the subnormal Thomé solutions [17] for the CHE and RCHE, respectively.

By the concepts of Ref. [7], the s-rank of the singularity at $z = \infty$ is 2 for the CHE, and 3/2 for the RCHE. However, more important is the fact that the solutions exhibit the above behaviour predicted by the normal or subnormal Thomé solutions, and fact that the Whittaker–Ince limit (3) may generate solutions to the RCHE. In effect, most of the known solutions for the RCHE [18–20] has been obtained from solutions of the CHE by means of the limit (3). On account of this, and for the sake of brevity, we restrict ourselves to integral relations among solutions of the CHE. We also do not consider kernels for double-confluent Heun equations which result by taking the Leaver limit $z_0 \to 0$ of Eqs. (1) and (2).

Integral relations, in principle, enable us to transform known solutions into solutions with different properties. However, apart from the Mathieu equation, only in rare cases this task has been accomplished successfully. One case is constituted by the solutions in series of associated Legendre functions for the Lamé equation, obtained by Erdélyi in 1948 as a transformation of solutions in Fourier–Jacobi series [21]; however, as far we are aware, his solutions have not been extended for the general Heun equation (of which Lamé equation is a particular case). Another example is an expansion in series of irregular confluent hypergeometric functions for the CHE, which was obtained by Leaver in 1985 as an integral transformation of a power-series solution [9]: the transformation was constructed for $\eta = \pm i(B_2/2 - 1)$ and, then, the result was extended for arbitrary η.

To establish integral relations for solutions the CHE it is necessary to get appropriate integral kernels. To this end, in Section 2 we proceed as in case of the general Heun equation [1]. In other words, firstly we insert into the integral connecting two solutions a weight function $w(z,t)$ which allows to write the CHE and the equation for its kernels in terms of differential operators functionally identical (respecting z and t). In this manner, by examining each variable substitution which leaves invariant the form of the CHE (one variable, z) we find prescriptions for the variables transformations which preserve the form of the equation for the kernels (two variables, z and t). By using these substitutions, we may systematically convert a given (initial) kernel into new kernels. As initial kernels we use the ones obtained as limits of kernels of the general Heun equation [1], adapting them to the form (1) for the CHE.

In Section 3 we find integral relations which transform the Jaffé power-series solutions [22] into known expansions in series of irregular confluent hypergeometric functions, including the aforementioned solution given by Leaver. Similarly, the power-series solutions of Baber and Hassé [23] are transformed into known expansions in series of regular confluent hypergeometric functions. We also consider non-integral transformations (involving only substitutions of variables) which do not modify the type of series: they transform, for example, a power-series solution into another power-series solution, and an expansion in series of special functions into another expansion in series special functions. In contrast, by applying an integral transformation on an asymptotic (Thomé) solution, in Section 4 we obtain a new solution in series of irregular confluent hypergeometric functions for the spheroidal equation. That solution is extended to any CHE (not just the spheroidal equation). Then, by substitutions of variables (non-integral transformations) we obtain a group of solutions for the CHE; we show that these solutions afford bounded and convergent solutions to the radial part of the Schrödinger equation for an electron in the field of two Coulomb centres [8] (the two-centre problem). In Section 5 we present concluding remarks and mention open issues, while in Appendix A we give some formulas concerning special functions, and in Appendix B we discuss asymptotic solutions for the CHE.

2. Kernels for the confluent Heun equation

In this section we regard kernels for the CHE (1). In particular,