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Solution of Dirac Equation with Generalized Hylleraas Potential

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Abstract *We employ the parametric generalization of the Nikiforov–Uvarov method to solve the Alhaidari formalism of the Dirac equation with a generalized Hylleraas potential of the form* $V(r) = V_0(a + \exp(\lambda r))/(b + \exp(\lambda r)) + V_1(d + \exp(\lambda r))/(b + \exp(\lambda r))$. *We obtain the bound state energy eigenvalue and the corresponding eigenfunction expressed in terms of the Jacobi polynomials. By choosing appropriate parameter in the potential model, the generalized Hylleraas potential reduces to the well known potentials as special cases.*

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Key words: Dirac equation, Alhaidari formalism, Nikiforov–Urarov method

1 Introduction

The solution of the Dirac equation has attracted a lot of attention of many authors in recent years.[1−2] It is well-known that the analytical solution of Dirac is only possible in few cases, such as the harmonic and hydrogen atom.[3] Recently, the relativistic bound states spectrum and its wave function for the triaxial and axially deformed oscillator with vector and scalar harmonic oscillator potential have been solved analytically for the general case.[4−5] The Dirac, Klein–Gordon, and Schrödinger equations have been solved analytically for some exponential-like type potential such as Woods–Saxon,[6] Hulthen,[7] Manning–Rosen,[8] the Eckart,[9] Hylleraas[10−12] potentials. Hylleras potential reduces to a special case of Morse potential which has raised a great deal of interest over the years and has been one of the most useful potential models to describe the interaction between two atoms in a diatomic molecule.[12−16] Various methods have been adopted to find the solutions of the Dirac equation. These methods include factorization method,[13] algebraic method,[14] Suppersymmetric quantum mechanics (SUSY) method,[15] asymptotic iteration method,[16] Nikiforov–Uvarov method[17] and others. A new formalism has been recently introduced by Alhaidari to the definition of the radial Dirac equation and solved for a class of shape invariant potentials.[18−19] Many attempts made by different authors to give analytical approximation of the Dirac equation for non-zero angular component involve the coupling $l(l+1)/r^2$. This is equivalent to the analytic approximation with the new orbital term $\kappa(\kappa \pm 1)/r^2$ in the second order differential equation that results from the Dirac equation, where κ is the spin orbit quantum number.[20] For the first time Alhaidari[21] obtained the solution of the Dirac equation with coupling to $1/r$ singular potential for all angular momentum. In addition several attempts have been made by different authors to obtain the solutions of the Dirac equation with different potential models under spin and pseudospin symmetry limits in recent years.[20−25] Nevertheless, with the formalism of Dirac equation proposed by Alhaidari[18−19] and the modified generalized parametric Nikiforov–Uvarov (NU) method,[17] we attempt to find analytical approximate solution of Dirac equation with generalized Hylleraas potential including the energy spectrum and the corresponding wave functions.

In this paper, the Dirac equation is solved by the NU method within the framework of the Alhaidari formalism (whose traditional name was known as Tricomi equation) with the generalized Hylleraas potential.

The organization of the paper is as follows: In Sec. 2 the Alhaidari formalism of the Dirac equation is presented. The NU method is given in Sec. 3. Section 4 is devoted to the solution of the Dirac equation. Finally, a brief conclusion is given in Sec. 5.

2 Alhaidari Formalism of Dirac Equation

In the relativistic units $\hbar = c = 1$ the Dirac equation with spherical symmetric coupling to scalar and vector $S(r)$ and $V(r)$ take the form[18−21]

$$\begin{pmatrix} m + S(r)\alpha^2 V(r) - \varepsilon & -\frac{\mathrm{d}}{\mathrm{d}r} + \frac{k}{r} \\ \frac{\mathrm{d}}{\mathrm{d}r} + \frac{k}{r} & -m - S(r)\alpha^2 V(r) - \varepsilon \end{pmatrix} \times \begin{pmatrix} \varphi^+(r) \\ \varphi^-(r) \end{pmatrix} = 0\,, \tag{1}$$

where $\varphi^{\pm}(r)$ are the upper and lower component spinor. Approximating $1/r$ orbital term by a singular potential function $W(r)$, the Dirac equation becomes

$$\begin{pmatrix} m + S(r)\alpha^2 V(r) - \varepsilon & -\frac{\mathrm{d}}{\mathrm{d}r} + kW(r) \\ \frac{\mathrm{d}}{\mathrm{d}r} + kW(r) & -m - S(r)\alpha^2 V(r) - \varepsilon \end{pmatrix} \times \begin{pmatrix} \varphi^+(r) \\ \varphi^-(r) \end{pmatrix} = 0\,. \tag{2}$$

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For a given value of the spin-orbit coupling parameter k, the Schrödinger-like relates the two potentials functions as $CS(r)+k(\sqrt{1-C^2})W(r)=V(r)/\xi$ where $C=\cos(\alpha\eta)$, and ξ is a real parameter. The global unitary transformation was proposed by Alhaidari[21] of the form $U(\eta)=\exp((1/2)\alpha\eta\sigma_2)$ in Eq. (2) to eliminate the first derivative, where η is a real constant and σ_2 is the 2×2 Pauli matrix that defines the two radial spinor components.[19] The recent revision of this formalism is given in Ref. [27]

$$\varphi^{\mp}(r)=\frac{\alpha}{mc\pm\varepsilon}\Big[\frac{\mathrm{d}}{\mathrm{d}r}\pm\frac{CV(r)}{\xi}-\xi\Big]\varphi^{\pm}(r)\,, \tag{3}$$

where $mC\neq\pm\varepsilon$. Substituting Eq. (3) into Eq. (2), we obtain the Schrödinger-like second order differential equation for the lower and upper spinor components as

$$\Big[-\frac{\mathrm{d}^2}{\mathrm{d}r^2}\pm\frac{CV^2(r)}{\xi^2}+2EV\mp\frac{C}{\xi}\frac{\mathrm{d}V}{\mathrm{d}r}-\frac{(E^2-m^2)}{\alpha^2}\Big]\varphi^{\pm}(r)=0\,, \tag{4}$$

where the "$\pm$" designate the upper and lower components respectively. With suitable parameter adjustment Eq. (4) reduces to purely Coulomb-like potential.[26]

3 Concept of the Nikiforov–Uvarov Method

The concept of the NU method[17] was proposed to solve the second order linear differential equation by reducing it to a generalized equation of hypergeometric-type of the form

$$\psi''(s)+\frac{\tilde{\tau}(s)}{\sigma(s)}\psi'(s)+\frac{\tilde{\sigma}(s)}{\sigma^2(s)}\psi(s)=0\,, \tag{5}$$

where the prime denotes the differential with respect to s, $\sigma(s)$ and $\tilde{\sigma}(s)$ are polynomials at most second degree and $\tilde{\tau}(s)$ is a first degree polynomials. The solution of Eq. (5) is obtained by using an ansatz for the wave function as

$$\psi(s)=\varphi(s)\chi_n(s)\,, \tag{6}$$

which reduces Eq. (5) into a hypergeometric type equation

$$\sigma(s)\chi_n''(s)+\tau(s)\chi_n'(s)+\lambda\chi_n(s)=0\,, \tag{7}$$

where $\varphi(s)$ is defined as a logarithmic derivative[17]

$$\frac{\varphi'(s)}{\varphi(s)}=\frac{\pi(s)}{\sigma(s)}\,, \tag{8}$$

and the other wave function is the hypergeometric-type function whose polynomial solution satisfies the Rodriques relation

$$\chi_n(s)=\frac{B_n}{\rho(s)}\frac{\mathrm{d}^n}{\mathrm{d}s^n}[\sigma^n(s)\rho(s)]\,, \tag{9}$$

where B_n is the normalization constant and the weight function $\rho(s)$ satisfies the condition

$$(\sigma(s)\rho(s))'=\tau(s)\rho(s)\,. \tag{10}$$

The required $\pi(s)$ and λ for the NU method are defined as

$$\pi(s)=\frac{\sigma'-\tilde{\tau}}{2}\pm\sqrt{\Big(\frac{\sigma'-\tilde{\tau}}{2}\Big)-\tilde{\sigma}(s)+k\sigma(s)}\,, \tag{11}$$

$$\lambda=k+\pi'(s)\,, \tag{12}$$

respectively. Therefore the determination of k in Eq. (11) is the necessary step in the calculation of $\pi(s)$ for which the discrimination of the square root in Eq. (11) is set to zero. The eigenvalues equation defined in Eq. (12) takes the form

$$\lambda=\lambda_n=-n\tau'-\frac{n(n-1)}{2}\sigma''\,,\quad n=0,1,2,\ldots\,, \tag{13}$$

where

$$\tau(s)=\tilde{\tau}(s)+2\pi(s)\,, \tag{14}$$

and its derivative is negative which is the necessary condition for bound state solutions. The energy eigenvalues is obtained by comparing Eqs. (12) and (13). The parametric generalization of the NU method that is valid for both central and non-central exponential-type potential[22] can be derived by comparing the generalized hypergeometric-type equation

$$\psi''(s)+\frac{(\alpha_1-\alpha_2 s)}{s(\alpha'-\alpha_3 s)}\psi'+\frac{1}{s^2(\alpha'-\alpha_3 s)^2}\times[-\zeta_1 s^2+\zeta_2 s-\zeta_3]\psi(s)=0\,, \tag{15}$$

with Eq. (5) and we obtain the following parametric polynomials

$$\tilde{\tau}(s)=(\alpha_1-\alpha_2 s)\,, \tag{16}$$

$$\sigma s=s(\alpha'-\alpha_3 s)\,, \tag{17}$$

$$\tilde{\sigma}(s)=-\zeta_1 s^2+\zeta_2 s-\zeta_3\,. \tag{18}$$

Substituting Eqs. (16)–(18) into Eq. (11), we find

$$\pi(s)=\alpha_4-\alpha_5 s\pm[(\alpha_6-\alpha_3 k_{\pm})s^2+(\alpha_7+k_{\pm})s+\alpha_8]^{1/2}\,, \tag{19}$$

where

$$\alpha_4=\frac{1}{2}(\alpha'-\alpha_1)\,,\quad \alpha_6=\alpha_5^2+\zeta_1\,,\quad \alpha_7=2\alpha_4\alpha_5-\zeta_2\,,\quad \alpha_8=\alpha_4^2+\zeta_3\,. \tag{20}$$

We obtain the parametric $k_{\pm}$ from the condition that the function under the square root be square of a polynomial,

$$k_{\pm}=-(\alpha_7+2\alpha_3\alpha_8)\pm 2\sqrt{\alpha_8\alpha_9}\,, \tag{21}$$

where

$$\alpha_9=\alpha_3\alpha_7+\alpha_3^2\alpha_8+\alpha_6\,. \tag{22}$$

Hence, the $\pi(s)$ in Eq. (19) becomes

$$\pi(s)=\alpha_4+\alpha_5 s-\big[(\sqrt{\alpha_9}+\alpha_3\sqrt{\alpha_8})s-\sqrt{(\alpha_8)}\,\big]\,, \tag{23}$$

for the negative k_- values

$$k_-=-(\alpha_7+2\alpha_3\alpha_8)-2\sqrt{\alpha_8\alpha_9}\,. \tag{24}$$

Thus, from the relation, $\tau(s)=\tilde{\tau}(s)+2\pi(s)$, we have

$$\tau(s)=\alpha_1+2\alpha_4-(\alpha_2-2\alpha_5)s-2\big[(\sqrt{\alpha_9}+\alpha_3\sqrt{\alpha_8})s-\sqrt{\alpha_8}\big]\,, \tag{25}$$

whose derivative must be negative,

$$\tau'(s)=-2\alpha_3-2\big[(\sqrt{\alpha_9}+\alpha_3\sqrt{\alpha_8})\big]<0\,. \tag{26}$$

Solving Eqs. (12) and (13), we obtain the parametric energy equation as

$$(\alpha_2-\alpha_3)n+\alpha_3 n^2-(2n+1)\alpha_5$$

$$+ (2n+1)\big[\sqrt{\alpha_9} + \alpha_3\sqrt{\alpha_8}\big] + \alpha_7 + 2\alpha_3\alpha_8 + 2\sqrt{\alpha_8\alpha_9} = 0\,. \tag{27}$$

The weight function $\rho(s)$ is obtained as

$$\rho(s) = s^{\alpha_{10}}(\alpha' - \alpha_3 s)^{\alpha_{11}}, \tag{28}$$

and together with Eq. (9), we get

$$\chi_n(s) = P_n^{(\alpha_{10},\alpha_{11})}(\alpha' - 2\alpha_3 s)\,, \tag{29}$$

where

$$\alpha_{10} = \alpha_1 + 2\alpha_4 + 2\sqrt{\alpha_8}\,, \tag{30}$$

$$\alpha_{11} = \alpha' - \alpha_1 - 2\alpha_4 + \frac{2}{\alpha_3}\sqrt{\alpha_9}\,. \tag{31}$$

Thus, the total wave function becomes

$$\Psi_n(s) = N_n s^{\alpha_{12}}(\alpha' - \alpha_3 s)^{\alpha_{13}} P_n^{(\alpha_{10},\alpha_{11})}(\alpha' - 2\alpha_3 s)\,, \tag{32}$$

where N_n is the normalization constant.

4 Solution of Dirac Equation

We considered the generalized modified Hylleraas potential of the form[10–12]

$$V(r) = \frac{V_0(a+\mathrm{e}^{\lambda r})}{(b+\mathrm{e}^{\lambda r})} + \frac{V_1(d+\mathrm{e}^{\lambda r})}{(b+\mathrm{e}^{\lambda r})}\,, \tag{33}$$

where V_0, V_1 are the depth of the potential, a, b, and d are the Hylleraas parameters. Substituting Eq. (33) into Eq. (4), we obtain the Dirac equation for the upper component of the spinor as

$$\Big[-\frac{\mathrm{d}^2\varphi^+}{\mathrm{d}r^2} + \frac{c^2}{\xi^2}\Big\{\frac{V_0^2(a+\mathrm{e}^{\lambda r})^2}{(b+\mathrm{e}^{\lambda r})^2} + \frac{2V_0V_1(a+\mathrm{e}^{\lambda r})(d+\mathrm{e}^{\lambda r})}{(b+\mathrm{e}^{\lambda r})^2} + \frac{V_1^2(d+\mathrm{e}^{\lambda r})^2}{(b+\mathrm{e}^{\lambda r})^2}\Big\}\varphi^+\Big] + 2E\Big(\frac{V_0(a+\mathrm{e}^{\lambda r})}{(b+\mathrm{e}^{\lambda r})} + \frac{V_1(d+\mathrm{e}^{\lambda r})}{(b+\mathrm{e}^{\lambda r})}\Big)\varphi^+ - \frac{C}{\xi}\Big\{\frac{\lambda\,\mathrm{e}^{\lambda r}}{(b+\mathrm{e}^{\lambda r})^2}(V_0(b-a) + V_1(b-d))\Big\}\varphi^+ - \Big(\frac{E^2-M^2}{\alpha^2}\Big)\varphi^+(r) = 0\,. \tag{34}$$

Defining a new variable $x = (b+\mathrm{e}^{\lambda r})$, Eq. (34) becomes

$$\frac{\mathrm{d}^2\phi^+}{\mathrm{d}x^2} - \frac{x}{x(b-x)}\frac{\mathrm{d}\phi^+}{\mathrm{d}x} + \frac{1}{x^2(b-x)^2}[-(\varepsilon^2 + A)x^2 + Bx - D]\varphi^+(x) = 0\,, \tag{35}$$

where

$$\varepsilon^2 = -\Big(\frac{E^2-M^2}{\lambda^2\alpha^2}\Big)\,, \tag{36}$$

$$\tilde{A} = \beta_1^2 + \frac{2(V_0+V_1)E}{\lambda^2}\,, \tag{37}$$

$$\tilde{B} = \beta_2^2 - 2\Big[\frac{V_0(a-b) + V_1(d-b)}{\lambda^2}\Big]E\,, \tag{38}$$

$$\tilde{D} = \frac{C^2}{\lambda^2\xi^2}\Big[V_0^2(a-b)^2 + 2V_0V_1(a-b)(d-b) + V_1^2(d-b)^2 + \frac{\lambda\xi V_0 b(b-a)}{C} + \frac{\xi V_1(b-a)}{C}\Big]\,, \tag{39}$$

$$\beta_1^2 = \frac{C^2}{\lambda^2\xi^2}[V_0^2 + 2V_0V_1 + V_1^2]\,, \tag{40}$$

$$\beta_2^2 = -\frac{C^2}{\lambda^2\xi^2}\Big[2(a-b)V_0^2 + 4(a+d-2b)V_0V_1 + 2(d-b)V_1^2 - \frac{\lambda\xi V_0 b(b-a)}{C}\Big]\,. \tag{41}$$

Comparing Eq. (35) with Eq. (15), we obtain the following parameters:

$$\alpha_1 = 0,\quad \zeta_1 = (\varepsilon^2 + \tilde{A}),\quad \alpha' = b,\quad \alpha_2 = -1,\quad \zeta_2 = \tilde{B},\quad \alpha_3 = -1,\quad \zeta_3 = \tilde{D}\,. \tag{42}$$

The values of the coefficients α_i $(i = 1, 2, \ldots, 13)$ together with ζ_i $(j = 1, 2, 3)$ are given in Table 1 for the Dirac equation with generalized Hylleraas potential model.

The energy eigenvalue of the Dirac equation with modified Hylleraas potential can be obtained from Eq. (27) as

$$E^2 - M^2 = \frac{-\lambda^2\xi^2}{4}\left[\frac{-\tilde{B} + \tilde{D} + ((n-1)/2)^2 + \big[n + 1/2 + \sqrt{\tilde{D} + b^2/4}\,\big]^2}{n + (1/2) + \sqrt{\tilde{D} + b^2/4}}\right]^2 + \lambda^2\xi^2\Big[\tilde{A} - \tilde{B} + \tilde{D} + \Big(\frac{b-1}{2}\Big)^2\Big]\,. \tag{43}$$

The energy defined explicitly by energy equation (43) is a rather complicated transcendental equation as there is no available literature to compare our results. However, we can impose an approximation values for the Hylleraas parameters to calculate the bound state energies of Dirac–Rosen Morse I and potential well as special cases. If we set $d = -1$, $V_1 = 0$, $a = 1$, $b = 1$, we obtain the Dirac–Rosen Morse I potential.[18]

$$V(r) = V_0 \tanh\Big(\frac{\lambda r}{2}\Big)\,. \tag{44}$$

Substituting these parameters into Eq. (43), we obtain the energy eigenvalue for the Dirac–Rosen Morse potential as

$$E^2-M^2=\frac{-\lambda^2\xi^2}{4}\Big[\frac{-4EV_0/\lambda_2+(n+1/2+\sigma)^2}{n+1/2+\sigma}\Big]^2 + V_0^2C^2\Big(1-\frac{\xi^2E}{2C^2V_0}\Big)\,, \tag{45}$$

where

$$\sigma=\frac{2CV_0}{\lambda\xi}\sqrt{1+\frac{\lambda\xi}{2V_1C}+\Big(\frac{\lambda\xi}{4CV_0}\Big)^2}\,.$$

Similarly, setting $a=-1$, $d=-1$, $V_1=0$ and mapping $V\to -V_0$, we obtain the energy eigenvalue for the potential well as

$$E^2-M^2=\frac{-\lambda^2\xi^2}{4}\Big(n+\frac{1}{2}\Big)^2. \tag{46}$$

We now look again at another special case for $b=0$ and the relationship between our results and some other existing results in the literature. For $a=-1$, $V_0=D_e$, the dissociation energy, $d=0$, $V_1=0$, we obtain the energy spectrum for the Morse potential as

$$E^2-M^2=-\frac{-\lambda^2\xi^2}{4}\left[\frac{\frac{3D_e^2C^2}{\lambda^2\xi^2}(1+\frac{\lambda\xi}{3D_eC})+(n+\delta)^2}{n+\delta}\right]^2 + 3D_e^2C^2\Big[1+\frac{\lambda\xi}{3D_eC}+\frac{2\xi^2}{3D_eC^2}\Big]\,, \tag{47}$$

where

$$\delta=\frac{1}{2}\Big(1+\sqrt{1+\frac{C^2D_e^2}{4\lambda^2\xi^2}}\Big)\,.$$

In order to calculate the Dirac wave function, we first obtain the function from Eqs. (28) and (32) as

$$\rho(r)=(b+\mathrm{e}^{\lambda r})^{\mu}(\mathrm{e}^{\alpha r})^{\nu}, \tag{48}$$

$$\varphi(r)=(b+\mathrm{e}^{\lambda r})^{\mu/2}(\mathrm{e}^{\alpha r})^{(\nu+1-b)/2}, \tag{49}$$

where $\mu=b+2(1+\sqrt{D+b^2/4})$ and

$$\nu=2\sqrt{\varepsilon^2+\tilde{A}+\tilde{D}-\tilde{B}+\Big(\frac{b-1}{2}\Big)^2}\,.$$

Hence, the second part $\chi_n(r)$ of the wave function can be obtained from the weight function as

$$P_n^{(\mu,\nu)}(1-2s)=\frac{(\mu+1)_n}{n!} \times {}_2F_1(-n,1+\mu+\nu+n;\mu+1;s)\,. \tag{50}$$

Finally, we find the unnormalized wave function as

$$\varphi_n^+=N_n(b+2\,\mathrm{e}^{\lambda r})^{\mu/2}(\mathrm{e}^{\lambda r})^{(\nu+1-b)/2}\frac{(\mu+1)_n}{n!} \times {}_2F_1(-n,1+\mu+\nu+n;\mu+1;(b+\mathrm{e}^{\lambda r}))\,. \tag{51}$$

In addition, the corresponding lower-spinor wave function can be obtained from Eq. (3) as

$$\varphi^-(r)=\frac{\alpha}{mC+\varepsilon}\Big(\frac{\mathrm{d}}{\mathrm{d}r}+\frac{CV(r)}{\xi}-\xi\Big)\phi^+(r). \tag{52}$$

Table 1 The specific value for the parametric constants necessary for the eigenvalue and eigen function of the Dirac equation.

Constant	Analytic value
α_1	0
α_2	1
α'	b
α_3	1
α_4	$\frac{b}{2}$
α_5	$-\frac{1}{2}$
α_6	$\frac{b^2}{4}+(\varepsilon^2+A)$
α_7	$\frac{b}{2}-\tilde{B}$
α_8	$\tilde{D}+\frac{b^2}{4}$
α_9	$\varepsilon^2+A-\tilde{B}+\tilde{D}+(\frac{b-1}{2})^2$
α_{10}	$b+2(1+\sqrt{\tilde{D}+\frac{b^2}{4}})$
α_{11}	$+2\sqrt{\varepsilon^2+\tilde{A}-\tilde{B}+\tilde{D}+(\frac{b-1}{2})^2}$
α_{12}	$\frac{1}{2}(b+\sqrt{4\tilde{D}+\frac{1}{4}})$
α_{13}	$-\frac{1}{2}[b+2(\sqrt{\varepsilon^2+\tilde{A}+\tilde{B}+\tilde{D}}+\frac{1}{2})]$

5 Conclusion

In this study, we investigated the analytical solution of the Dirac equation for the generalized Hylleraas potential within the framework of Alhaidari formalism of Dirac theory using the parametric generalization of Nikiforov-Uvarov method. Within this formalism, energy eigenvalues have been obtained. We also found the radial upper and lower wave functions in terms of hypergeometric functions. Special cases of this potential are also deduced.

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