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Rodrigues solution of the Dirac equation for fields obtained from the master function formalism

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Abstract
We show that the radial Dirac equation with constant electrostatic potential and for a large class of the field potentials which are obtained from the master function formalism can be solved by the Rodrigues representation of the orthogonal polynomials. We also show that the Schrödinger-like differential equation obtained from the Dirac equation satisfies the supersymmetry and shape invariant conditions in non-relativistic quantum mechanics. The relativistic energy spectrum for a given potential function is calculated from its corresponding non-relativistic energy spectrum.

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1. Introduction

Exact solutions of the wave equations are very important because an understanding of physics can only be brought about through these solutions. Moreover, these solutions are valuable for testing and improving the numerical methods introduced to solve problems. Because they have attracted much interest, various techniques such as point canonical transformations [1–3], Lie algebraic techniques [4, 5], the factorization method [6], supersymmetric quantum mechanics and shape invariance techniques [7–9] have been developed to increase the number of exactly solvable potentials. Also, the solutions of the Dirac equation with physical potentials such as the harmonic oscillator [10–12], Mörse [13, 14] and the Coulomb [15–19] potentials have been considered as a relativistic extension of these potentials. So, there are a number of investigations in the literature that show how the methods used to obtain analytical solutions of the Schrödinger equation can be extended to the Dirac case [20–23]. On the other hand, in [24–26], the authors have shown that by choosing a polynomial of a degree not exceeding two, called the master function, one can factorize the associated differential equation into the product of raising and lowering operators. In fact, they have shown that almost all solvable potentials with supersymmetry and the shape invariance property are obtainable from the master function by an algebraic method.

Now, in the present work, for the radial Dirac equation, we apply the master function formalism and obtain the field potentials on the basis of superpotentials given in [24–26]. We then calculate the relativistic energy in correspondence to the non-relativistic energy. In fact, we show that for a constant electrostatic potential, we can derive a second-order differential equation which can be factorized as the product of two first-order differential operators and so the upper spinor wave function can be expressed in terms of the Rodrigues representation of the orthogonal polynomials. In other words, for a given master function, we obtain a potential function for the radial Dirac equation with constant electrostatic potential such that the relativistic energy is calculated from the non-relativistic energy spectrum and the upper spinor wave function is easily obtained from the Rodrigues representation. The lower spinor wave function is also obtained from the upper component.

This paper is organized as follows. In section 2, we review the master function formalism and factorize the general associated differential equation which has shape invariant symmetry. In section 3, we will briefly study the approach that is proposed to solve the Dirac equation with a given interaction potential in the vector coupling scheme and, by performing some calculations, we derive a second-order differential equation with shape invariant symmetry in the framework of the master function formalism for the radial Dirac equation. We complete our calculation with an example in section 4. In section 5, the paper ends with the conclusion.

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2. The master function formalism: the Rodrigues polynomials and superpotential

In the framework of the master function formalism, the general form of the associated second-order differential equation in mathematical physics is written as [24–26]

$$A(x)\psi''_{n,m}(x)+\frac{(A(x)W(x))'}{W(x)}\psi'_{n,m}(x)+\left[-\frac{1}{2}(n^2+n-m^2)A''(x)+(m-n)\left(\frac{A(x)W'(x)}{W(x)}\right)'-\frac{m^2}{4}\frac{(A'(x))^2}{A(x)}-\frac{m}{2}\frac{A'(x)W'(x)}{W(x)}\right]\psi_{n,m}(x)=0, \quad (2.1)$$

where $A(x)$ as the master function is a polynomial of order up to two and $W(x)$ as the weight function is a non-negative function in the interval $[a, b]$. For a given $A(x)$, the weight function $W(x)$ is chosen such that the expression $\frac{1}{W(x)}\frac{\mathrm{d}}{\mathrm{d}x}(A(x)W(x))$ will be a first-order polynomial or a constant with the condition $A(a)W(a)=A(b)W(b)=0$. Also, for a given positive integer n, the Rodrigues solutions of the orthogonal polynomials $\psi_{n,m}(x)$ are calculated as

$$\psi_{n,m}(x)=(-1)^m A^{\frac{m}{2}}(x)\left(\frac{\mathrm{d}}{\mathrm{d}x}\right)^m\psi_n(x), \quad m=0,1,2,\ldots,n, \quad (2.2)$$

where

$$\psi_n(x)=\frac{N_n}{W(x)}\left(\frac{\mathrm{d}}{\mathrm{d}x}\right)^n(A^n(x)W(x)) \quad (2.3)$$

and N_n is a constant parameter.

One can see easily that for different choices of $A(x)$ and $W(x)$, equation (2.1) will be transformed into well-known second-order differential equations in mathematical physics such as Laguerre, Hermite, Jacobi and so on [24–26]. As an example, in order to obtain the Jacobi polynomial, we choose the master function $A(x)$ as $A(x)=(x^2-1)$. After solving the expression $\frac{1}{W(x)}\frac{\mathrm{d}}{\mathrm{d}x}((x^2-1)W(x))$, which must be a polynomial of at most degree one, we obtain the possible non-negative weight function $W(x)$ as $W(x)=(x-1)^{\lambda}(x+1)^{\gamma}$; $\lambda>-1$, $\gamma>-1$ and the condition $A(a)W(a)=A(b)W(b)=0$ also give the related interval as $x\in[-1,+1]$. The Rodrigues representation of the Jacobi polynomial, which satisfies the Jacobi differential equation, is $P_n^{(\lambda,\gamma)}\equiv\psi_n(x)=N_n(x-1)^{-\lambda}(x+1)^{-\gamma}\left(\frac{\mathrm{d}}{\mathrm{d}x}\right)^n\left((x-1)^{n+\lambda}(x+1)^{n+\gamma}\right)$.

Also, in order to obtain the Schrödinger equation, the first-order derivative in (2.1) should be eliminated; hence, by changing the variable $\frac{\mathrm{d}x}{\mathrm{d}r}=\sqrt{A(x)}$ and introducing the following new function,

$$\Phi_{n,m}(r)=A^{1/4}(x)W^{1/2}(x)\psi_{n,m}(x), \quad (2.4)$$

we have

$$-\frac{\mathrm{d}^2}{\mathrm{d}r^2}\Phi_{n,m}(r)+V_m(x(r))\Phi_{n,m}(r)=E(n,m)\Phi_{n,m}(r), \quad (2.5)$$

where

$$V_m(x)=-\frac{1}{2}\left(\frac{A(x)W'(x)}{W(x)}\right)'-\frac{2m-1}{4}A''(x)+\frac{1}{4A(x)}\left(\frac{A(x)W'(x)}{W(x)}\right)^2+\frac{m}{2}\frac{A'(x)W'(x)}{W(x)}+\frac{4m^2-1}{16}\frac{A'^2(x)}{A(x)}, \quad (2.6)$$

and the energy spectrum $E(n,m)$ is

$$E(n,m)=-(n-m+1)\left[\left(\frac{A(x)W'(x)}{W(x)}\right)'+\tfrac{1}{2}(n+m)A''(x)\right], \quad m=0,1,2,\ldots,n. \quad (2.7)$$

On the other hand, a pair of raising and lowering operators can be introduced as

$$B_{\pm}(m)=\pm\frac{\mathrm{d}}{\mathrm{d}r}+W_m(x(r)), \quad (2.8)$$

where the superpotential $W_m(x(r))$ is expressed in terms of the master function $A(x)$ and weight function $W(x)$ as

$$W_m(x(r))=-\frac{\frac{1}{2}\left(\frac{A(x)W'(x)}{W(x)}\right)+\frac{2m-1}{4}A'(x)}{\sqrt{A(x)}}, \quad (2.9)$$

and the Schrödinger equation (2.5) can be factorized to the following form with respect to index m:

$$B_+(m)B_-(m)\Phi_{n,m}(r)=E(n,m)\Phi_{n,m}(r), \quad (2.10)$$

$$B_-(m)B_+(m)\Phi_{n,m-1}(r)=E(n,m)\Phi_{n,m-1}(r). \quad (2.11)$$

We see from these equations that the operator $B_+(m)$ raises the index m and the operator $B_-(m)$ lowers it for a given n. Also, from equation (2.7), it is clear that the energy spectrum $E(n,m)$ vanishes for $m=n+1$ and so the highest state $\Phi_{n,n}(r)$ can be obtained by solving the first-order differential equation $B_+(n+1)\Phi_{n,n}(r)=0$. Hence, we can obtain the algebraic solution of equation (2.5) by the consecutive action of the lowering operator on the highest state. By using the ladder operators (2.8) and corresponding to (2.10) and (2.11), the solvable potentials $V_m^{\pm}(r)$, as the pair of supersymmetry partner potentials, can be obtained from the superpotential (2.9) as

$$V_m^{\pm}(r)=W_m^2(r)\pm\frac{\mathrm{d}W_m(r)}{\mathrm{d}r}. \quad (2.12)$$

According to [9], if the pair of supersymmetry partners become similar in shape and differ only in parameters, then we say that they are shape invariant and so the quantum system is a solvable model and its solution can be obtained by an algebraic method.

Hence, in the next section, we try to construct the conditions of (2.12) for solvable potentials of a Schrödinger-like equation which is derived from the radial Dirac equation for the upper spinor component. In fact, we see that for the constant electrostatic potential of the radial Dirac equation, the field of the potential with spherical symmetry can be written in terms of the superpotential (2.9). Moreover, we obtain the upper spinor field in terms of the Rodrigues representation of the orthogonal polynomials in terms of the master function formalism.

3. Superpotential as a potential function for the Dirac equation with constant electrostatic potential

In atomic units ($m = e = \hbar = 1$) and taking the speed of light $c = \alpha^{-1}$, the Hamiltonian for a Dirac spinor in the four-component electromagnetic potential $(A_0, \vec{A})$ can be written as

$$H = \begin{pmatrix} 1+\alpha A_0 & -\mathrm{i}\alpha\vec{\sigma}\cdot\nabla+\alpha\vec{\sigma}\cdot\vec{A} \\ -\mathrm{i}\alpha\vec{\sigma}\cdot\nabla+\alpha\vec{\sigma}\cdot\vec{A} & -1+\alpha A_0 \end{pmatrix}, \quad (3.1)$$

where α is the fine structure constant and $\vec{\sigma}$ are the three 2×2 Pauli matrices [13]. We consider the form of electromagnetic potential for static charge distribution with spherical symmetry as

$$(A_0, \vec{A}) = (\alpha\upsilon(r), \hat{r}\omega(r)), \quad (3.2)$$

where $\hat{r}$ is the radial unit vector, $\upsilon(r)$ is the electrostatic potential and $\omega(r)$ is a field that does not contribute to the magnetic field. By substituting the two off-diagonal terms $\alpha\vec{\sigma}\cdot\vec{A}$ by $\pm\mathrm{i}\alpha\vec{\sigma}\cdot\vec{A}$ in equation (3.1), the Hamiltonian leads to the following two-component radial Dirac equation [15]:

$$\begin{pmatrix} 1+\alpha^2\upsilon(r) & \alpha\left(\frac{k}{r}+\omega(r)-\frac{\mathrm{d}}{\mathrm{d}r}\right) \\ \alpha\left(\frac{k}{r}+\omega(r)+\frac{\mathrm{d}}{\mathrm{d}r}\right) & -1+\alpha^2\upsilon(r) \end{pmatrix}\begin{pmatrix}\Phi(r)\\ \Theta(r)\end{pmatrix} = \varepsilon\begin{pmatrix}\Phi(r)\\ \Theta(r)\end{pmatrix}, \quad (3.3)$$

where ε is the relativistic energy and k is the spin–orbit coupling parameter defined as $k = \pm(j+\frac{1}{2})$ for $l = j\pm\frac{1}{2}$. Equation (3.3) gives two coupled first-order differential equations for the radial spinor components where, after some calculation, we obtain the following equation:

$$-\frac{\mathrm{d}^2\Phi(r)}{\mathrm{d}r^2} + \left[\left(\frac{k}{r}+\omega(r)\right)^2 - \left(\frac{\mathrm{d}\omega(r)}{\mathrm{d}r}-\frac{k}{r^2}\right) - \left(\frac{(\alpha^2\upsilon(r)-\varepsilon)^2-1}{\alpha^2}\right)\right]\Phi(r) - \left(\alpha\frac{\mathrm{d}\upsilon(r)}{\mathrm{d}r}\right)\Theta(r) = 0. \quad (3.4)$$

Now, if we assume that $\frac{\mathrm{d}\upsilon}{\mathrm{d}r} = 0$, i.e. the electrostatic potential is considered as a constant parameter such as η, then the above equation will transform to the following Schrödinger-like equation:

$$-\frac{\mathrm{d}^2\Phi(r)}{\mathrm{d}r^2} + \left[\left(\frac{k}{r}+\omega(r)\right)^2 - \left(\frac{\mathrm{d}\omega}{\mathrm{d}r}-\frac{k}{r^2}\right) - \left(\frac{(\alpha^2\eta-\varepsilon)^2-1}{\alpha^2}\right)\right]\Phi(r) = 0. \quad (3.5)$$

In the above equation, it is easy to see that the potential function can be written as the Riccati equation; that is, it will have the condition of equation (2.12). Hence, if we consider the function $\omega(r)+\frac{k}{r}$ as the superpotential, then we can relate the superpotential of the master function formalism to the potential function of the radial Dirac equation as

$$\omega(r) = W_m(r) - \frac{k}{r}. \quad (3.6)$$

Indeed, $\omega(r)$ will be related to the superpotential (2.9) and so we can obtain the potential functions in terms of the master function $A(x)$ and weight function $W(x)$ which are given in [24–26]. On the other hand, the relativistic energy spectrum can be obtained by comparing of equation (3.5) with equation (2.5) as

$$\varepsilon_n = \alpha^2\eta \mp \sqrt{\alpha^2 E(n,m)+1}. \quad (3.7)$$

Therefore, choosing various functions of $A(x)$ and $W(x)$, we specify the superpotential and non-relativistic energy spectrum according to equations (2.9) and (2.7), and therefore, substituting them into equations (3.6) and (3.7), we determine $\omega(r)$, which is satisfied in the Dirac equation. By this procedure, in fact, we can obtain a large number of the potential functions in which the relativistic energy spectrum can be easily obtained from the non-relativistic energy spectrum (3.7), and the upper spinor field can be expressed in terms of Rodrigues solution of the orthogonal polynomials (2.4) and (2.2). The lower spinor wave function can also be calculated from the upper spinor by one of the first-order differential equations which are given by (3.3). In the next section, as an example, we choose $A(x) = x$ and obtain $\omega(r)$ from the above procedure in some detail. Moreover, in table 1, we list other functions of $\omega(r)$ corresponding to different choices of $A(x)$.

4. Three-dimensional (3D) oscillator superpotential as an example

Let $A(x) = x$; taking into account that $(1/W(x))\frac{\mathrm{d}}{\mathrm{d}x}(xW(x))$ is a polynomial of a degree not exceeding one, we obtain the weight function $W(x)$ as

$$W(x) = x^{\lambda}\mathrm{e}^{-\gamma x}, \quad x = \frac{r^2}{4}, \quad 0 < x < +\infty, \quad (4.1)$$

where $\lambda > -1$ and $\gamma > 0$. Substituting the master and weight functions into equations (2.9) and (2.7), we obtain the superpotential and non-relativistic energy as

$$W_m(r) = -(\lambda+m-\tfrac{1}{2})\tfrac{1}{r} + \tfrac{\gamma}{4}r, \quad E(n,m) = \gamma(n-m+1), \quad m = 0, 1, 2, \ldots, n. \quad (4.2)$$

Using these expressions in (3.6) and (3.7), we obtain the field potential and relativistic energy as

$$\omega(r) = -(\lambda+m+k-\tfrac{1}{2})\tfrac{1}{r} + \tfrac{\gamma}{4}r, \quad (4.3)$$

$$\varepsilon_n = \alpha^2\eta \mp \left(\alpha^2\gamma(n-m+1)+1\right)^{1/2}, \quad m = 0, 1, 2, \ldots, n. \quad (4.4)$$

Substituting (4.3) and (4.4) into (3.5), the differential equation for the upper spinor $\Phi_{n,m}(r)$ is written as

$$-\frac{\mathrm{d}^2}{\mathrm{d}r^2}\Phi_{n,m}(r) + \left[\frac{\gamma^2}{16}r^2 + (\lambda+m-\tfrac{1}{2})(\lambda+m-\tfrac{3}{2})\tfrac{1}{r^2} - \frac{\gamma}{2}(\lambda+m)\right]\Phi_{n,m}(r) = \gamma(n-m+1)\Phi_{n,m}(r). \quad (4.5)$$

Table 1. List of the field potentials $\omega(r)$, the relativistic energy ε_n and the upper spinor wavefunctions $\Phi_{n,m}(x)$ that can be obtained for every choice of the master function $A(x)$ and weight function $W(x)$.

$A(x)$ / $x(r)$	$W(x)$ / Interval of x	Field function $\omega(r)$ / Relativistic energy ε_n	$\Phi_{n,m}(x)\cdot(N(-1)^m)^{-1}$
1	$e^{-\frac{1}{2}\gamma x^2}$	$\frac{1}{2}\gamma r-\lambda-\frac{k}{r}$	$e^{\frac{1}{4}\gamma x^2}\left(\frac{d}{dx}\right)^{n-m}(e^{-\frac{1}{2}\gamma x^2})$
$x=r-\frac{2\lambda}{\gamma}$	$-\infty<x<+\infty$	$\alpha^2\eta\mp\left[\alpha^2\gamma(n-m+1)+1\right]^{1/2}$	
x	$x^{\lambda}e^{-\gamma x}$	$\frac{1}{4}\gamma r-\frac{A}{r}-\frac{k}{r}$	$x^{-\frac{A}{2}}e^{\frac{\gamma x}{2}}\left(\frac{d}{dx}\right)^{n-m}[x^{\lambda+n}e^{-\gamma x}]$
	$\lambda>-1$	$A=m+\lambda-\frac{1}{2}$	
	$\gamma>0$		
$x=\frac{1}{4}r^2$	$0<x<+\infty$	$\alpha^2\eta\mp\left[\alpha^2\gamma(n-m+1)+1\right]^{1/2}$	
x^2	$x^{\lambda}e^{-\frac{\gamma}{x}}$	$-\frac{\gamma}{2}e^{-r}-\frac{k}{r}-A$	
	$\lambda<-2$	$A=m+\frac{\lambda}{2}-\frac{1}{2}$	$x^{-A}e^{\frac{\gamma}{2x}}\left(\frac{d}{dx}\right)^{n-m}[x^{2n+\lambda}e^{-\frac{\gamma}{x}}]$
	$\gamma>0$		
$x=e^r$	$0<x<+\infty$	$\alpha^2\eta\mp\left[-\alpha^2(\lambda+n+m)(n-m+1)+1\right]^{1/2}$	
$1+x^2$	$(1+x^2)^{\lambda}e^{\gamma\arctan x}$	$-A\tanh r-\frac{\gamma}{2\cosh r}-\frac{k}{r}$	
	$\lambda<-1$	$A=m+\lambda-\frac{1}{2}$	$(1+x^2)^{-\frac{A}{2}}e^{-\frac{\gamma}{2}\arctan x}\times\left(\frac{d}{dx}\right)^{n-m}[(1+x^2)^{\lambda+n}e^{\gamma\arctan x}]$
	$-\infty<\gamma<+\infty$		
$x=\sinh r$	$-\infty<x<+\infty$	$\alpha^2\eta\mp\left[-\alpha^2(2\lambda+n+m)(n-m+1)+1\right]^{1/2}$	
$x(1-x)$	$x^{\lambda}(1-x)^{\gamma}$	$A\tan r-B\sec r-\frac{k}{r}$	
	$\lambda,\gamma>-1$	$A=\frac{\lambda+\gamma+2m-1}{2}$	$x^{\frac{B-A}{2}}(1-x)^{-\frac{A+B}{2}}\times\left(\frac{d}{dx}\right)^{n-m}[x^{n+\lambda}(1-x)^{n+\gamma}]$
		$B=\frac{\lambda-\gamma}{2}$	
$x=\frac{1+\sin r}{2}$	$0<x<+1$	$\alpha^2\eta\mp\left[\alpha^2(\lambda+\gamma+n+m)(n-m+1)+1\right]^{1/2}$	
x^2-1	$(x-1)^{\lambda}(x+1)^{\gamma}$	$-A\coth r+\frac{B}{\sinh r}-\frac{k}{r}$	
	$\lambda,\gamma>-1$	$A=\frac{\lambda+\gamma+2m-1}{2}$	$(x-1)^{\frac{B-A}{2}}(x+1)^{-\frac{A+B}{2}}\times\left(\frac{d}{dx}\right)^{n-m}[(x-1)^{n+\lambda}(x+1)^{n+\gamma}]$
		$B=\frac{\gamma-\lambda}{2}$	
$x=\cosh r$	$-1<x<+1$	$\alpha^2\eta\mp\left[-\alpha^2(\lambda+\gamma+n+m)(n-m+1)+1\right]^{1/2}$	
$4x^2-1$	$(2x-1)^{\lambda}(2x+1)^{\gamma}$	$-A\tanh r+B\coth r-\frac{k}{r}$	
	$\lambda,\gamma>-1$	$A=\gamma+m-\frac{1}{2}$	$(2x-1)^{-\frac{B}{2}}(2x+1)^{-\frac{A}{2}}\times\left(\frac{d}{dx}\right)^{n-m}[(2x-1)^{\lambda+n}(2x+1)^{\gamma+n}]$
		$B=-(\lambda+m-\frac{1}{2})$	
$x=\frac{1}{2}\cosh 2r$	$-\frac{1}{2}<x<+\frac{1}{2}$	$\alpha^2\eta\mp\left[-4\alpha^2(\lambda+\gamma+n+m)(n-m+1)+1\right]^{1/2}$	

We have thus obtained the Schrödinger equation for the 3D oscillator potential. It is easy to see that the potential is shape invariant and can be represented as an operator product of raising and lowering operators as follows:

$$B_{+}(m)B_{-}(m)\Phi_{n,m}(r)=\gamma(n-m+1)\Phi_{n,m}(r), \tag{4.6}$$

$$B_{-}(m)B_{+}(m)\Phi_{n,m-1}(r)=\gamma(n-m+1)\Phi_{n,m-1}(r), \tag{4.7}$$

where

$$B_{\pm}(m)=\pm\frac{\mathrm{d}}{\mathrm{d}r}+\left[\frac{\gamma}{4}r-(\lambda+m-\tfrac{1}{2})\tfrac{1}{r}\right]. \tag{4.8}$$

Introducing a new function according to (2.4) as

$$\Phi_{n,m}(r)=x^{(\frac{\lambda}{2}+\frac{1}{4})}\exp\left(-\frac{\gamma}{2}x\right)\psi_{n,m}(x) \tag{4.9}$$

and changing the variable $\frac{\mathrm{d}x}{\mathrm{d}r}=\sqrt{x}$, the differential equation (4.5) can be transformed into the following associated differential equation:

$$x\frac{\mathrm{d}^2}{\mathrm{d}x^2}\psi_{n,m}(x)+[(\lambda+\tfrac{1}{2})-\gamma x]\tfrac{\mathrm{d}}{\mathrm{d}x}\psi_{n,m}(x)+\Big[\gamma(n-m+\tfrac{1}{2})-\frac{\lambda\gamma}{2}-\frac{(m-1)(2\lambda+1)}{4}\,x^{\frac{-1}{2}}\Big]\psi_{n,m}(x)=0, \tag{4.10}$$

where $\psi_{n,m}(x)$ is defined based on (2.2) as

$$\psi_{n,m}(x)=(-1)^m x^{\frac{m}{2}}\left(\frac{\mathrm{d}}{\mathrm{d}x}\right)^m\psi_n(x), \tag{4.11}$$

and $\psi_n(x)$ satisfies the Laguerre differential equation which has the following Rodrigues representation:

$$\psi_n(x)=N_n x^{-\lambda}\mathrm{e}^{\gamma x}\left(\frac{\mathrm{d}}{\mathrm{d}x}\right)^n(x^{\lambda+n}\mathrm{e}^{-\gamma x}). \tag{4.12}$$

The lower spinor field can easily be obtained from the upper component that we have not calculated here.

By taking other different choices of $A(x)$, $W(x)$ and using the above procedure, we have solved the radial Dirac equation for the other potentials that can be found in table 1.

5. Conclusion

We have investigated a procedure for solving the radial Dirac equation with spherical symmetric potentials. We have shown that for constant electrostatic potential, if the potential functions are written on the basis of the superpotentials that be obtained from the master function formalism, then the upper spinor wave functions can be expressed in terms of the Rodrigues representation of orthogonal polynomials. For each case of electromagnetic potentials, the relativistic spectra of the bound states have also been obtained in terms of the non-relativistic energy spectra.

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