Effective-mass Klein–Gordon equation for non-PT/non-Hermitian generalized Morse potential

Altuğ Arda and Ramazan Sever

Department of Physics Education, Hacettepe University, 06800 Ankara, Turkey
Department of Physics, Middle East Technical University, 06531 Ankara, Turkey
E-mail: arda@hacettepe.edu.tr and sever@metu.edu.tr

Received 27 April 2010
Accepted for publication 6 October 2010
Published 10 November 2010
Online at stacks.iop.org/PhysScr/82/065007

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. Energy eigenvalues and corresponding eigenfunctions are obtained. They are also calculated for the constant mass case.

PACS numbers: 03.65.Fd, 03.65.Ge

1. Introduction
In the past few decades, there has been an increased interest in finding the exact solutions of non-relativistic and relativistic equations. The solutions of the Schrödinger equation have been studied using different methods based on perturbative and non-perturbative approaches [1–5]. The Klein–Gordon (KG) and Dirac equations have also been 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 PT-symmetric quantum mechanics. Following the initial studies of Bender et al [21], PT-symmetric theory has been successfully developed by many authors because of its importance, and also for its use in different research areas such as quantum field theory and nuclear physics [22], (23) and references therein. In the present study, we take into account the form of the generalized Morse potential also having the non-PT symmetric property to achieve solutions within the position-dependent mass formalism, and study the effects of mass varying with spatial coordinates against the solutions of the case of constant mass. It could be of interest to solve the relativistic KG equation from 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. Solving the above equations for the case of spatially dependent mass has been studied by many authors [26–34] for different types of mass distributions such as exponential and quadratic mass functions [27], inverse-quadratic mass dependence [35], trigonometric mass distributions [36], and mass functions of the form \( m(r) = r^n \), particularly for three-dimensional problems [36, 37]. We will also use a mass distribution with an exponential form and study it in the half-plane to achieve a physically acceptable (finite) mass function which has a decreasing 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 the generalized Morse potential in the case of coordinate-dependent 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 potential forms with two or more terms [38, 39]. We also obtain 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 2, we obtain the exact bound-state energy spectra for real, and non-PT symmetric/non-Hermitian cases of the generalized Morse potential. We also find and the corresponding eigenfunctions by taking an infinite series for the wave function.
function in the case of a convenient mass distribution. We summarize the numerical results in one table and two figures to show the effects of mass coordinate dependence. To this aim, we carry out the numerical analysis for three different diatomic molecules H₂, LiH and HCl. We also give the results for the case of constant mass and present our conclusions in section 3.

2. Bound state solutions

2.1. Real generalized Morse case

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

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

(1)

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

\[
\frac{d^2 \psi(x)}{dx^2} + \frac{2m}{\hbar^2} (E - V_s(x)) \psi(x) = 0, \quad (2)
\]

which is a Schrödinger-like equation with the energy eigenvalue \( \varepsilon = \frac{E^2}{2mc^2} - \frac{m^2 c^4}{\hbar^2} \). We deal with the KG equation in the case where the vector part of the potential is absent, since we are trying to obtain the analytical solutions of the KG equation for the generalized Morse potential within the position-dependent mass formalism based on the definition of mass function defined below.

We consider the scalar potential \( V_s(x) \) in (2) a generalized Morse potential, which can be used to describe the vibrations of a two-atomic molecule \( V_s(x) \) is of the form

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

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

Here, we prefer to use the following mass distribution:

\[
m(x) = m_0 + m_1 e^{-\beta x},
\]

(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 (3) and (4) into (2) yields

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

(5)

By using the coordinate and wave function transformations

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

(6)

and with the help of the following parameters:

\[
A_1 = Q^2 (E^2 - m_0^2 c^4) + \frac{1}{2},
A_2 = 2Q^2 (V_2 m_0 c^2 - m_0 m_1 c^4),
A_3 = Q^2 (V_1^2 + 2V_2 m_0 c^2 - 2V_1 m_1 c^2 + m_1^2 c^4),
A_4 = 2Q^2 (V_1 m_1 c^2 - V_1 V_2),
A_5 = Q^2 V_1^2,
\]

(7)

we obtain

\[
\frac{d^2 \phi(z)}{dz^2} + \left( -A_3 + \frac{A_1}{z} + \frac{A_2}{z^2} - A_4 z - A_5 z^2 \right) \phi(z) = 0,
\]

(8)

where \( Q^2 = 1/\hbar^2 c^2 \beta^2 \) in the above expressions \( 0 \leq z \leq 1 \). It would be interesting to look at the results obtained from the last equation for a special case \( A_2 = A_4 = 0 \). Doing so, we find that

\[
\frac{d^2 \phi(z)}{dz^2} + \left( \frac{A_1}{z^2} - A_5 z^2 \right) \phi(z) = A_3 \phi(z).
\]

(9)

This equation has a similar form to the one given by equation (7) in [17] where \( A_5 \rightarrow \omega^2, A_1 \rightarrow -\ell' (\ell' + 1) \) and \( A_3 \rightarrow -\lambda (\alpha, \ell', \lambda) \) are the parameters used in (17).

Our equation (9) corresponds to the differential equation of a harmonic oscillator with centrifugal potential barrier, so we obtain the energy eigenvalues

\[
\varepsilon_n = \left[ m_0 c^2 + Q^2 V_1^2 \right] \left[ 2(n + 1) + \sqrt{4 \bar{V}_1^2 Q^2 + 1} \right] - \frac{1}{4Q^2} \right)^{1/2},
\]

(10)

which could be used to obtain the bound state energies of the non-relativistic generalized Morse problem. The non-relativistic limit is obtained by taking \((1/c) \rightarrow 0 \) and \( \varepsilon_n \approx m_0 c^2 + \frac{1}{2} E_{NR} \) in (10) to obtain

\[
E_{NR} = -D + h \omega (2n + \frac{1}{2}),
\]

(11)

which is the energy eigenvalues of the Schrödinger equation for the Morse potential with a potential depth

\[
D = \frac{1}{16m_0} \left( \frac{\hbar^2 \beta^4}{8m_0^3} + V_1^2 \right)
\]

(12)

for low-energy vibrations with frequency \[41\]

\[
\omega = \frac{V_1^2}{8m_0} = \frac{1}{\hbar} \left( 2D - \frac{\hbar^4 \beta^4}{64m_0^3} \right).
\]

(13)

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

\[
\phi(z) = e^{\phi_0(z)} \sum_{n=0}^{\infty} a_n z^{2n + \lambda + 1/2}.
\]

(14)

Substituting (14) into (8) and equating coefficients, we obtain the following identities among coefficients:

\[
X_0 a_0 + Y_{n+1} a_{n+1} + Z_{n+2} a_{n+2} = 0,
\]

(15)
where
\begin{align}
X_n &= 2q(2n + L + 1) - A_3, \\
Y_n &= A_2 + p(4n + 2L + 1), \\
Z_n &= 4n(n + L) + 2L^2,
\end{align}
and expressions for \( p \) and \( q \)
\begin{equation}
q^2 = A_5, \tag{19}
\end{equation}
\begin{equation}
2pq = A_4, \tag{20}
\end{equation}
where the new parameter \( L \) is defined as \( L^2 \rightarrow Q^2(E^2 - m_0^2c^4) \) and we choose the parameters \( p = Q(V_2 - m_1c^2) \) and \( q = -QV_1 \) to obtain a physically realistic solution.

\( X_n, Y_n \) and \( Z_n \) must satisfy the following condition to determine the coefficients in the system of equations given by (16)–(18):
\begin{equation}
\det \begin{vmatrix}
Y_0 & Z_1 & \cdots & \cdots & \cdots & 0 \\
X_0 & Y_1 & Z_2 & \cdots & \cdots & 0 \\
X_1 & Y_2 & Z_3 & \cdots & \cdots & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\
0 & 0 & 0 & 0 & \cdots & Y_n
\end{vmatrix} = 0. \tag{21}
\end{equation}

In the case where \( a_n \neq 0 \) but \( a_{n+1} = a_{n+2} = \cdots = 0 \) in (15), we impose the condition \( X_n = 0 \). This leads to the following algebraic equation:
\begin{equation}
2q(2n + L + 1) = A_3. \tag{22}
\end{equation}

Substituting the values of the parameters defined in (7) into (22) and by using \( p \) and \( q \) obtained from (19) and (20), we may write the relativistic energy eigenvalues of the generalized Morse potential as
\begin{equation}
E_n = \pm \left\{ \sqrt{m_0^2c^4 + Q^2(2n + 1 + Q\tilde{V}_1)^2 + \frac{m_1c^2\tilde{V}_2}{Q}} \times \sqrt{2(2n + 1) + 2Q\tilde{V}_1 + Qm_1c^2\tilde{V}_2} \right\}^{1/2}, \tag{23}
\end{equation}
where
\begin{equation}
\tilde{V}_1 = \frac{V_2^2}{2V_1} + m_0c^2, \quad \tilde{V}_2 = -\frac{V_2}{V_1} + \frac{m_1c^2}{2V_1}. \tag{24}
\end{equation}

It is seen that the energy levels of the particle and antiparticle 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 \( V_2 \).

### Table 1. The dependence of bound states on \( n \) in \( \text{MeV} \) for \( \text{H}_2 \)

| \( n \) | \( \pm E_n(\text{H}_2) \) | \( \pm E_n(\text{LiH}) \) | \( \pm E_n(\text{HCl}) \) |
|-----|-----------------|-----------------|-----------------|
| 0   | 663.819         | 1159.420        | 1291.130        |
| 2   | 663.827         | 1159.430        | 1291.140        |
| 4   | 663.835         | 1159.440        | 1291.150        |
| 6   | 663.859         | 1159.470        | 1291.190        |
| 8   | 663.899         | 1159.520        | 1291.260        |
| 10  | 663.939         | 1159.570        | 1291.330        |
| 12  | 664.979         | 1159.620        | 1291.390        |
| 14  | 664.020         | 1159.670        | 1291.460        |

**Figure 1.** The variation of \( \text{H}_2 \) molecule ground states with \( m_1 \).

The corresponding wave functions can be written as follows:
\begin{equation}
\phi_n(z) = (a_0z^{1/2} + a_1z^{3/2} + \cdots)z^L \times \exp\left[ Q(V_2 - m_1c^2)z - \frac{QV_1}{2}z^2 \right], \tag{25}
\end{equation}
where \( a_i \) \((i = 0, 1, \ldots)\) 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 set \( m_1 = 0 \) in (23) which gives
\begin{equation}
E_{n=0}^{\text{const}} = \pm \left[ 2n + 1 + Q\tilde{V}_1 \right]^{1/2} \left( \frac{m_0c^2}{2n + 1 + Q\tilde{V}_1} \right)^2. \tag{26}
\end{equation}

According to (26), the energy levels of the particle and antiparticle are symmetric about zero in the case 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 1 for \( \text{H}_2 \), LiH and HCl molecules in the case of constant mass \( m_0 \) obtained from (26). We give the bound state energies of the particles \((+E_n)\), and antiparticles \((-E_n)\) for different \( n \)-values in table 1. Further, we plot the dependence of the ground states of the above molecules on \( m_1 \) in figure 1, and LiH, HCl.
molecules in figure 2. We conduct the numerical analysis in the range $10^{-6} < \frac{m_1}{m} < 10^{-2}$, where $M = m_0/m_1$, where (p) denotes the particle case, and (a) denotes the antiparticle one in the figures. Note that the corresponding eigenfunctions in the case of constant mass can be obtained from (25) by setting $m_1 = 0$.

2.2. Non-PT symmetric and non-Hermitian generalized Morse case

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

$$
V_1 = u_1^2 - u_2^2 + 2i\bar{u}_1 u_2,
V_2 = u_1 + i\bar{u}_2 + 2\bar{v}_2 (u_1 + i\bar{u}_2),
$$

where $u_i$ $(i = 1, 2, 3)$ are the real parameters and $\beta = 1$. This complex form of the generalized Morse potential is called the non-PT symmetric/non-Hermitian potential form [42, 43].

From (23), we obtain the energy spectra of the non-PT symmetric/non-Hermitian generalized Morse potential by substituting (27) into (24) to get

$$
E_n = \pm \left\{ m_c^2 c^4 + \frac{1}{Q^2} \left[ 2n + 1 + Q' \tilde{V}_1 \right]^2 \right\}^{1/2} \left\{ 2n + 1 + 2 Q' \tilde{V}_1 + Q' m_i c^2 \tilde{V}_2 \right\}^{1/2},
$$

where

$$
\tilde{V}_1 = \frac{2(u_1 + 1)^2}{2} + m_0 c^2, \quad \tilde{V}_2 = \frac{2u_3 + 1}{u_1 + iu_2} + \frac{m_1 c^2}{2(u_1 + iu_2)^2},
$$

$$
Q' = \frac{1}{\hbar^2 c^2}.
$$

The corresponding eigenfunctions can be written as

$$
\phi_n(z) = (a_0 z^{L+1/2} + a_1 z^{L+5/2} + \cdots) \exp \left[ Q (V_2 - m_1 c^2) z - \frac{Q \tilde{V}_1}{2} z^2 \right].
$$

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

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

(31)

It is clear that the energy eigenvalues of the non-PT symmetric/non-Hermitian generalized Morse potential have real and imaginary parts, which come 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 are symmetric about zero as in the real potential case. Note that the eigenfunctions for the case of constant mass are obtained by setting $m_1 = 0$ in (30).

3. Conclusion

We have obtained solutions of the KG equation for real and non-PT symmetric/non-Hermitian generalized Morse potential with position-dependent mass. The energy spectra and corresponding wave functions have been obtained by using an infinite series for the wave function. We have found that real generalized Morse potential has real energy eigenvalues in the case of position-dependent mass. We summarized first the energy eigenvalues of three diatomic molecules for different values of $n$, and then plotted two different graphs where the energy eigenvalues vary with mass to see the effects of mass depending on spatial coordinates. We also studied the non-PT symmetric/non-Hermitian case and pointed out that the energy eigenvalues are imaginary in this case. We found that energy levels are purely real in the case of constant mass as given in (26) and (31) for both forms of the generalized Morse potential.

Acknowledgments

This research was partially supported by the Scientific and Technical Research Council of Turkey.

References

[1] Killingbeck J P, Grosjean A and Jolicard G 2001 J. Phys. A: Math. Gen. 34 8309
[2] Arda A 2004 Turk. J. Phys. 28 223
[3] Chen J, Kweck L C and Oh C H 2003 Phys. Rev. A 67 012101
[4] Biswas S N et al 1973 J. Math. Phys. 14 1190
[5] Khare A and Sukhatme U P 1993 J. Phys. A: Math. Gen. 26 L901–4
[6] Hagen C R 1993 Phys. Rev. D 48 5935
[7] Villalba V M 1994 Phys. Lett. A 193 218
[8] de Castro A S 2007 Int. J. Mod. Phys. A 22 2609
[9] de Castro A S 2005 Phys. Lett. A 338 81
[10] de Castro A S 2005 Phys. Lett. A 346 71
[11] de Castro A S 2005 Phys. Lett. A 342 53
[12] Qiang W C, Zhou R-S and Gao Y 2007 Phys. Lett. A 371 201
[13] Saad N 2007 Phys. Scr. 76 623
[14] Giachetti R and Sorace E 2008 Phys. Rev. Lett. 101 190401
[15] Bhattacharya K 2007 (arXiv: 0705.4275)
[16] de Souza Dutra A and Hott M 2006 Phys. Lett. A 356 215
[17] Gang C, Zi-Dong C and Zhi-Mei L 2004 Chin. Phys. 13 279
[18] Gang C 2005 Phys. Lett. A 339 300
[19] Gang C 2001 Acta. Phys. Sin. 50 1651
[20] Yi L, Z, Diao Y F, Liu J Y and Jia C S 2004 Phys. Lett. A 333 212
[21] Bender C M, Boettcher S and Meisinger P N 1999 J. Math. Phys. 40 2201
[22] Ikhdair S M and Sever R 2007 Ann. Phys. 16 218
[23] Jia C S, Wang P Q, Liu J Y and He S 2008 Int. J. Theor. Phys. 47 2513
[24] Mostafazadeh A 1998 J. Phys. A: Math. Gen. 31 6495
[25] Mostafazadeh A 1997 Phys. Rev. A 55 4084
[26] Alhaidari A D 2004 Phys. Lett. A 322 72
[27] Dutra A S and Almeida C A S 2000 Phys. Lett. A 275 25
[28] Gönül B, Gönül B, Tutcu D and Ozer O 2002 Mod. Phys. Lett. A 17 2057
[29] Gönül B, Ozer O, Gönül B and Uzgun F 2002 Mod. Phys. Lett. A 17 2453
[30] Gönül B and Kocak M 2005 Chin. Phys. Lett. 20 2742
[31] Gönül B and Kocak M 2006 J. Math. Phys. 47 102101
[32] Tezcan C and Sever R 2007 J. Math. Chem. 42 387
[33] Vakarchuk I O 2005 J. Phys. A: Math. Gen. 38 4727
[34] Gang C and Chen Z 2004 Phys. Lett. A 331 312
[35] Jiang L, Yi L-Z and Jia C S 2005 Phys. Lett. A 335 249
[36] Alhaidari A D 2002 Phys. Rev. A 66 042116
[37] Ju G X, Xiang Y and Ren Z Z 2006
[38] Dong S H, Ma Z and Espozito G 1999 Found. Phys. Lett. 12 465
[39] Dong S H 2000 Int. J. Theor. Phys. 39 1119
Dong S H 2001 Int. J. Theor. Phys. 40 569
[40] de Castro A S 2005 Phys. Lett. A 338 81
[41] Flügge S 1971 Practical Quantum Mechanics I (Berlin: Springer) p 183
[42] Ahmed Z 2001 Phys. Lett. A 282 343
[43] Bagchi G and Quesne C 2000 Phys. Lett. A 273 285
[44] Filho E D and Ricotta R M 2000 Phys. Lett. A 269 269