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Solution of Klein Gordon Equation for Some Diatomic Molecules with New Generalized Morse-like Potential Using SUSYQM

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We present the solution of Klein Gordon equation with new generalized Morse-like potential using SUSYQM formalism. We obtained approximately the energy eigenvalues and the corresponding wave function in a closed form for any arbitrary l state. We computed the numerical results for some selected diatomic molecules.

Key Words : New generalized Morse-like potential, Supersymmetric quantum mechanics, Klein Gordon equation

Introduction

In quantum mechanics, the study of exact solutions of relativistic and non-relativistic equation with different potentials plays a significant role in Physics.[1-5] The bound state solution of Klein Gordon equation (KGE) is of great important in nuclear and high energy physics.[6] Klein Gordon equation is a relativistic wave equation that describes spin-zero particles. It contains of two major objects, the vector potential $V(r)$ and the scalar potential $S(r)$. In D-dimension, the Klein Gordon equation[5] is written as

$$\left[\frac{d^2}{dr^2} + E_{nl}^2 + V^2(r) - 2E_{nl}V(r) - m^2 - S^2(r) - 2mS(r) - \frac{(D+2l+1)(D+2l+3)}{4r^2}\right]\Psi_{nl}(r) = 0 \quad (1)$$

where E_{nl} is the energy and m is rest mass.[7,8] However, different authors have adopted several techniques to obtain the exact or approximate solutions of KGE with various potential interactions. These techniques include asymptotic iteration method (AIM),[9] the Nikiforov-Uvarov method (NU),[10] supersymmetric quantum mechanices,[11] and others. Amongst the potentials studied with these techniques are the Manning-Rosen Potential,[12,13] Hulthen Potential,[14,15] Eckart-type Potential,[16,17] Wood-Saxon Potential,[18,19] Poschl-Teller Potential.[20] Many contributions from different authors shows that the analytical solution of KGE are possible only in the s-wave case $(l=0)$ while for $l \neq 0$, it is solved by using suitable approximation scheme.[21,22] The Morse Potential is one of the known potentials model used in describing diatomic molecules. It given as

$$V(r) = D_e\left(e^{-2a(r-r_0)} - e^{-a(r-r_0)}\right), \quad D_e > 0,\, a > 0 \quad (2)$$

Where D_e is the dissociation energy, r_0 is the equilibrium internuclear distance and a is a parameter controlling the width of potential well.[23] Nevertheless, several authors have done investigations with this potential, Berkdemir investigated Pseudospin symmetry in relativistic Morse potential including the spin-orbit coupling,[23] Jia *et al.* studied Equivalence of the deformed Rosen-Morse Potential energy model and Tietz potential energy model,[24] Zarezadeh *et al.* investigated the solution of the Schrodinger wave equation for a particular form of Morse Potential using Laplace transform,[25] Erkol *et al.* studied the Exact solutions for a Hamiltonian with Morse Potential and Dirac Delta shell interactions.[26]

In this work, we introduced a novel potential and call it the New Generalized Morse-like potential (NGMP) model recently proposed by Ikot *et al.*[27] having the same behaviours as MP, attractive radial potential and Deng-Fan potential models. It is defined as

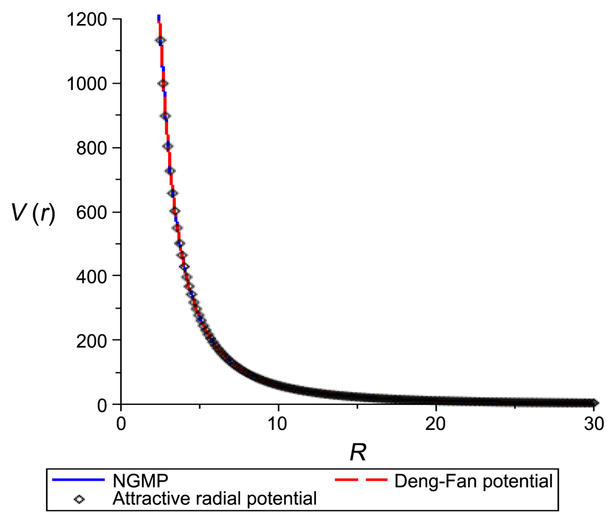

Figure 1. Behavior of potentials for $\alpha = 0.01$ fm^{-1}, $a = 1$, $b = -2$, $c = 1$, $d = -1$, $D_e = -0.8$ fm^{-1}.

$$V(r) = D_e\left[1-\left(\frac{a+be^{-\alpha r}}{c+de^{-\alpha r}}\right)^2\right] \tag{3}$$

where a, b, c, d, are constant coefficients and the term in the bracket is the Mobius square potential proposed recently (see Fig. 1).

The purpose of our work is to investigate the Solution of Klein Gordon equation for some diatomic molecules with NGMP using Supersymmetry Quantum mechanics.

Klein-Gordon in D-dimension

The Klein-Gordon equation in higher dimension for spherically symmetric potential reads,[22-25]

$$-\Delta_D\psi_{n,l,m}(r,\Omega_D) = \{[E_{n,l}-V(r)]^2-[m+S(r)]^2\}\,\psi_{n,l,m}(r,\Omega_D) \tag{4}$$

Where $E_{n,l}$, m, $V(r)$ and $S(r)$ are the relativistic energy ,rest mass, the repulsive vector potential and the attractive scalar potential respectively and Δ_D is defined as

$$\Delta_D = \nabla_D^2 = \frac{1}{r^{D-1}}\frac{\partial}{\partial}\left(r^{D-1}\frac{\partial}{\partial r}\right)-\frac{\Lambda_D^2(\Omega_D)}{r^2} \tag{5}$$

The total wave function in D-dimension is written as,

$$\psi_{n,l,m}(r,\Omega_D) = R_{n,l}(r)Y_l^m(\Omega_D) \tag{6}$$

The term $\Lambda_D^2(\Omega_D)/r^2$ is the generalization of the centrifugal term for the higher dimensional space. The eigenvalues of $\Lambda_D^2(\Omega_D)$ are defined by the relation,

$$\Lambda_D^2(\Omega_D)Y_l^m(\Omega_D) = l(l+D-2)Y_l^m(\Omega_D) \tag{7}$$

Where $Y_l^m(\Omega_D)$, $R_{n,l}$ and l represent the hyperspherical harmonics, the hyperradial wave function and the orbital angular momentum quantum number respectively.

Now substituting ansatz $R_{n,l}(r) = r^{-\frac{(D-1)}{2}}F_{n,l}(r)$ for the wave function into Eq. (4) yields,

$$\left[\frac{d^2}{dr^2} + E_{nl}^2 + V^2(r) - 2E_{nl}V(r) - m^2 - S^2(r) - 2mS(r) - \frac{(D+2l+1)(D+2l+3)}{4r^2}\right]\Psi_{nl}(r) = 0 \tag{8}$$

Solutions of the Radial Klein-Gordon Equation in D-dimension

Now considering equal scalar and vector potentials as the NGMP, $S(r) = V(r)$ in Eq. (7), we obtain the second order Schrodinger-like equation For equal scalar and vector potentials $V(r) = S(r)$, substituting Eqn. (3) into Eqn. (1), we have

$$\left[\frac{d^2}{dr^2} + E_{nl}^2 - m^2 - 2(E_{nl}+m)D_e1-\left(\left(\frac{a+be^{-\alpha r}}{c+de^{-\alpha r}}\right)^2\right) - \frac{(D+2l+1)(D+2l+3)}{4r^2}\right]\Psi_{nl}(r) = 0 \tag{9}$$

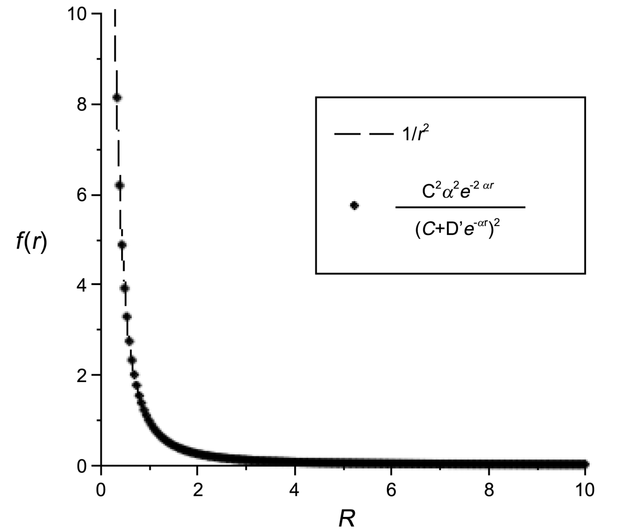

Figure 2. The centrifugal term ($1/r^2$) and its approximation for $\alpha = 0.01$ fm^{-1}, $c = 1$, $d = -1$.

The good approximation for the centrifugal term is given as,[28]

$$\frac{1}{r^2} = \alpha^2\left(\frac{ce^{-\alpha r}}{c+de^{-\alpha r}}\right)^2, \tag{10}$$

$$= \lim_{\alpha\to 0}\left(\frac{1}{r^2}+\frac{\alpha}{r}+\frac{5}{12}\alpha^2+\frac{1}{12}\alpha^3 r+\frac{1}{240}\alpha^4 r^2 -\frac{1}{720}\alpha^5 r^3-\frac{1}{6045}\alpha^6 r^4+O(r^5)\right)$$

where $c = -d$, Eq. (10) gives a good approximation for the centrifugal term (see in Fig. (2)). When performing a power series expansion and setting $\alpha\to 0$ gives the desired r^{-2} suggested by Greene and Aldrich.[29]

Now, Substituting Eq. (10) into (9) we have,

$$\frac{d^2\psi_{nl}}{dr^2}+\frac{1}{\left(1+\frac{de^{-\alpha r}}{c}\right)}\left[\begin{array}{c}\left(\frac{2D_e b^2(E_{nl}+m)}{c}-\frac{\alpha^2(D+2l-1)(D+2l-3)}{4}\right)e^{-2\alpha r}\\ +4D_e ab(E_{nl}+m)e^{-\alpha r}+2D_e a^2(E_{nl}+m)\end{array}\right]\psi_{nl}(r)$$

$$= [m^2-E_{nl}^2+2D_e(E_{nl}+m)]\,\psi_{nl}(r) \tag{11}$$

Furthermore, we can rewrite Eq. (11) as follows:

$$-\frac{d^2\psi_{nl}}{dr^2} + V_{eff}(r)\psi_{nl}(r) = \tilde{E}\psi_{nl}(r), \tag{12}$$

Where,

$$V_{eff}(r) = \frac{Xe^{-2\alpha r} + Ye^{-\alpha r} + Z}{\left(1+\frac{de^{-\alpha r}}{c}\right)^2} \tag{13}$$

$$X = -\frac{2D_e b^2(E_{nl}+m)}{c} + \frac{\alpha^2(D+2l-1)(D+2l-3)}{4} \tag{14}$$

$$Y = -4D_e ab(E_{nl}+m) \tag{15}$$

$$Z = -2D_e a^2(E_{nl}+m) \tag{16}$$

$$\tilde{E}_{nl} = E_{nl}^2 - m^2 - 2D_e(E_{nl}+m) \tag{17}$$

To be able to solve Eq. (12), we have to solve the associated Riccati equation

$$W^2(r) \mp W'(r) = V_{eff}(r) - \tilde{E}_{0,l}, \tag{18}$$

for which we propose a solution of the form

$$W(r) = \frac{fe^{-\alpha r}}{\left(1+\frac{de^{-\alpha r}}{c}\right)} + q. \tag{19}$$

Substituting Eq. (19) into Eq. (18), we get

$$\frac{f^2e^{-2\alpha r}}{\left(1+\frac{de^{-\alpha r}}{c}\right)^2} + (q)^2 + \frac{2fqe^{-\alpha r}}{\left(1+\frac{de^{-\alpha r}}{c}\right)^2} + \frac{\alpha fe^{-\alpha r}}{\left(1+\frac{de^{-\alpha r}}{c}\right)^2}$$

$$= \frac{Xe^{-2\alpha r}+Ye^{-\alpha r}+Z}{\left(1+\frac{de^{-\alpha r}}{c}\right)^2} - \tilde{E}_{0,l} \tag{20}$$

Solving Eq. (20), we obtain the following three set of parameters

$$\tilde{E}_{0,l} = -(q)^2 + Z \tag{21}$$

$$f = \frac{\left(\frac{d\alpha}{c}\right) \pm \sqrt{\left(\frac{d\alpha}{c}\right)^2 + 4\left(X+\frac{d^2Z}{c^2}-\frac{dY}{c}\right)}}{2}, \tag{22}$$

$$q = \frac{\left(-f^2+X-\frac{d^2Z}{c^2}\right)}{2f\frac{d}{c}} \tag{23}$$

Now based on Eq. A.2, we can obtain the supersymmetric partner potentials as,

$$V_{eff+}(r) = \frac{f\left(f+\frac{d\alpha}{c}\right)e^{-2\alpha r}}{\left(1+\frac{de^{-\alpha r}}{c}\right)^2} + \frac{2fqe^{-\alpha r}}{\left(1+\frac{de^{-\alpha r}}{c}\right)} + (q)^2$$

$$V_{eff-}(r) = \frac{f\left(f-\frac{d\alpha}{c}\right)e^{-2\alpha r}}{\left(1+\frac{de^{-\alpha r}}{c}\right)^2} + \frac{2fqe^{-\alpha r}}{\left(1+\frac{de^{-\alpha r}}{c}\right)} + (q)^2 \tag{24}$$

Therefore, it is shown that $V_{eff+}(r)$ and $V_{eff-}(r)$ are shape invariant, satisfying the shape-invariant condition

$$V_+(r, \rho_0) = V_-(r, \rho_1) + R(\rho_1), \tag{25}$$

with $\rho_0 = f$ and ρ_1 is a function of ρ_0, *i.e* $\rho_i = f(\rho_0) = \rho_0 + \frac{d\alpha}{c}$. Therefore, $\rho_n = \rho_0 + \left(\frac{d\alpha n}{c}\right)$. Thus, we can see that the shape invariance holds *via* a mapping of the form $f \to f + \left(\frac{d\alpha}{c}\right)$.

From Eq. (A.5), we have

$$R(a_1) = \left(\frac{-\rho_0^2+X-\frac{Zd^2}{c^2}}{2\rho_0\frac{d}{c}}\right)^2 - \left(\frac{-\rho_1^2+X-\frac{Zd^2}{c^2}}{2\rho_1\frac{d}{c}}\right)^2,$$

$$R(a_2) = \left(\frac{-\rho_1^2+X-\frac{Zd^2}{c^2}}{2\rho_1\frac{d}{c}}\right)^2 - \left(\frac{-\rho_2^2+X-\frac{Zd^2}{c^2}}{2\rho_2\frac{d}{c}}\right)^2,$$

$$\vdots \tag{26}$$

$$R(a_n) = \left(\frac{-\rho_{n-1}^2+X-\frac{Zd^2}{c^2}}{2\rho_{n-1}\frac{d}{c}}\right)^2 - \left(\frac{-\rho_n^2+X-\frac{Zd^2}{c^2}}{2\rho_n\frac{d}{c}}\right)^2,$$

The energy eigenvalues can be obtained as follows

$$\tilde{E}_{nl} = \tilde{E}_{nl}^- + \tilde{E}_{0,l}, \tag{27}$$

where,

$$\tilde{E}_{nl}^- = \sum_{k=1}^{n} R(a_k) = \left(\frac{-\rho_0^2+X-\frac{Zd^2}{c^2}}{2\rho_0\frac{d}{c}}\right)^2 - \left(\frac{-\rho_n^2+X-\frac{Zd^2}{c^2}}{2\rho_n\frac{d}{c}}\right)^2, \tag{28}$$

By substituting Eqs. (23) and (28) into Eq. (27), We have

$$\tilde{E}_{nl} = -\left(\frac{-\rho_n^2+X-\frac{Zd^2}{c^2}}{2\rho_n\frac{d}{c}}\right)^2 + Z \tag{29}$$

More explicitly, we obtain the energy equation for the Klein Gordon equation with NGMP as

$$E_{nl}^2 - m^2 - 2D_e(E_{nl}+m) + \frac{c^2}{4d^2}\left[\frac{\left(\frac{-\frac{2D_eb^2(E_{nl}+m)}{c}+\frac{\alpha^2(D+2l-1)(D+2l-3)}{4}+2D_ea^2(E_{nl}+m)d^2}{c^2}\right)}{\left(\frac{d\alpha}{c}\right)[n+\sigma]} - 1\right]$$

$$+ 2D_ea^2(E_{nl}+m) = 0 \tag{30}$$

Where

$$\rho_n = \left(\frac{d\alpha}{c}\right)[n+\sigma], \tag{31}$$

$$\sigma = 1 \pm 1\sqrt{1+\frac{4c^2\left(\frac{-\frac{2D_eb^2(E_{nl}+m)}{c}+\frac{\alpha^2(D+2l-1)(D+2l-3)}{4}}{-\frac{2d^2D_ea^2(E_{nl}+m)}{c^2}+\frac{4dD_eab(E_{nl}+m)}{c}}\right)}{d^2\alpha^2}} \tag{32}$$

Furthermore, in order to calculate the radial wave function we used the coordinate transform, $s = e^{-\alpha r}$ in Eq. (12) to get,

$$\frac{d^2\psi_{nl}}{ds^2} + \frac{\left(1+\frac{d}{c}s\right)}{s\left(1+\frac{d}{c}s\right)}\frac{d\psi_{nl}}{ds} + \frac{1}{s^2\left(1+\frac{d}{c}s\right)^2}$$

$$\left[-\left(\frac{X}{\alpha^2}-\frac{\tilde{E}_{nl}d^2}{\alpha^2c^2}\right)s^2+\left(\frac{2\tilde{E}_{nl}d}{c\alpha^2}-\frac{Y}{\alpha^2}\right)s-\left(\frac{Z}{\alpha^2}-\frac{\tilde{E}_{nl}}{\alpha^2}\right)\right]\psi_{nl}(s)=0\,, \quad (33)$$

The corresponding radial wave function is obtain from Eq. (33) as follows,

$$R_{nl}(r) = N_{nl}(e^{-\alpha r})^{\sqrt{\frac{Z}{\alpha^2}-\frac{\tilde{E}_{nl}}{\alpha^2}}}\left(1+\frac{d}{c}e^{-\alpha r}\right)^{\frac{-d}{2c}-\left(\sqrt{\frac{d^2}{4c^2}+\frac{X}{\alpha^2}-\frac{Yd}{c\alpha^2}+\frac{Zd^2}{c^2\alpha^2}}-\frac{d}{c}\sqrt{\frac{Z}{\alpha^2}-\frac{\tilde{E}_{nl}}{\alpha^2}}\right)}$$

$$P_n^{\left(2\sqrt{\frac{Z}{\alpha^2}-\frac{\tilde{E}_{nl}}{\alpha^2}},\, 2\sqrt{\frac{d^2}{4c^2}+\frac{X}{\alpha^2}-\frac{Yd}{c\alpha^2}+\frac{Zd^2}{c^2\alpha^2}}\right)}\left(1+2\frac{d}{c}e^{-\alpha r}\right) \quad (34)$$

where N_{nl} is the normalization constant

In order to test for the accuracy of our work, we use the potential parameters given in Ref. [30] Table 1 to compute the energy eigen values for some diatomic molecules of HF_2, N_2, I_2, H_2 and O_2 as shown in Tables 2-16, where we have chosen $\hbar=1$ in our calculation.

Conclusion

In this work, we solve the Klein Gordon Equation for NGMP with proper approximation to the centrifugal term using the SUSQM technique. We obtain explicitly, the bound state energy eigenvalues and the corresponding wave function in a closed form. We employed the Aldrich and Greene approximation scheme[29] to deal with centrifugal term in d-dimension. However, one may find the improved approximation scheme in Ref. [31, 32] for comparison. Finally, we computed the energy eigenvalues of our work numerically in order to check the accuracy of our results and our result may find many applications in molecular and chemical physics. As compared to the one reported by Chen *et al.*[33] in D-dimension

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