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On the Schrödinger equations of rotating harmonic, three-dimensional and doubly anharmonic oscillators and a class of confinement potentials in connection with the biconfluent Heun differential equation

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Abstract. The Schrödinger equations of rotating harmonic, three-dimensional and doubly anharmonic oscillators and a class of confinement potentials are examined simultaneously with the biconfluent Heun equation. The eigenvalue problems lead us to compute a transcendent constant function of the corresponding physical parameters.

1. Introduction

It is well known that the eigenvalue problems are often very difficult to solve. This is true in the so-called cases of rotating harmonic [1], three-dimensional [2] and doubly anharmonic [3] oscillators and a class of confinement potentials [2].

In these four cases we get radial Schrödinger equations. Several methods are used to solve these equations with the help of numerical techniques.

We intend to investigate in this paper these four radial Schrödinger equations simultaneously. These equations can in fact be expressed in the canonical form of the biconfluent Heun differential equation (BCH) [4]. This linear differential equation, which has one regular singularity at the origin and one irregular singularity at $+\infty$ of fourth species [4], is characterised in the Ince [5] classification by the formula $[0, 1, 1_4]$. We intend to examine the possibility of quasi-polynomial solutions and to point out how the eigenvalue problem comes to find values of a transcendent expression depending only on the parameters of the corresponding differential equation. This problem is strictly connected with the so-called 'connection coefficients' problem [6] which, to our knowledge, in this case of non-Fuchsian-type equations is not entirely solved, particularly when the irregular singularity is at $+\infty$.

In a previous paper we have also shown how the Schrödinger equation corresponding to the interaction potential [7]

$$V(x) = x^2 + (\lambda x^2/(1+gx^2))$$

can be solved using the confluent Heun equation formalism.

2. Radial Schrödinger equations and the corresponding biconfluent Heun equations

2.1. Schrödinger equations

2.1.1. Radial Schrödinger equation for the harmonic oscillator [1].

$$F''+\left(\frac{\lambda_m+\frac{1}{2}}{\alpha_m}-\frac{(r-1)^2}{4\alpha_m^2}-\frac{l_m(l_m+1)}{r^2}\right)F=0 \tag{1}$$

where $0\leqslant r<\infty$, λ_m is the eigenvalue, l_m is the rotational quantum number and $\alpha_m>0$ is a coupling parameter.

Equation (1) is of the form

$$F''+[A_0+A_1r+A_2r^2+(A_3/r^2)]F=0. \tag{2}$$

Following Masson [1], let

$$F=r^{l_m+1}\exp[-(r-1)^2/2\alpha_m]\chi(r). \tag{3}$$

We obtain

$$\chi''+\left(\frac{2l_m+2}{r}-\frac{(r-1)}{\alpha_m}\right)\chi'+\left(\frac{\lambda_m-l_m-1}{\alpha_m}+\frac{l_m+1}{\alpha_m r}\right)\chi=0. \tag{4}$$

With the substitution

$$r=\sqrt{2\alpha}\,\rho \tag{5}$$

equation (4) becomes

$$\rho\chi''+[(2l_m+2)+(2/\alpha_m)^{1/2}\rho-2\rho^2]\chi'$$
$$+[(2/\alpha_m)^{1/2}(l_m+1)+2(\lambda_m-l_m-1)\rho]\chi=0. \tag{6}$$

2.1.2. Radial Schrödinger equation of a three-dimensional anharmonic oscillator [2].

$$y''+[E-(\nu/r^2)-\mu r^2-\lambda r^4-\eta r^6]y=0 \tag{7}$$

where $\nu=l(l+1)$, $\mu>0$, $\eta>0$ and E is the energy.

With the transformations

$$z=(\eta/4)^{1/4}r^2 \qquad y=z^{1/4}Y(z)$$

equation (7) becomes

$$z^2Y''+zY'+(B_0+B_1z+B_2z^2+B_3z^3-z^4)Y=0 \tag{8}$$

where

$$\alpha_1=(\eta/4)^{1/4}$$
$$B_0=-\tfrac{1}{4}(\tfrac{1}{4}+\nu) \qquad B_1=E/4\alpha_1$$
$$B_2=-(\mu/4\alpha_1^2) \qquad B_3=-(\lambda/4\alpha_1^3).$$

If one requires solutions in the form

$$Y(z)=z^{-\rho_1}\exp(-az-\tfrac{1}{2}z^2)\varphi(z)$$

with

$$\rho_1=-\tfrac{1}{2}(\tfrac{1}{4}+\nu)^{1/2} \qquad a=\lambda/8\alpha_1^3$$

equation (8) becomes

$$z\varphi''+[(1+\alpha)-\beta z-2z^2]\varphi'+\{(\gamma-\alpha-2)z-\tfrac{1}{2}[\delta+\beta(1+\alpha)]\}\varphi=0 \tag{9}$$

where

$$\alpha = (\tfrac{1}{4} + \nu)^{1/2} \qquad \delta = -E/2\alpha_1$$

$$\beta = \lambda/4\alpha_1^3 \qquad \gamma = \frac{1}{4\alpha_1^2}\left(\frac{\lambda^2}{16\alpha_1^4} - \mu\right).$$

2.1.3. Radial equation of a class of confinement potentials. The confinement potential has the form [3]

$$V(r) = -(a/r) + br + cr^2 \qquad c > 0.$$

The Schrödinger equation is

$$R'' + \left[\left(\frac{2\mu}{h^2}\right)\left(E + \frac{a}{r} - br - cr^2\right) - \frac{l(l+1)}{r^2}\right]R = 0 \tag{10}$$

with E being the energy.

This equation is of the form

$$R'' + \left(C_0 + C_1 r + C_2 r^2 + \frac{C_3}{r} + \frac{C_4}{r^2}\right)R = 0. \tag{11}$$

Seeking solutions in the form

$$R(r) = r^{l+1}\exp(-\tfrac{1}{2}r^2\alpha_F - \beta_F r)g(r)$$

we obtain the following differential equation for $g(r)$:

$$g'' + 2\left(\frac{l+1}{r} - \alpha_F r - \beta_F\right)g' + \left(\varepsilon_F - (2l+3)\alpha_F + \frac{[a - 2\beta_F(l+1)}{r}\right)g = 0. \tag{12}$$

Putting $\rho = \sqrt{\alpha_F}\, r$ equation (12) becomes

$$\rho g'' + 2g'\left((l+1)\sqrt{\alpha_F} - \rho^2 - \frac{\beta_F}{\sqrt{\alpha_F}}\rho\right) + \left[\left(\frac{\varepsilon_F}{\alpha_F} - (2l+3)\right)\rho + \frac{[a - 2\beta_F(l+1)]}{\sqrt{\alpha_F}}\right]g = 0 \tag{13}$$

with

$$\alpha_F = [(2\mu/h^2)c]^{1/2} \qquad \beta_F = (2\mu/h^2)^{1/2}(b/c^{1/2}) \qquad \varepsilon_F = \beta_F^2 + (2\mu/h^2)E.$$

2.1.4. Schrödinger equation for the doubly anharmonic oscillator. $V(x) = \mu x_1^2 + \lambda x_1^4 + \eta x_1^6$, with $\eta > 0$ [3]. The corresponding Schrödinger equation is

$$y'' + (E - \mu x_1^2 - \lambda x_1^4 - \eta x_1^6)y = 0 \tag{14}$$

where $-\infty < x_1 < +\infty$.

Equation (14) leads to a 'radial' equation with the transformation

$$y(x_1) = \exp(-\tfrac{1}{4}\alpha_c x_1^4 + \tfrac{1}{2}\beta_c x_1^2)\varphi(x_1)$$

where

$$\alpha_c = \sqrt{\eta} \qquad \beta_c = -\tfrac{1}{2}\lambda/\sqrt{\eta}.$$

Let $u = (\alpha_c/2)^{1/2}x_1^2$, then equation (14) becomes

$$u\varphi'' + [-2u^2 + \beta_c(2/\alpha_c)^{1/2}u + \tfrac{1}{2}]\varphi'$$
$$+ \tfrac{1}{4}(2/\alpha_c)^{1/2}[(\beta_c^2 - 3\alpha_c - \mu)(2/\alpha_c)^{1/2}u + (E + \beta_c)]\varphi = 0$$

and finally with

$$\varphi = u^{1/2}\psi$$

$$u\psi'' + [-2u^2 + \beta_c(2/\alpha_c)^{1/2}u + \tfrac{3}{2}]\psi' + \{[(1/2\alpha_c)(\beta_c^2 - 3\alpha_c - \mu) - 1]u + \tfrac{1}{4}(2/\alpha_c)^{1/2}(E + 3\beta_c)\}\psi = 0. \qquad (15)$$

2.2. Canonical form of equations (6), (9), (13), and (15)

Equations (6), (9), (13) and (15) are of the form

$$xy'' + (1 + \alpha - \beta x - 2x^2)y' + \{(\gamma - \alpha - 2)x - \tfrac{1}{2}[\delta + \beta(1+\alpha)]\}y = 0. \qquad (16)$$

For equation (6)

$$x = r/\sqrt{2\alpha} \qquad \alpha = 2l_m + 1 \qquad \gamma = 1 + 2\lambda_m$$
$$\beta = -(2/\alpha_m)^{1/2} \qquad \delta = 0. \qquad (17)$$

For equation (9)

$$x = (\eta/4)^{1/4}r^2 \qquad \alpha = (\tfrac{1}{4} + \nu)^{1/2} \qquad \gamma = \frac{1}{2\sqrt{\eta}}\left(\frac{\lambda^2}{4\eta} - \mu\right)$$
$$\beta = \frac{\lambda}{4}\left(\frac{4}{\eta}\right)^{3/4} \qquad \delta = -\frac{E}{2}\left(\frac{4}{\eta}\right)^{1/4}. \qquad (18)$$

For equation (13)

$$x = \sqrt{\alpha_F}\, r \qquad \alpha = 2(l+1)\sqrt{\alpha_F} - 1 \qquad \gamma = \frac{\varepsilon_F}{\alpha_F} + 2(l+1)(\sqrt{\alpha_F} - 1)$$
$$\beta = \frac{2\beta_F}{\sqrt{\alpha_F}} \qquad \delta = \frac{2}{\sqrt{\alpha_F}}[-a + 2\beta_F(l+1)(1 - \sqrt{\alpha_F})]. \qquad (19)$$

We suppose $\alpha > 0$. If $\alpha < 0$, we take at the origin the solutions of (16) in the form

$$y(\alpha, \beta, \gamma, \delta; x) = x^{-\alpha}N(-\alpha, \beta, \gamma, \delta; x).$$

For equation (15)

$$x = (\tfrac{1}{2}\alpha_c)^{1/2}x_1^2 \qquad \alpha = \tfrac{1}{2} \qquad \gamma = \frac{1}{2\alpha_c}(\beta_c^2 - 3\alpha_c - \mu) + \tfrac{3}{2}$$
$$\beta = -\beta_c(2/\alpha_c)^{1/2} \qquad \delta = -\frac{E}{\sqrt{2\alpha_c}}. \qquad (20)$$

Equation (16) is the canonical form of the BCH equation $[0, 1, 1_4]$.

When α is not a negative whole number, at the origin, the suitable solution is defined by [4]

$$N(\alpha, \beta, \gamma, \delta; r) = \sum_{\nu=0}^{\infty} \frac{A_\nu(\alpha, \beta, \gamma, \delta)}{(1+\alpha)_\nu \nu!} r^\nu \qquad (21)$$

with

$$A_0 = 1 \qquad A_1 = \tfrac{1}{2}[\delta + \beta(1+\alpha)]$$

and the following recurrence relation for $A_\nu (\nu \geq 1)$,

$$A_{\nu+2} - A_{\nu+1}\{(\nu+1)\beta + \tfrac{1}{2}[\delta + \beta(1+\alpha)]\} + A_\nu(\gamma - 2 - \alpha - 2\nu)(\nu+1)(\nu+1-\alpha) = 0 \quad (22)$$

where

$$(\alpha)_\nu = \frac{\Gamma(\alpha+\nu)}{\Gamma(\alpha)} = \begin{cases} \alpha(\alpha+1)\dots(\alpha+\nu-1) & \nu = 1, 2, 3, \dots \\ 1 & \nu = 0. \end{cases}$$

Taking account of these results, we obtain the solutions of equations (6), (9), (13) and (15) in the form

$$F(r) = r^{l_m+1} \exp[-(r-1)^2/2\alpha_m] N[\alpha, \beta, \gamma, \delta; r/\sqrt{2\alpha_m}] \quad (23)$$

where $\alpha, \beta, \gamma, \delta$ are defined by (17);

$$y(r) = r^{(1/2)-2\rho_l} \exp[-a(\tfrac{1}{4}\eta)^{1/4} r^2 - \tfrac{1}{2}(\tfrac{1}{4}\eta)^{1/2} r^4] N[\alpha, \beta, \gamma, \delta; (\tfrac{1}{4}\eta)^{1/4} r^2] \quad (24)$$

where $\alpha, \beta, \gamma, \delta$ are defined by (18);

$$R(r) = r^{l+1} \exp(-\tfrac{1}{2} r^2 \alpha_F - r\beta_F) N[\alpha, \beta, \gamma, \delta; \sqrt{\alpha_F}\, r] \quad (25)$$

where $\alpha, \beta, \gamma, \delta$ are defined by (19) and

$$y(x_1) = \exp(-\tfrac{1}{4}\alpha_c x_1^4 + \tfrac{1}{2}\beta_c x_1^2) N[\alpha, \beta, \gamma, \delta; (\tfrac{1}{2}\alpha_c)^{1/2} x_1^2] \quad (26)$$

where $\alpha, \beta, \gamma, \delta$ are defined by (20).

3. Quasi-polynomial solutions of the four Schrödinger equations

As is well known [4], we see immediately, looking at the recurrence relations (22), that the BCH admit polynomial solutions if

$$\gamma - 2 - \alpha = 2n \qquad n = 0, 1, 2, \dots \quad (27)$$

and

$$A_{n+1} = 0. \quad (28)$$

A_{n+1} is a polynomial of degree $n+1$ in $\theta = \tfrac{1}{2}[\delta + \beta(1+\alpha)]$, whose roots are the eigenvalues corresponding to these particular solutions. The roots of these polynomials in the four examined cases are all real and different since $1+\alpha > 0$ and $\beta \in R$ [4].

For equation (6)

$$\theta = -(2/\alpha_m)^{1/2}(1+l_m). \quad (29)$$

For equation (9)

$$\theta = \frac{1}{4}\left(\frac{4}{\eta}\right)^{1/4}\left[\frac{\lambda}{2}\left(\frac{4}{\eta}\right)^{1/2}[1 + (\tfrac{1}{4}+\nu)^{1/2}] - E\right]. \quad (30)$$

For equation (13)

$$\theta = (2\beta_F - a)(1+l)/\sqrt{\alpha_F}. \quad (31)$$

For equation (15)

$$\theta = -\tfrac{1}{4}\beta_c(2/\alpha_c)^{1/2}[1 + 2(E+\beta_c)]. \quad (32)$$

The explicit calculation of these roots cannot be performed without the help of numerical techniques as soon as n is increasing.

The physically suitable eigenfunctions corresponding to these eigenvalues are quasi-polynomial solutions which, in the four cases, may be put in the form

$$Z(r) = r^q \exp(dr + er^2 - f^2 r^4) N[\alpha, \beta, (\alpha + 2n + 2), \delta_p^n; kr] \tag{33}$$

where N is the polynomial solution of the canonical BCH equation. In cases (23) and (25) $f^2 = 0$ and $e < 0$. We note that Flessas [2] has given the polynomial condition (27) when $n = 0$.

4. Asymptotic behaviour of the solution

The asymptotic expansions of the solutions are determined by that of the $N(\alpha, \beta, \gamma, \delta; x)$ function, defined at $n = 0$. The problem is also that of the connection between solutions defined at $x = 0$ and solutions at x, ∞. One requires that the N solutions defined at $n = 0$ vanish in the limit $x \to \infty$.

Without going into all the details of proofs we intend to use some results obtained by Decarreau *et al* [4] and Batola [8] in connection with the BCH equation. The results allow us to determine the values of a parameter of the equation, δ, as functions of the three others and consequently permit us to calculate, as a rule, the eigenvalues corresponding to these non-polynomial solutions.

The solutions concerned are thus solutions of polynomial order.

The solution of the canonical equation (16), the function $N(\alpha, \beta, \gamma, \delta; x)$, at x, ∞ admits the following asymptotical behaviour [8]:

$$N(\alpha, \beta, \gamma, \delta; x) \underset{x \to \infty}{\sim} K_2(\alpha, \beta, \gamma, \delta) \exp(\beta x + x^2) x^{-(\gamma + \alpha + 2)/2}. \tag{34}$$

The constant K_2 is a non-elementary constant, defined by

$$K_2(\alpha, \beta, \gamma, \delta) = \frac{\Gamma(1+\alpha)}{\Gamma\frac{1}{2}(\alpha - \gamma)\Gamma(1 + \frac{1}{2}(\alpha + \gamma))} J(\tfrac{1}{2}(\alpha + \gamma), \beta, \tfrac{1}{2}(3\alpha - \gamma), \delta + \beta\tfrac{1}{2}(\gamma - \alpha)) \tag{35}$$

where J is defined by

$$J(\lambda, \mu, \nu, \sigma) = \int_0^\infty x^\lambda \exp(-\mu x - x^2) N(\lambda, \mu, \nu, \sigma; x)\, dx. \tag{36}$$

This integral is defined when $\operatorname{Re} \lambda > 0$ and $\operatorname{Re}(\nu - \lambda) > 0$. Here the condition becomes $\alpha > |\gamma|$; in the four cases, we have the following conditions.

For equation (6), taking (17) into account,

$$2l_m + 1 > |1 + 2\lambda_m|.$$

For equation (9), taking (18) into account,

$$(\tfrac{1}{4} + \nu)^{1/2} > \frac{1}{2\sqrt{\eta}} \left| \frac{\lambda^2}{4\eta} - \mu \right|.$$

For equation (13), taking (19) into account,

$$2(l+1)\sqrt{\alpha_F} - 1 > |(\varepsilon_F/\alpha_F) + 2(l+1)(\sqrt{\alpha_F} - 1)|.$$

For equation (15), taking (20) into account,

$$|(1/\alpha_c)(\beta_c^2 - 3\alpha_c - \mu) + 3| < 1.$$

The eigenvalues corresponding to solutions of the form (33) with the boundary condition $Z(r) = 0$ at r, ∞ are the roots $\sigma(\alpha, \beta, \gamma)$ of the transcendent equation [8]:

$$J[\lambda, \mu, \nu, \sigma(\lambda, \mu, \nu)] = 0. \tag{37}$$

This difficult problem can be reduced with the help of the Faxen integral [9]:

$$\Gamma^x(\alpha, \lambda; x) = \int_0^\infty t^{x-1} \exp(-\lambda t^\alpha - t)\, \mathrm{d}t.$$

If $\lambda = 0$, Γ^x becomes the Euler Γ function and the constant $J(\lambda, \mu, \nu, \sigma)$ can be usefully written as

$$J(\lambda, \mu, \nu, \sigma) = \frac{1}{2} \sum_{k=0}^{\infty} \frac{A_k(\lambda, \mu, \nu, \sigma)}{(1+\lambda)_k k!} \Gamma^x(\tfrac{1}{2}, \mu; \tfrac{1}{2}(\lambda + k + 1)).$$

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