

Effective-mass Klein-Gordon Equation for non-PT/non-Hermitian Generalized Morse Potential

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Abstract

The one-dimensional effective-mass Klein-Gordon equation for the real, and non-PT-symmetric/non-Hermitian generalized Morse potential is solved by taking a series expansion for the wave function. The energy eigenvalues, and the corresponding eigenfunctions are obtained. They are also calculated for the constant mass case.

Keywords: position dependent mass, Klein-Gordon Equation, generalized Morse potential, PT-symmetry, energy eigenvalues, eigenfunctions.

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I. INTRODUCTION

In the past few decades, there has been an increased interest to find the exact solutions of the non-relativistic and relativistic equations. The solutions of the Schrödinger equation has been studied by using different methods based on perturbative and non-perturbative approaches [1-5]. The Klein-Gordon (KG) and Dirac equations have been also studied for different type of potentials such as Aharonov-Bohm (AB) potential [6], the AB plus Dirac monopole potential [7, 11], generalized Hulthen, harmonic, and linear potentials, generalized asymmetrical Hartmann potentials, for a uniform magnetic field, pseudoharmonic oscillator, and exponential-type potentials [12-20].

Recently, there has been considerable work on the PT-symmetric quantum mechanics. Following the initially studies of Bender et al. [21], the PT-symmetric theory has been successfully studied by many authors because of their importance, and also for using in different research areas, such as quantum field theory, and nuclear physics [22, 23]. In the present study, we take into account the form of the generalized Morse potential having also non-PT symmetric property to achieve the solutions within the position-dependent mass formalism, and study the effects of the mass varying with spatially coordinate on the solutions of the case of constant mass. It could be interested to solve the relativistic KG equation in this point of view.

The solutions of the above wave equations are taken in general for constant or time-dependent masses [24, 25]. There are also many examples of physically important systems, for which the mass depends on coordinates. So far, solving the above equations for the case of spatially dependent mass has been studied by many authors [26-34] for different types of the mass distributions such as an exponentially, and quadratic mass functions [27], inverse-quadratic dependence of mass [35], trigonometric mass-distributions [36], and mass functions of the forms $m(r)=r^\alpha$, especially for three-dimensional problems [36, 37]. We will use also a mass distribution having an exponential form, and study in the half-plane to achieve a physically acceptable (finite) mass function, which has a decreasingly behavior in this range.

In the present work, we study the bound state solutions of the KG equation with real and non-PT symmetric/non-Hermitian forms of generalized Morse potential in the case of a coordinate-dependence mass distribution. In order to find the energy spectra, and the

corresponding wave functions we prefer to use an infinite series for the wave function. This approach is a powerful technique to solve second order differential equations especially for the potential forms having two and/or more terms [38, 39]. We obtain also the energy spectrum, and the corresponding eigenfunctions in the case of constant mass for two potential types.

The organization of the work as follows. In section II, we obtain the exact bound-state energy spectra for real, and non-PT symmetric/non-Hermitian cases of generalized Morse potential, and the corresponding eigenfunctions by taking an infinite series for the wave function in the case of a convenient mass distribution. We summarize the numerical results in one table, and two figures to see the effects of the mass depending on coordinate. For this aim we do the numerical analysis for three different diatomic molecules such as H₂, LiH, and HCl. We give also the results for the case of constant mass, and present our conclusions in Section III.

II. BOUND STATE SOLUTIONS

A. Real Generalized Morse Case

The one-dimensional KG equation is written in terms of scalar and vector potential as following [40]

$$\frac{d^2\psi(x)}{dx^2} + \frac{1}{\hbar^2 c^2} \left[[E - V_v(x)]^2 - [mc^2 + V_s(x)]^2 \right] \psi(x) = 0, \quad (1)$$

where m is the mass of the particle, E denotes the energy, and $V_s(x)$ and $V_v(x)$ are the scalar and vector parts of the potential, respectively, and c is the velocity of light. In the absence of the vector potential, the KG equation can be written as

$$\frac{d^2\psi(x)}{dx^2} + \frac{2m}{\hbar^2} \left(\varepsilon - \frac{V_s^2(x)}{2mc^2} - V_s(x) \right) \psi(x) = 0, \quad (2)$$

which is a Schrödinger-like equation with the energy eigenvalue $\varepsilon = \frac{E^2}{2mc^2} - \frac{mc^2}{2}$.

We consider the scalar potential $V_s(x)$ in Eq. (2) as generalized Morse potential, which can be used to describe the vibrations of a two-atomic molecule, as the following

$$V_s(x) = V_1 e^{-2\beta x} - V_2 e^{-\beta x}, \quad (0 \leq x \leq +\infty). \quad (3)$$

where V_1 , and V_2 are two real parameters, and $x = (r - r_0)/r_0$. The parameter β is a/r_0 , here, a is the potential width, and r_0 is the equilibrium distance.

Here, we prefer to use the following mass-distribution

$$m(x) = m_0 + m_1 e^{-\beta x}, \quad (4)$$

where m_0 , and m_1 are real parameters. This distribution is finite at infinity, and enables us to analyze the results in the case of constant mass.

Substituting Eqs. (3) and (4) into Eq. (2), than we have

$$\begin{aligned} \frac{d^2\psi(x)}{dx^2} + \left\{ \frac{1}{\hbar^2 c^2} [E^2 - m_0^2 c^4] + \frac{2}{\hbar^2 c^2} [V_2 m_0 c^2 - m_0 m_1 c^4] e^{-\beta x} \right. \\ - \frac{1}{\hbar^2 c^2} [V_2^2 + 2V_1 m_0 c^2 - 2V_2 m_1 c^2 + m_1^2 c^4] e^{-2\beta x} \\ \left. + \frac{2}{\hbar^2 c^2} [V_1 V_2 - V_1 m_1 c^2] e^{-3\beta x} - \frac{V_1^2}{\hbar^2 c^2} e^{-4\beta x} \right\} \psi(x) = 0, \end{aligned} \quad (5)$$

By using the transformations on coordinate and wave function

$$z = e^{-\beta x}, \quad \psi(z) = \frac{1}{\sqrt{z}} \phi(z), \quad (6)$$

and with the help of the following parameters

$$\begin{aligned} A_1 &= Q^2 (E^2 - m_0^2 c^4) + \frac{1}{4}, \\ A_2 &= 2Q^2 (V_2 m_0 c^2 - m_0 m_1 c^4), \\ A_3 &= Q^2 (V_2^2 + 2V_1 m_0 c^2 - 2V_2 m_1 c^2 + m_1^2 c^4), \\ A_4 &= 2Q^2 (V_1 V_2 - V_1 m_1 c^2), \\ A_5 &= Q^2 V_1^2. \end{aligned} \quad (7)$$

we get

$$\frac{d^2\phi(z)}{dz^2} + \left(-A_3 + \frac{A_1}{z^2} + \frac{A_2}{z} - A_4 z - A_5 z^2 \right) \phi(z) = 0. \quad (8)$$

where $Q^2 = 1/\hbar^2 c^2 \beta^2$ in the above expressions ($0 \leq z \leq 1$). It would be interested the results obtained from the last equation for a special case $A_2=A_4 = 0$, which gives

$$\frac{d^2\phi(z)}{dz^2} + \left(\frac{A_1}{z^2} - A_5 z^2 \right) \phi(z) = A_3 \phi(z), \quad (9)$$

This equation has a similar form with the ones given by Eq. (7) in Ref. [17] for $A_5 \rightarrow \alpha^2$, $A_1 \rightarrow -\ell'(\ell' + 1)$, and $A_3 \rightarrow -\lambda$ (α , ℓ' , and λ are the parameters used in Ref. [17]). Eq. (9) corresponds to the equation of the harmonic oscillator with centrifugal potential barrier, so we could give the solutions as

$$\varepsilon_n = \mp \left\{ m_0^2 c^4 + \frac{4c^2}{\beta^2 \hbar^2} (m_1 c^2 + m_0)^2 [2n + 1 + \sqrt{\frac{1}{4} - V_1^2 Q^2}]^{-2} - \frac{1}{4Q^2} \right\}^{1/2}. \quad (10)$$

We turn to the solution of Eq. (8), and write the wave function as [38, 39]

$$\phi(z) = e^{pz+(1/2)qz^2} \sum_{n=0}^{\infty} a_n z^{2n+L+1/2}. \quad (11)$$

Substituting Eq. (11) into Eq. (8), and equating of the coefficients to zero, we get the following identities among coefficients, and the expressions for p, and q

$$X_n a_n + Y_{n+1} a_{n+1} + Z_{n+2} a_{n+2} = 0, \quad (12)$$

where

$$X_n = 2q(2n + L + 1) - A_3, \quad (13)$$

$$Y_n = A_2 + p(4n + 2L + 1), \quad (14)$$

$$Z_n = 4n(n + L) + 2L^2. \quad (15)$$

and

$$q^2 = A_5 \quad (16)$$

$$2pq = A_4. \quad (17)$$

where the new parameter L is defined as $L^2 \rightarrow Q^2(E^2 - m_0^2 c^4)$, and we choose the parameters as $p = Q(V_2 - m_1 c^2)$, and $q = -QV_1$ to obtain a physically solution.

On the other hand, X_n , Y_n and Z_n must satisfy the following condition to determine the coefficients in the system of equations given in Eqs. (13)-(15)

$$\det \begin{vmatrix} Y_0 & Z_1 & \dots & \dots & \dots & 0 \\ X_0 & Y_1 & Z_2 & \dots & \dots & 0 \\ X_1 & Y_2 & Z_3 & \dots & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & X_{n-1} & Y_n \end{vmatrix} = 0, \quad (18)$$

In the case of $a_n \neq 0$, but $a_{n+1} = a_{n+2} = \dots = 0$ in Eq. (12), we impose $X_n = 0$. This leads to the following algebraic equation

$$2q(2n + L + 1) = A_3. \quad (19)$$

Substituting the values of the parameters defined in Eq. (7) into Eq. (19), and by using p , and q obtained from Eqs. (16)-(17), we have the energy eigenvalues of the generalized Morse potential as

$$E_n = \pm \left\{ m_0^2 c^4 + \frac{1}{Q^2} [2n + 1 + Q\tilde{V}_1]^2 + \frac{m_1 c^2 \tilde{V}_2}{Q} [2(2n + 1) + 2Q\tilde{V}_1 + Qm_1 c^2 \tilde{V}_2] \right\}^{1/2}, \quad (20)$$

where

$$\tilde{V}_1 = \frac{V_2^2}{2V_1} + m_0 c^2, \quad \tilde{V}_2 = -\frac{V_2}{V_1} + \frac{m_1 c^2}{2V_1}, \quad (21)$$

It is seen that the energy levels of the particle and antiparticles are split around zero. On the other hand, the energy spectrum of the generalized Morse potential for the position-dependent mass is real. The part of the energy eigenvalues coming from the coordinate dependence of the mass is dependent on the quantum number n , and also on the potential parameters V_1 , and V_2 .

The corresponding wave functions can be written as the following

$$\phi_n(z) = (a_0 z^{1/2} + a_1 z^{5/2} + \dots) z^L \exp \left[Q(V_2 - m_1 c^2) z - \frac{QV_1}{2} z^2 \right]. \quad (22)$$

where $a_i (i = 0, 1 \dots)$ are the coefficients of the series.

In order to obtain the energy spectrum of the real generalized Morse potential for the case of constant mass, we have to set $m_1 = 0$ in Eq. (20), than we get

$$E_n^{m_1=0} = \pm \left(2n + 1 + Q\tilde{V}_1 \right) \sqrt{\frac{1}{Q^2} + \left(\frac{m_0 c^2}{2n + 1 + Q\tilde{V}_1} \right)^2}, \quad (23)$$

According to Eq. (23), the energy levels of the particle and antiparticles are symmetric about the zero in the limit of the constant mass. On the other hand, the energy spectrum of the real generalized Morse potential is purely real as in the first case.

We summarize the numerical results in Table I for the H₂, LiH, and HCl molecules in the case of the constant mass m_0 obtained from Eq. (23). We give the bound state energies of the particles (+ E_n), and antiparticles (- E_n) for different n-values in Table I. Further, we plot the dependence of the ground states of the above molecules on m_1 for H₂, and LiH, HCl molecules in Fig.1, and Fig.2, respectively. We do the numerical analysis in the range $10^{-6} < \frac{1}{M} < 10^{-4}$, where $M = m_0/m_1$, and (p) denotes the particle case, and (a) denotes the antiparticle one in figures.

The corresponding eigenfunctions in the case of the constant mass can be obtained from Eq. (22) by setting $m_1 = 0$.

B. Non-PT Symmetric and non-Hermitian Generalized Morse Case

Now we consider the complex case of the generalized Morse potential, where the potential parameters are written as

$$\begin{aligned} V_1 &= v_1^2 - v_2^2 + 2iv_1v_2, \\ V_2 &= v_1 + iv_2 + 2v_3(v_1 + iv_2). \end{aligned} \quad (24)$$

where v_i 's ($i = 1, 2, 3$) are the real parameters, and $\beta = 1$. This complex form of the generalized Morse potential is called non-PT symmetric/non-Hermitian potential form of the potential [41, 42].

Substituting Eq. (24) into Eq. (21), than we have from Eq. (20) for the energy spectra of the non-PT symmetric/non-Hermitian generalized Morse potential the following

$$E_n = \pm \left\{ m_0^2 c^4 + \frac{1}{Q'^2} [2n + 1 + Q' \tilde{V}'_1]^2 + \frac{m_1 c^2 \tilde{V}'_2}{Q'} [2(2n + 1) + 2Q' \tilde{V}'_1 + Q' m_1 c^2 \tilde{V}'_2] \right\}^{1/2}, \quad (25)$$

where

$$\tilde{V}'_1 = \frac{2(v_3 + 1)^2}{2} + m_0 c^2, \quad \tilde{V}'_2 = \frac{2v_3 + 1}{v_1 + iv_2} + \frac{m_1 c^2}{2(v_1 + iv_2)^2}, \quad Q' = \frac{1}{\hbar^2 c^2}. \quad (26)$$

The corresponding eigenfunctions can be written as

$$\phi_n(z) = (a_0 z^{L+1/2} + a_1 z^{L+5/2} + \dots) \exp \left[Q(V_2 - m_1 c^2)z - \frac{QV_1}{2} z^2 \right]. \quad (27)$$

The energy spectrum for the case of constant mass is given as

$$E_n^{m_1=0} = \pm (2n + 1 + Q' \tilde{V}'_1) \sqrt{\frac{1}{Q'^2} + \left(\frac{m_0 c^2}{2n + 1 + Q' \tilde{V}'_1} \right)^2}, \quad (28)$$

It is clearly seen that the energy eigenvalues of the non-PT symmetric/non-Hermitian generalized Morse potential has real and imaginary parts, which is coming from the coordinate dependence of the mass, but in the constant mass limit the energy spectrum is real. On the other hand, the energy levels of the non-PT symmetric/non-Hermitian generalized Morse potential is symmetric about zero as in the real potential case. The eigenfunctions for the case of constant mass are obtained by setting $m_1 = 0$ in Eq. (27).

III. CONCLUSION

We have obtained the solutions of the KG equation for the real and non-PT symmetric/non-Hermitian generalized Morse potential with position dependent mass. The

energy spectra and the corresponding wave functions have been obtained by using an infinite series for the wave function. We have found that the real generalized Morse potential has a real energy eigenvalues in the case of the position-dependent mass. We have summarized first the energy eigenvalues of three diatomic molecules for different values of n , and then plot two different graphs where the energy eigenvalues varying with mass to see the effects of the mass depending on spatially coordinate. We have also studied the non-PT symmetric/non-Hermitian case of the potential, and pointed out that the energy eigenvalues are imaginary in this case. We have found that the energy levels are purely real in the case of the constant mass as given in Eqs. (23), and (28) for both form of the generalized Morse potential.

IV. ACKNOWLEDGMENTS

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TABLE I: The dependence of bound states on n in MeV for H_2 ($D=38267.76 \text{ cm}^{-1}$, $a=1,9426 \text{ \AA}^{-1}$, $r_0 = 0,7416 \text{ \AA}$, and $m_0 = 0,50391 \text{ amu}$), LiH ($D=20287 \text{ cm}^{-1}$, $a=1,1280 \text{ \AA}^{-1}$, $r_0 = 1,5956 \text{ \AA}$, and $m_0 = 0,8801221 \text{ amu}$), and HCl molecule ($D=37255 \text{ cm}^{-1}$, $a=1,8677 \text{ \AA}^{-1}$, $r_0 = 1,2746 \text{ \AA}$, and $m_0 = 0,9801045 \text{ amu}$) [43] with $\ell = 0$.

n	$\pm E_n(H_2)$	$\pm E_n(LiH)$	$\pm E_n(HCl)$
0	663,819	1159,420	1291,130
2	663,827	1159,430	1291,140
4	663,835	1159,440	1291,150
10	663,859	1159,470	1291,190
20	663,899	1159,520	1291,260
30	663,939	1159,570	1291,330
40	663,979	1159,620	1291,390
50	664,020	1159,670	1291,460

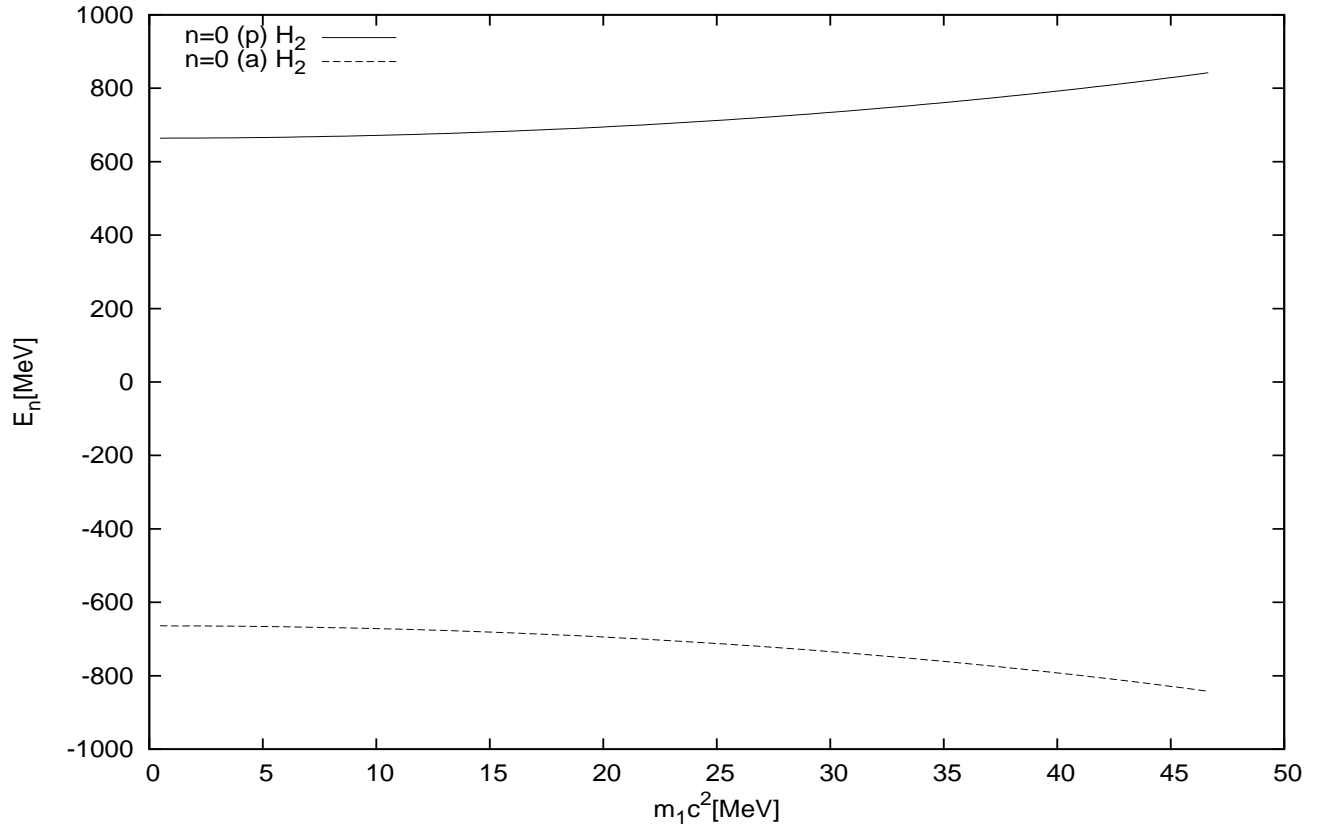


FIG. 1: The variation of ground states of the H_2 molecule with m_1 .

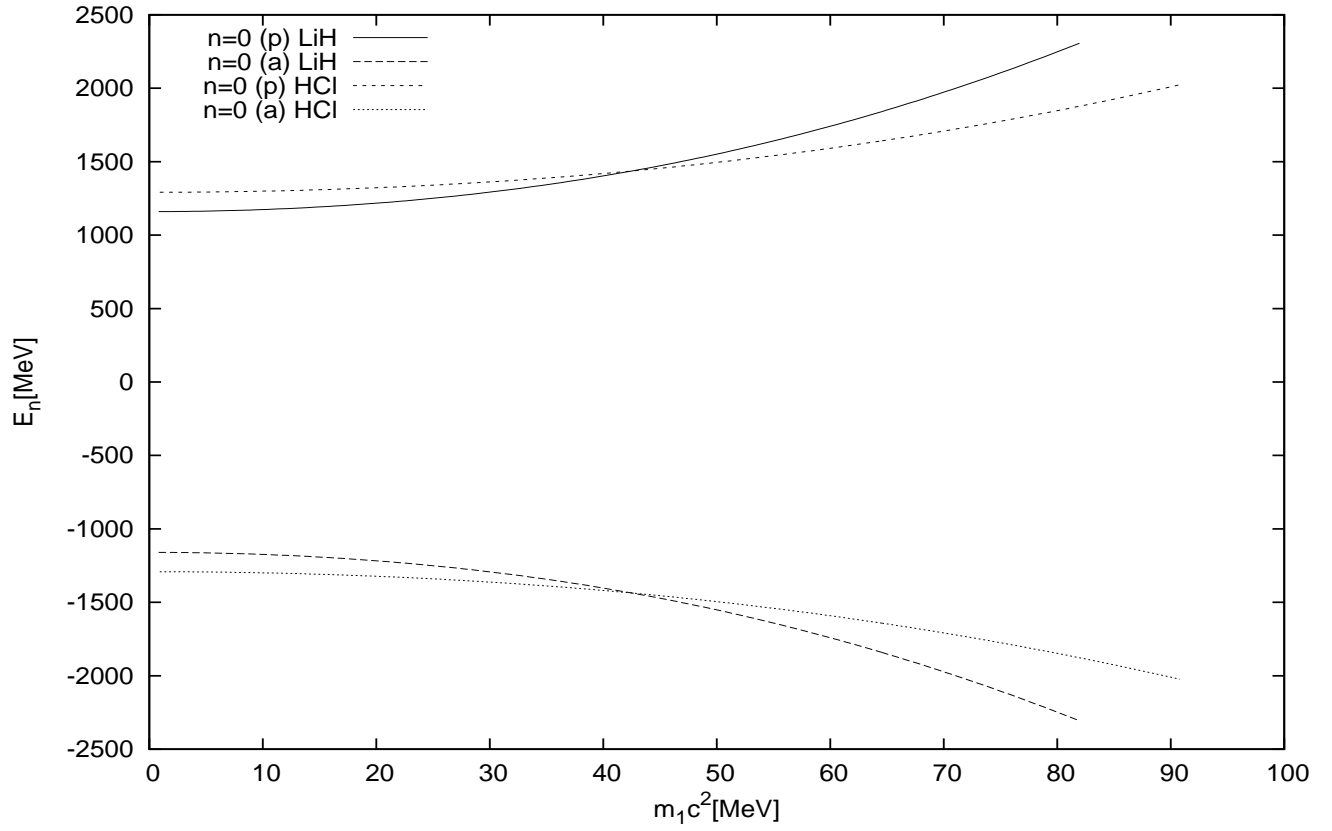


FIG. 2: The variation of ground states of the LiH, and HCl molecules with m_1 .