Energy eigenfunctions for position-dependent mass particles in a new class of molecular hamiltonians

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Abstract

Based on recent results on quasi-exactly solvable Schrödinger equations, we review a new phenomenological potential class lately reported. In the present paper we consider the quantum differential equations resulting from position dependent mass (PDM) particles. We focus on the PDM version of the hyperbolic potential $V(x) = a \sech^2 x + b \sech^4 x$, which we address analytically with no restrictions on the parameters and the energies. This is the celebrated Manning potential, a double-well widely known in molecular physics, until now not investigated for PDM. We also evaluate the PDM version of the sixth power hyperbolic potential $V(x) = a \sech^6 x + b \sech^4 x$ for which we could find exact expressions under some special settings. Finally, we address a triple-well case $V(x) = a \sech^6 x + b \sech^4 x + c \sech^2 x$ of particular interest for its connection to the new trends in atomtronics. The PDM Schrödinger equations studied in the present paper yield analytical eigenfunctions in terms of local Heun functions in its confluents forms. In all the cases PDM particles are more likely tunneling than ordinary ones. In addition, a merging of eigenstates has been observed when the mass becomes nonuniform.

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I. INTRODUCTION

Over the years, the dynamics of quantum particles in every single substance has been a target for analytical studies in order to have a full understanding of condensed matter systems. This is certainly an ambitious task but, although generally frustrating, several phenomenologically relevant models have had its differential equations analytically solved \[1\text{–}17\].

New models involving hyperbolic potentials, typically found in molecular physics, have been reported very recently and in some cases have yield exact wavefunctions for certain relations among the parameters \[18\text{–}20\]. In the present paper it is our aim to deal with the family of potentials reported in \[18\] in connection with the issue of position-dependent mass (PDM) particles.

If the number of solvable potentials is not large in ordinary quantum mechanics, when we assume the particle mass has a nontrivial space distribution the mathematical difficulties grow considerably. For some relevant mass distributions some phenomenological potentials have been solved in recent years \[21\text{–}28\].

The origin of the PDM approximation can be traced back in the domain of solid state physics \[29\text{–}36\]. For instance, the dynamics of electrons in semiconductor heterostructures has been tackled with an effective mass model related to the envelope-function approximation \[36\text{–}38\]. Besides this, position dependent mass particles have been used to set to several important issues of low-energy physics related to the understanding of the electronic properties of semiconductors, crystal-growth techniques \[39\text{–}41\], quantum wells and quantum dots \[42\], Helium clusters \[43\], graded crystals \[44\], quantum liquids \[45\], and nanowire structures under size variations, impurities, dislocations, and geometrical imperfections \[46\], among others.

In this paper, assuming a PDM distribution in the Schrodinger equation, we take up on a new class of potentials \[18\] recently reported, viz.

\[
V(x) = -A \text{sech}^6 x - B \text{sech}^4 x - C \text{sech}^2 x. \tag{1}
\]

For a large variety of constants, this family represents symmetric asymptotically flat double-well potentials, related to problems of solid state and condensed matter physics. Double-well potentials are emblematic since they allow studying typical quantal situations involving
bound states and particle tunneling through a barrier. For example, the case \( A = 0 \) of Eq. (1) results in the renowned Manning potential originally used to address the vibrational normal modes of the \( \text{NH}_3 \) and \( \text{ND}_3 \) molecules and found also appropriate for the understanding of the infrared spectra of organic compounds such as ammonia, formamide and cyanamide. Coincidentally, the family given in also includes this potential when the parameter \( g >> 1 \). This class, also phenomenologically rich, was originally related to the double sine-Gordon kink but is known for its interest in different physical subjects such as the study of anti-ferromagnetic chains and experimentally accessible systems like \((\text{CH}_3)_4 \text{NMnCl}_3 \) (TMMC). In both papers the ordinary constant-mass Schrodinger equations have been found some analytical solutions proportional to Heun functions. These special functions are not very well-known but have been receiving increasing attention, particularly in the last decade.

Interestingly, although not explored in, the class given by Eq. (1) also includes three parameter triple-well potentials particularly interesting in atomtronics, associated with atomic diodes and transistors and laser optics. Triple-well semiconductor structures have been used in experiments of light transfer in optical waveguides as well as in models of dipolar condensates with phase transitions and metastable states.

In the present work we analyze the new potentials given by Eq. (1) with a physically significant input, namely a nonuniform mass. This phenomenological upgrade of course induces highly nontrivial consequences in the associated differential equations and yields new mathematical and physical results. Our goal is to analytically handle the resulting equations and find their general solutions. We succeed in some cases which we detail in what follows and find Heun functions in their confluent forms. In the case of triple-wells we manage it numerically for its high analytical complexity. In every case we compare the PDM results with the equivalent constant mass situations.

In the next section, we first address the problem of determining the correct kinetic operator of the PDM Schrodinger equation and then, in Sec. III we obtain an effective potential in a convenient space. In Sec. III A we consider the \( \text{PDM-Manning} \) potential, a particularly important member of the class, and find a complete set of eigenstates built in terms of confluent Heun solutions. We plot all the six eigenstates of the PDM differential equation together with those of the constant mass problem to show their deviation from the ordinary ones. Next, in section III B we find exact expressions for the \( E = 0 \) eigenfunctions
of the PDM version of the sixth power potential \( V(x) = a \sech^6 x + b \sech^4 x \) under some special settings. In this case, the eigenstates are proportional to triconfluent forms of the Heun functions. Finally, we address the triple-well phase of the potential class, with and without PDM, and discuss our results. The final remarks are drawn in Sec IV.

II. THE PDM KINETIC OPERATOR

The effective hamiltonian of a PDM nonrelativistic quantum particle has received much attention along the years for both phenomenological and mathematical reasons [32–37, 39, 69–80]. The full expression for the kinetic-energy hermitian operator for a position-dependent mass \( m(x) \) reads

\[
\hat{T} = \frac{1}{4} \hat{T}_0 + \frac{1}{8} \left\{ \hat{P}^2 m^{-1}(x) + m^\alpha(x) \hat{P} m^\beta(x) \hat{P} m^\gamma(x) + m^\gamma(x) \hat{P} m^\beta(x) \hat{P} m^\alpha(x) \right\},
\]

(2)

where, for constant mass, \( \hat{T}_0 = \frac{1}{2} \hat{P}^2 \) is the standard quantum kinetic energy and \( \hat{P} = -i \hbar \frac{d}{dx} \) is the momentum operator. The above parameters have to fulfill the condition \( \alpha + \beta + \gamma = -1 \) [33].

Recalling the basic postulate \([\hat{X}, \hat{P}] = i \hbar\), we get

\[
\hat{T} = \frac{1}{2m} \hat{P}^2 + \frac{i \hbar}{2} \frac{1}{m^2} \frac{dm}{dx} \hat{P} + U_K (x),
\]

(3)

where

\[
U_K (x) = \frac{-\hbar^2}{4m^3(x)} \left[ (\alpha + \gamma - 1) \frac{m(x)}{2} \left( \frac{d^2 m}{dx^2} \right)^2 + (1 - \alpha \gamma - \alpha - \gamma) \left( \frac{dm}{dx} \right)^2 \right]
\]

(4)

is an effective potential of kinematic origin. This is of course a source of ambiguity in the hamiltonian for it depends on the values of \( \alpha, \beta, \gamma \). In order to fix this issue, we can kill the kinematic potential by adding the constraint \( \alpha + \gamma = 1 = \alpha \gamma + \alpha + \gamma \). Its solution is \( \alpha = 0 \) and \( \gamma = 1 \), or \( \alpha = 1 \) and \( \gamma = 0 \), which corresponds to the Ben-Daniel–Duke \( \hat{T} \) ordering [36].

Now, the hamiltonian is free of ambiguities but the resulting effective Schrödinger equation still looks weird for it now includes a first order derivative term. For an arbitrary external potential \( V(x) \) the PDM-Schrödinger equation turns out

\[
\frac{d^2 \psi(x)}{dx^2} - \left( \frac{1}{m(x)} \frac{dm(x)}{dx} \right) \frac{d\psi(x)}{dx} + \frac{2}{\hbar^2} m(x) [E - V(x)] \psi(x) = 0.
\]

(5)

Noticeably, not only the last term has been strongly modified from the ordinary Schrödinger equation but the differential operator turned out to be dramatically changed. This will have of course deep consequences on the physical wave solutions of the system.
III. EFFECTIVE NEW PDM POTENTIAL

Here we will adopt a solitonic smooth effective mass distribution

\[ m(x) = m_0 \sech^2(x/d) \quad (6) \]

(see e.g. [24] and [27]). Besides its convenient analytical nature, its shape is familiar in effective models of condensed matter and low energy nuclear physics and depicts a soft symmetric distribution. The effective Schrödinger equation (5) thus reads

\[ \psi''(x) + 2 \tanh(x) \psi'(x) + \frac{2m_0}{\hbar^2} (E - V(x)) \sech^2(x) \psi(x) = 0, \quad (7) \]

but for the ansatz solution

\[ \psi(x) = \cosh^n(x) \varphi(x), \quad (8) \]

becomes

\[ \varphi''(x) + 2(n+1) \tanh(x) \varphi'(x) + \left[ n(n+2) \tanh^2 x + \left( n + \frac{2m_0}{\hbar^2} (E - V(x)) \right) \sech^2(x) \right] \varphi(x) = 0. \quad (9) \]

Now, a change of variables

\[ \sech x = \cos z, \quad (10) \]

maps the domain \((-\infty, \infty) \to (-\frac{\pi}{2}, \frac{\pi}{2})\) and provides

\[ \varphi''(z) + (2n + 1) \tan(z) \varphi'(z) + \left[ n + n(n+2) \tan^2(z) + \frac{2m_0}{\hbar^2} (E - V(z)) \right] \varphi(z) = 0 \quad (11) \]

(we call \(\varphi(x(z)) = \varphi(z)\), etc.). The choice \(n = -1/2\) allows the removal of the first derivative and grants an ordinary Schrödinger equation

\[ \left[ -\frac{d^2}{dz^2} + V(z) \right] \varphi(z) = \mathcal{E} \varphi(z) \quad (12) \]

where \(\mathcal{E} = \frac{2m_0}{\hbar^2} E\). The potential class we are dealing with is

\[ V(x) = -A \sech^6 x - B \sech^4 x - C \sech^2 x, \quad (13) \]

where the adjustable parameters determine a large variety of possible shapes. Thus, in Eq. (12) we shall employ

\[ V(z) = \frac{1}{2} + \frac{3}{4} \tan^2 z - A \cos^6 z - B \cos^4 z - C \cos^2 z, \quad (14) \]
where $A, B, C$ incorporated the factor $\frac{2m_0}{\hbar^2}$, e.g. $A = \frac{2m_0}{\hbar^2} \mathcal{A}$. The dynamics of the original PDM particle is therefore described by one of constant mass $m_0$ moving in $z$-space in a non-ambiguous effective potential with no kinematical contributions. Although restricted to within $z = (-\frac{\pi}{2}, \frac{\pi}{2})$, with $\varphi(z) = 0$ at the borders, we can eventually transform everything back to the original $x$-variable and $\psi$ wave-function to obtain the real space solution.

### A. The PDM-Manning potential

The celebrated Manning potential, $V(x) = a \sech^2 x + b \sech^4 x$, very much used in molecular physics, is here addressed in the very interesting situation of an effective spatially dependent mass. This phenomenological potential corresponds to the case $A = 0$ of Eq. (13). Note that when $B < 0, C > 0$ and $-C/2B < 1$, the Manning potential is a double-well potential with two minima at $x = \pm \text{arcsech}(\sqrt{-C/2B})$. In Fig. 1 we show this potential for several values of the free parameters.

![Figure 1. From top to bottom, plot of the Manning potential $V(x)$ (left) and $V(z)$ (right), for $(B, C) = (-500, 500)$, $(-1000, 1300)$, $(-1000, 1600)$; and $(-1000, 1800)$.](image)

In $z$-space we have

$$V(z) = \frac{1}{2} + \frac{3}{4} \tan^2 z - B \cos^4(z) - C \cos^2(z),$$

(15)

to be considered in eq. (12). By means of the ansatz

$$\varphi(z) = \cos^k z \phi(z)$$

(16)
we obtain
\[ \phi''(z) - 2\mu \tan(z) \phi'(z) + \left[ (\mu^2 - \mu - 3/4) \tan^2 z - \mu + \mathcal{E} - 1/2 + B \cos^4 z + C \cos^2 z \right] \phi(z) = 0 \] (17)
which can be simplified by choosing \( \mu^2 - \mu - 3/4 = 0 \), namely \( \mu = 3/2 \) or \( \mu = -1/2 \). If we now transform coordinates by \( y = \sin^2 z \), the above equation results in
\[ y (1 - y) \phi''(y) + \left[ \frac{1}{2} - (1 + \mu) y \right] \phi'(y) + \frac{1}{4} \left[ - \mu + \mathcal{E} - \frac{1}{2} + B(1 - y)^2 + C(1 - y) \right] \phi(y) = 0. \] (18)
A further transformation
\[ \phi(y) = e^{\nu y} H(y), \] (20)
puts in evidence its Heun nature
\[ h''(y) + \left( 2\nu + \frac{1}{2} + \frac{\mu + 1/2}{y - 1} \right) h'(y) + \frac{1}{4y(y-1)} \left[ \mu + \frac{1}{2} - 2\nu - \mathcal{E} - B - C \right. \\
\left. - 4 \left( \nu^2 - \nu - \mu \nu - \frac{B}{2} - \frac{C}{4} \right) y + (B - 4\nu^2) y^2 \right] h(y) = 0. \] (21)
Since \( \mu = -1/2 \) is misleading and \( \nu \) is arbitrary we choose \( \mu = 3/2 \) and \( 2\nu = \sqrt{B} \). This yields
\[ h''(y) + \left( \frac{\sqrt{B} + \frac{1}{2} + \frac{2}{y - 1}}{y(y-1)} \right) h'(y) + \\
\frac{1}{y(y-1)} \left[ \frac{1}{4} \left( B + C + 5\sqrt{B} \right) y + \frac{1}{2} - \frac{\sqrt{B} + \mathcal{E} + B + C}{4} \right] h(y) = 0, \] (22)
which is a canonical non-symmetric confluent Heun equation \([53, 60, 61]\) of the form
\[ Hc''(y) + \left( \alpha + \frac{\beta + 1}{y} + \frac{\gamma + 1}{y-1} \right) Hc'(y) + \frac{1}{y(y-1)} \left[ \left( \delta + \frac{\alpha}{2} (\beta + \gamma + 2) \right) y + \eta + \frac{\beta}{2} + \frac{1}{2}(\gamma - \alpha)(\beta + 1) \right] Hc(y) = 0, \] (23)
with
\[ \alpha = \sqrt{B} \]
\[ \beta = -1/2 \]
\[ \gamma = 1 \]
\[ \delta = \frac{1}{4} (B + C) \]
\[ \eta = \frac{1}{2} - \frac{\mathcal{E} + B + C}{4}. \]
Figure 2. Plot of the normalized symmetric solutions $\psi(1)(x)$ [Eq. (28)], when $B = -C = -500$ (see top (red) curve in Fig. 1), in their three symmetric bound states $\mathcal{E}_0 = -102.25913969050$ (left), $\mathcal{E}_2 = -61.4581676270$ (center) and $\mathcal{E}_4 = -25.9419535530$ (right). Below are shown the corresponding probability densities.

Therefore, the solutions of Eq. (22) are

$$h^{(1)}(y) = Hc \left( \sqrt{B}, -\frac{1}{2}, 1, \frac{1}{4}(B + C), \frac{1}{2} - \frac{\mathcal{E} + B + C}{4}; y \right)$$

$$h^{(2)}(y) = \sqrt{y} Hc \left( \sqrt{B}, \frac{1}{2}, 1, \frac{1}{4}(B + C), \frac{1}{2} - \frac{\mathcal{E} + B + C}{4}; y \right),$$

which in $z$-space result

$$\varphi^{(1)}(z) = \cos^2 z e^{\sqrt{\mathcal{E} + B} \sin^2 z} Hc \left( \sqrt{B}, -\frac{1}{2}, 1, \frac{1}{4}(B + C), \frac{1}{2} - \frac{\mathcal{E} + B + C}{4}; \sin^2 z \right)$$

$$\varphi^{(2)}(z) = \sin z \cos^2 z e^{\sqrt{\mathcal{E} + B} \sin^2 z} Hc \left( \sqrt{B}, \frac{1}{2}, 1, \frac{1}{4}(B + C), \frac{1}{2} - \frac{\mathcal{E} + B + C}{4}; \sin^2 z \right),$$

and in $x$-space read finally

$$\psi^{(1)}(x) = \text{sech}^2 x e^{\sqrt{\mathcal{E} + B} \tanh^2 x} Hc \left( \sqrt{B}, -\frac{1}{2}, 1, \frac{1}{4}(B + C), \frac{1}{2} - \frac{\mathcal{E} + B + C}{4}; \tanh^2 x \right)$$

$$\psi^{(2)}(x) = \tanh x \text{sech}^2 x e^{\sqrt{\mathcal{E} + B} \tanh^2 x} Hc \left( \sqrt{B}, \frac{1}{2}, 1, \frac{1}{4}(B + C), \frac{1}{2} - \frac{\mathcal{E} + B + C}{4}; \tanh^2 x \right).$$
Figure 3. Plot of the normalized antisymmetric solutions $\psi^{(2)}(x)$ [Eq. (29)], in their three antisymmetric bound-states when $B = -500 = -C$ (see top (red) curve in Fig. 1), for $\varepsilon_1 = -102.2558018532$ (left), $\varepsilon_3 = -61.3388827970$ (center) and $\varepsilon_5 = -24.20206500$ (right). Below are shown the corresponding probability densities.

In Figs. 2 and 3 we plot the solutions and probability densities of a PDM particle in the six bound-states of this PDM-Manning potential. Although the three pairs of probability distributions are very close, the corresponding solutions are certainly different (all the symmetric solutions are nonzero at the origin while the antisymmetric ones are of course null). This is particularly apparent for the third pair of eigenfunctions where the tunneling effect is highly manifest in the $\varepsilon_4$ eigenstate. As we foreseen, the PDM analytic expressions are quite different from the ordinary constant-mass solutions to the Manning potential found in [18]

$$\chi^{(1)}(x) = (\text{sech } x)^{\sqrt{-E}} H_c \left(0, -\frac{1}{2}, \sqrt{-E}, \frac{1}{4}B, \frac{1}{4} - \frac{E + B + C}{4}; \tanh^2 x \right)$$

$$\chi^{(2)}(x) = \tanh x (\text{sech } x)^{\sqrt{-E}} H_c \left(0, \frac{1}{2}, \sqrt{-E}, \frac{1}{4}B, \frac{1}{4} - \frac{E + B + C}{4}; \tanh^2 x \right).$$

In Figs. 4 and 5 we show both pairs of curves for the closest possible eigenenergies found for the two problems. We observe similar shapes in both sets with a rapidly increasing deviation from the ordinary constant-mass case for the higher eigenstates. Note that in all
the eigenstates the PDM particle has more probability to be near the origin of coordinates and thus keep on tunneling across the potential barrier. Another remarkable point is that while in the constant-mass case there exist fourteen bound-states in the PDM case there are only six. This shows a kind of merging of eigensates and a lower number of physical possibilities for growing energies assuming PDM (see Table I).

Figure 4. In solid line, the normalized PDM solutions $\psi^{(1)}(x)$ [Eq. (28)] for the three symmetric bound states $E_0 = -102.25913969050$ (left), $E_2 = -61.4581676270$ (center) and $E_4 = -25.9419535530$ (right). In dashed line the normalized ordinary solutions $\chi^{(1)}(x)$ [Eq. (30)] for the first three symmetric bound states $E_0 = -109.94122211881$ (left), $E_2 = -81.887958347499$ (center) and $E_4 = -57.567702358602$ (right). Here $B = -C = -500$; see top (red) Manning potential curve in Fig. I.
Figure 5. In solid line, the normalized PDM solutions $\psi^{(2)}(x)$ [Eq. (29)] for the three antisymmetric bound states $E_1 = -102.25580185320$ (left), $E_3 = -61.3388827970$ (center) and $E_5 = -24.20206500$ (right). In dashed line the normalized ordinary solutions $\chi^{(2)}(x)$ [Eq. (31)] for the first three antisymmetric bound states $E_1 = -109.9940489854443$ (left), $E_3 = -81.87558412881$ (center) and $E_5 = -57.474984727067$ (right). Here $B = -C = -500$; see top (red) Manning potential curve in Fig. 1.
B. The \textit{PDM} sixth-order hyperbolic potentials

Regarding the sixth-order members of family \[1\] we have tried to analytically disentangle the full problem but it seems too complex. In any case, we have been able to find the exact solution to the \textit{PDM}-modified differential equation for one free parameter in two specific cases: $B = 0, C = 0$, namely $V(x) = -A \sech^6(x)$, and $A = -B, C = 0$, that is $V(x) = -A(\sech^6(x) - \sech^4(x))$, for $E = 0$, both yielding \textit{triconfluent} Heun eigenfunctions [53] (see also e.g. [81]). In Fig. 6 and Fig. 9 we show these potentials for several values of the free parameter.

Table I. Complete list of the energy eigenvalues of the \textit{PDM} and constant-mass Manning Hamiltonians for $A = 0$ and $B = -C = -500$. The $\text{S}$ and $\text{A}$ subindexes at left indicate symmetric and antisymmetric states.

\begin{center}
\begin{tabular}{lll}
\hline
Constant mass & \textit{PDM} \\
\hline
$E_1^\text{S}$ & -109.9412221188093 & -102.2591396905 \\
$E_2^\text{A}$ & -109.9940489854443 & -102.2558018532 \\
$E_3^\text{S}$ & -81.887958347499 & -61.458167627 \\
$E_4^\text{A}$ & -81.875584128810 & -25.941953553 \\
$E_5^\text{S}$ & -57.567702358602 & -13.736298720 \\
$E_6^\text{A}$ & -57.474984727067 & -16.879030280 \\
$E_7^\text{S}$ & -37.240150270295 & -20.021459510 \\
$E_8^\text{A}$ & -36.841246822072 & -24.202065000 \\
$E_9^\text{S}$ & -21.195042009000 & -- \\
$E_10^\text{A}$ & -20.147434878873 & -- \\
$E_11^\text{S}$ & -9.457236339000 & -- \\
$E_12^\text{A}$ & -7.8621835775695 & -- \\
$E_13^\text{S}$ & -2.02308205000 & -- \\
$E_14^\text{A}$ & -0.961473079820 & -- \\
\hline
\end{tabular}
\end{center}
Figure 6. From top to bottom, plot of well potentials $V(x) = A \text{sech}^6(x)$ (left) and the corresponding effective potentials $V(z)$ (right) for $A = 10, 30, 50$ and $100$.

1. Case free $A$ and $B = C = 0$

In the first case, the $z$-space eq. (12) to solve is

$$\varphi''(z) - \left(\frac{1}{2} + \frac{3}{4} \tan^2(z) - A \cos^6(z)\right) \varphi(z) = 0.$$  \hspace{1cm} (32)

We first factorize $\varphi(z) = \cos^\sigma(z) \phi(z)$, bearing

$$\varphi''(z) - 2\sigma \tan(z) \phi'(z) + \left[(\sigma^2 - \sigma - \frac{3}{4}) \tan(z)^2 - \sigma - \frac{1}{2} + A \cos(z)^6\right] \phi(z) = 0.$$ \hspace{1cm} (33)

We then cut down this equation by choosing $\sigma = -1/2$. Now we transform the variable by means of $y = \sin^2 z$ and get

$$(-y^2 + 1) \phi''(y) + (A(-y^2 + 1)^3) \phi(y) = 0.$$ \hspace{1cm} (34)

It looks as the representative form of the triconfluent Heun equation and therefore we try with an exponential ansatz of the form $\phi(y) = e^{ay^3 + by} h(y)$ (see Proposition E.1.2.1 in [53]), so that Eq. (34) results

$$h''(y) + (6ay^2 + 2b)h'(y) + \left[6ay + (3ay^2 + b)^2 + A(-y^2 + 1)^2\right] h(y) = 0.$$ \hspace{1cm} (35)

This can be further shorten by means of $a = -\frac{1}{3} \sqrt{-A}$ and $b = \sqrt{-A}$ and if we next define the variable

$$\bar{y} = \left(\frac{2\sqrt{-A}}{3}\right)^{\frac{1}{3}} y$$

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we obtain
\[ h''(y) = \left[ 3 \ddot{y}^2 - (-12A)^{1/3} \right] h'(y) - 3 \dot{y} h(y) = 0. \] (36)

Now, this can be readily compared with
\[ H''(u) - (\gamma + 3u^2)H'(u) + [\alpha + (\beta - 3)u]H(u) = 0 \] (37)

which is known as the **canonical** triconfluent form of the Heun equation. Its L.I. solutions are
\[ H^{(1)}(u) = Ht(\alpha, \beta, \gamma; u) \] (38)
\[ H^{(2)}(u) = e^{u^3 + \gamma u} Ht(\alpha, -\beta, \gamma; -u). \] (39)

The triconfluent Heun equation is obtained from the **biconfluent** form through a process in which two singularities coalesce by redefining parameters and taking the appropriate limits. See [53] for a detailed discussion about the confluence procedure in the case of the Heun equation and its different forms. The function \( Ht(\alpha, \beta, \gamma; u) \) is a local solution around the origin, which is a regular point. Because the single singularity is located at infinity, this series converges in the whole complex plane and consequently its solutions can be related to the Airy functions \( 82 \).

Our solutions are thus
\[ h^{(1)}(y) = Ht \left( 0, 0, -(-12A)^{1/3}; (2/3 \sqrt{-A})^{1/3} y \right) \] (40)
\[ h^{(2)}(y) = \exp \left[ 2/3 \sqrt{-A} y (y^2 - 3) \right] Ht \left( 0, 0, -(-12A)^{1/3}; (2/3 \sqrt{-A})^{1/3} y \right), \] (41)

namely
\[ \phi^{(1)}(y) = \exp \left[ -1/3 \sqrt{-A} y (y^2 - 3) \right] Ht \left( 0, 0, -(-12A)^{1/3}; (2/3 \sqrt{-A})^{1/3} y \right) \] (42)
\[ \phi^{(2)}(y) = \exp \left[ 1/3 \sqrt{-A} y (y^2 - 3) \right] Ht \left( 0, 0, -(-12A)^{1/3}; -(2/3 \sqrt{-A})^{1/3} y \right). \] (43)

In variable \( z \), recalling that \( \varphi(z) = \cos z \phi(z) \), they result
\[ \varphi^{(1)}(z) = \cos z \exp \left[ -1/3 \sqrt{-A} \cos z (\cos^2 z - 3) \right] Ht \left( 0, 0, -(-12A)^{1/3}; (2/3 \sqrt{-A})^{1/3} \cos z \right) \] (44)
\[ \varphi^{(2)}(z) = \cos z \exp \left[ 1/3 \sqrt{-A} \cos z (\cos^2 z - 3) \right] Ht \left( 0, 0, -(-12A)^{1/3}; -(2/3 \sqrt{-A})^{1/3} \cos z \right) \] (45)

and finally, for \( \psi(x) = \text{sech}^{3/2} x \varphi(x) \) we have
\[ \psi^{(1)}(x) = \text{sech}^{3/2} x e^{\left[ \frac{1}{3} \sqrt{-A} \tanh (\text{sech}^2 x - 3) \right]} Ht \left( 0, 0, -(-12A)^{1/3}; (2/3 \sqrt{-A})^{1/3} \tanh x \right) \] (46)
\[ \psi^{(2)}(x) = \text{sech}^{3/2} x e^{\left[ \frac{1}{3} \sqrt{-A} \tanh (\text{sech}^2 x - 3) \right]} Ht \left( 0, 0, -(-12A)^{1/3}; -(2/3 \sqrt{-A})^{1/3} \tanh x \right). \] (47)
Figure 7. Plot of symmetric solutions $\psi_s(x)$ [up] and the corresponding probability densities $|\psi_s(x)|^2$ [down] given $B = C = 0$ and $E = 0$, for $A = 3.131784324$ (left); $A = 41.919051$ (center); and $A = 125.162981$ (right).

Note that although these solutions, Eqs. (46) and (47), are both complex functions, their symmetric and antisymmetric combinations are real. Furthermore, only the symmetric and antisymmetric solutions satisfy the border conditions and make physical sense. There is a discrete number of potential wells with an $E = 0$ eigenstate. We show these eigenfunctions for the first six values of $A$, see Fig. 7 and 8. It can be seen that the number of nodes of the zero-modes depends directly on the depths of the wells.
Figure 8. Plot of antisymmetric solutions $\psi_a(x)$ [up] and the corresponding probability densities $|\psi_a(x)|^2$ [down] given $B = C = 0$ and $E = 0$, for (left) $A = 16.962907791$; (center) $A = 77.987131$; and (right) $A = 183.4448166$.

2. Case free $B = -A$, and $C = 0$

Figure 9. From top to bottom, plot of double-well potentials $V(x) = A(\text{sech}^6(x) - \text{sech}^4(x))$ (left) and the corresponding effective potentials $V(z)$ (right) for $-A = 10, 20, 40$ and $80$.

The second case we managed to analytically solve corresponds to the hyperbolic sixth-order double-well plotted in Fig. 9.

In order to show this we have to analyze the following instance of the modified Schrödinger
eq. (12)
\[ \varphi''(z) - \left( \frac{1}{2} + \frac{3}{4} \tan^2(z) - \mathcal{A} \cos^6(z) + \mathcal{A} \cos^4(z) \right) \varphi(z) = 0. \] (48)

After transformation \( \varphi(z) = \cos^\mu(z) \phi(z) \) we get
\[ \phi''(z) - \left( \frac{1}{2} + \frac{3}{4} \tan^2(z) - \mu - 1/2 + \mathcal{A} \cos^6 z - \mathcal{A} \cos^4 z \right) \phi(z) = 0 \] (49)
which shortens to
\[ \phi''(z) + \tan(z) \phi'(z) + \left[ \mathcal{A} (1 - y^2)^2 - \mathcal{A} (1 - y^2) \right] \phi(y) = 0, \] (50)
provided one chooses \( \mu = -1/2 \).

Now, we change coordinates by \( y = \sin(z) \) yielding
\[ \phi''(y) + \left[ \mathcal{A} (1 - y^2)^2 - \mathcal{A} (1 - y^2) \right] \phi(y) = 0. \] (51)

As in the previous case, we try the ansatz \( \phi(y) = e^{ay^2+by} h(y) \) and get
\[ h''(y) + (6ay^2 + 2b) h'(y) + \left[ 6ay + b^2 + (\mathcal{A} + 9a^2) y^4 + (-\mathcal{A} + 6ab) y^2 \right] h(y) = 0, \] (52)
which simplifies conveniently when we adopt \( 3a = -\sqrt{\mathcal{A}} \) and \( 2b = \sqrt{-\mathcal{A}} \). We thus obtain
\[ h''(y) + \sqrt{-\mathcal{A}} \left( -2y^2 + 1 \right) h'(y) + \left( -2\sqrt{-\mathcal{A}} y - \mathcal{A}/4 \right) h(y) = 0 \] (53)
which, by redefining \( \bar{y} = \left( \frac{2\sqrt{-\mathcal{A}}}{3} \right)^{1/3} y \), gives
\[ h''(\bar{y}) - \left[ 3 \bar{y}^2 - \left( -\frac{3A}{2} \right)^{1/3} \right] h'(\bar{y}) + \left[ -3 \bar{y} + \left( \frac{-3A}{16} \right)^{2/3} \right] h(\bar{y}) = 0. \] (54)

This is the canonical triconfluent Heun equation
\[ H''(u) - (3u^2 + \gamma) H'(u) + [(\beta - 3)u + \alpha] H(u) = 0, \] (55)
as soon as we identify
\[ \alpha = \left( -\frac{3A}{16} \right)^{2/3} \]
\[ \beta = 0 \]
\[ \gamma = -\left( -\frac{3A}{2} \right)^{1/3}. \]
The solutions of eq. (54) are then
\[ h^{(1)}(y) = Ht \left( \left( -\frac{3A}{16} \right)^{2/3}, 0, -\left( -\frac{3A}{2} \right)^{1/3}, \left( \frac{2\sqrt{-A}}{3} \right)^{1/3} y \right) \] (56)
\[ h^{(2)}(y) = \exp \left[ \frac{2}{3} \sqrt{-A} y (y^2 - 3/2) \right] Ht \left( \left( -\frac{3A}{16} \right)^{2/3}, 0, -\left( -\frac{3A}{2} \right)^{1/3}, -\left( \frac{2\sqrt{-A}}{3} \right)^{1/3} y \right). \] (57)
Finally, by transforming everything back to the original $x$-space, we have the starting eigenfunctions of the PDM hamiltonian

$$
\psi^{(1)}(x) = e^{\sqrt{A} \tanh x (1/2 - 1/3 \tanh^2 x)} H t \left( \left(-\frac{3A}{16}\right)^{2/3}, 0, -\left(\frac{3A}{2}\right)^{1/3} \tanh x \right) \tag{58}
$$

$$
\psi^{(2)}(x) = e^{\sqrt{A} \tanh x (1/3 \tanh^2 x - 1/2)} H t \left( \left(-\frac{3A}{16}\right)^{2/3}, 0, -\left(\frac{3A}{2}\right)^{1/3} \tanh x \right) \tag{59}
$$

In this case, we found again that just the symmetric and antisymmetric combinations of Eqs. (58) and (59) are real functions and the only that fit the boundary conditions (as expected from the parity of the potential). After a numerical survey of the parameter space we found a discrete set of values of potential depths compatible with a zero energy eigenstate. In Figs. 10 and 11 we plot the eigenfunctions in the first six cases, three being even and the other antisymmetric, as indicated.

![Figure 10. Plot of symmetric PDM zero-modes $\psi_s(x)$ of $V(x) = A(\text{sech}^6(x) - \text{sech}^4(x))$ [up], and the corresponding probability densities $|\psi_s(x)|^2$ [down], for $A = -25.125695463186$ (left); $A = -209.2999338840$ (center); and $A = -571.605964500$ (right).](image)

For a constant mass, the general solution for this potential is

$$
\chi^{(1)}(x) = e^{1/2 \sqrt{A} \tanh^2 x (\text{sech} x) \sqrt{-E}} H c \left( \sqrt{A}, -\frac{1}{2}, \sqrt{-E}, 0, -\frac{1}{4} \text{ tanh}^2 x \right) \tag{60}
$$

$$
\chi^{(2)}(x) = e^{1/2 \sqrt{A} \tanh^2 x (\text{sech} x) \sqrt{-E}} \tanh x \ H c \left( \sqrt{A}, \frac{1}{2}, \sqrt{-E}, 0, -\frac{1}{4} \text{ tanh}^2 x \right) \tag{61}
$$
It is noteworthy that we found no zero-energy modes in the ordinary constant mass cases of neither $V(x) = A \text{sech}^6 x$ nor $V(x) = A(\text{sech}^6 x - \text{sech}^4 x)$ potentials.

3. Three-term potentials

The three-term potentials given by Eq. (1) have three possible phases: hyperbolic single-wells, hyperbolic double-wells and hyperbolic triple-wells. Since we have already analyzed in detail the first two situations, among which the PDM Poschl-Teller [21] and PDM Manning potentials respectively, we now focus on the triple-well case which oblige the three terms.

In Fig. 12 we show a sequence of triple-wells based on the Manning potential, already represented at the top of Fig. 1 now with the addition of a "sinh$^6 x"$$ term. It can be seen that in this case the bigger is $A$ the softer is the barrier. In Fig. 13 (up) we show the eigenstates of this three-term $PDM$-potential $A = 60$ (solid) together with the $A = 0$ (dashed) Manning potential. In Fig. 13 (down) we show again the $A = 60$ and $A = 0$ eigenstates but for an ordinary constant mass. We put the figures altogether in two lines for a more comprehensive comparison. In all the eigenstates we see a higher probability density.
around the origin in the $V_A(x)$ potential and, remarkably, the PDM particle is always more probably tunneling than the ordinary one. We have numerically computed the full spectrum of the $A = 60$ potential and found that for a constant-mass particle there are 14 eigenstates that for PDM merge into eight (see Table II).

Table II. Full list of the energy eigenvalues of the $PDM$ and constant-mass hamiltonians for $B = -C = -500$ and $A = 60$. The $S$ and $A$ subindexes indicate symmetric and antisymmetric states.

| Constant mass | $PDM$ |
|---------------|--------|
| $E^1_S$       | $E^1_A$ |
| $-119.74469342961597$ | $-113.818781855$ |
| $E^2_A$       | $E^2_A$ |
| $-119.7247052343852$ | $-113.7572364242$ |
| $E^3_S$       | $E^3_S$ |
| $-93.74280924014700$ | $-79.9396818103$ |
| $E^4_A$       | $E^4_A$ |
| $-93.3985291361313$ | $-78.185815300$ |
| $E^5_S$       | $E^5_S$ |
| $-72.4166803691808$ | $-55.2994525270$ |
| $E^6_A$       | $E^6_A$ |
| $-70.0578863544200$ | $-44.8009029700$ |
| $E^7_S$       | $E^7_S$ |
| $-55.5196963894542$ | $-26.8437685530$ |
| $E^8_A$       | $E^8_A$ |
| $-49.0703204490206$ | $-9.3961914300$ |
| $E^9_S$       | $E^9_S$ |
| $-38.5023159579192$ | $-9.4951818181818$ |
| $E^{10}_A$    | $E^{10}_A$ |
| $-30.432820320680$ | $-9.4951818181818$ |
| $E^{11}_S$    | $E^{11}_S$ |
| $-22.074924478020$ | $-9.4951818181818$ |
| $E^{12}_A$    | $E^{12}_A$ |
| $-15.125970648791$ | $-9.4951818181818$ |
| $E^{13}_S$    | $E^{13}_S$ |
| $-9.091694203800$ | $-9.4951818181818$ |
| $E^{14}_A$    | $E^{14}_A$ |
| $-4.5142592000$ | $-9.4951818181818$ |
Figure 12. Plot of $V(x) = -A \text{sech}^6 x - B \text{sech}^4 x - C \text{sech}^2 x$ for $A = 0$ (black), 60 (red), 120 (orange), 500 (blue) and $B = -C = -500$. The first is the Manning case already represented at the top of Fig. 1 and the following double-wells result from an $A$ term added to it.
Figure 13. Plot of symmetric eigenstates of $V_A(x) = V(x)_{Mann} - 60 \text{sech}^6(x)$ (solid) versus $V(x)_{Mann}$ (dashed) for PDM [up] and constant mass [down].

Likewise, when we add a “sech$^2 x$” term the zero-modes found in the previous section III B 2 and the values of $A$ for them to exist, deviate increasingly as $C$ goes bigger. In Fig. 14 we show the first zero-modes for $C = 10$ and $C = 2$ with respect to $C = 0$. These zero-modes take place for $A$ as listed in Table III. Adding a $C = 10$ term has a stronger effect and the first two $A$ values with a zero-mode are in this case positive. Note that as $C$ increases the zero energy particle tends to stay closer to the origin. Table III and the corresponding figures show that, as $A$ grows, the values of $A$ and the curves themselves rapidly converge to a unique one for all the three columns. In any case, the number of nodes of these eigenstates grows accordingly.
Figure 14. Comparative plot of $C = 10$ (orange solid) vs. $C = 2$ (blue dotted) vs. $C = 0$ (red dashed) for the first PDM zero-modes of potential $V(x) = A(\text{sech}^6(x) - \text{sech}^4(x)) + C \text{sech}^2 x$; see values of $A$ in Table III.
Now, let us finally deal with the triple-well phase of the family. In Fig. 15 we display a sequence of triple-well potentials constructed by setting specific relations among the parameters. In the first (left) figure the potential is about starting the triple-well phase. In this case, the first and second derivatives are zero at \( x = \pm \text{arcsech} \sqrt{-B/3A}, B/A < 0 \), for \( B^2 = 3AC \). We adopt \( A > 0 \) so that \( C > 0 \) and \( B < 0 \). In the second figure we let \( B^2 > 3AC \) and we get a couple of maxima, one at each side of the origin, resulting in three cleanly defined wells. In the third figure we let \( B^2 = 4AC \) when both maxima make simultaneously \( V'(x) = 0 \) and \( V(x) = 0 \). For \( B^2 > 4AC \) the potential develops a nonnegative barrier (see fourth figure).

![Figure 15. Plot of a sequence of potentials \( V(x) = -240 \text{sech}^6 x - B \text{sech}^4 x - 160 \text{sech}^2 x \) as described in the text.](image)

Table III. List of \( A \) values for which potential \( V(x) = A(\text{sech}^6(x) - \text{sech}^4(x)) + C \text{sech}^2 x \) has PDM zero-modes. The \( S \) and \( A \) subindexes at left indicate symmetric and antisymmetric states.

| \( C \)  | \( A_S^1 \) | \( A_A^1 \) | \( A_S^2 \) | \( A_A^2 \) | \( A_S^3 \) | \( A_A^3 \) | \( A_S^4 \) | \( A_A^4 \) | \( A_S^5 \) | \( A_A^5 \) | \( A_S^6 \) | \( A_A^6 \) | \( A_S^7 \) | \( A_A^7 \) | \( A_S^8 \) | \( A_A^8 \) |
|-------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|
|       | -25.125695463186 | -5.12163713219 | 119.20733625954 |
|       | -56.05506043240 | -45.04829005631 | 0.77393328576 |
|       | -209.2999338840 | -186.17085929030 | -96.85687735639 |
|       | -284.9369967664 | -270.878712213 | -213.6783204354 |
|       | -571.60596450 | -546.7836421587 | -447.94257185326 |
|       | -691.7230772070 | -676.0837563001 | -612.9440054961 |
|       | -1111.7112347 | -1085.76152523664 | -981.980281775 |
|       | -1276.268835001 | -1259.5595989779 | -1192.32726360 |

... ... ...
Figure 16. Plot of the potential \( V_T(x) = -800 \text{sech}^6 x + \sqrt{4AC} \text{sech}^4 x - 449 \text{sech}^2 x \).

For the triple-well represented in Fig. 16, \( V_T(x) = -A \text{sech}^6 x + \sqrt{4AC} \text{sech}^4 x - C \text{sech}^2 x \) \((A = 800, C = 449)\), we show the full PDM bound spectrum of eigenfunctions and probability densities in Fig. 17. As shown in Table IV, there is once again a reduction or merging of eigenstates for PDM in which case the ten (constant-mass) eigenstates result in just four eigenstates when the mass depends on the position.

Figure 17. Plot of PDM eigenfunctions and probabilities for \( V_T(x) = -800 \text{sech}^6 x + \sqrt{4AC} \text{sech}^4 x - 449 \text{sech}^2 x \). The full sequence of eigenergies has been numerically computed, see Table IV.
IV. CONCLUSION

In the present paper we have studied the new hyperbolic potential class recently reported in [18]. This time the mass of the particle has gained a position-dependent status in order to enrich the phenomenological possibilities of the models involved and explore its mathematical consequences. After properly setting up the PDM problem we have payed special attention to the celebrated Manning potential, of great interest in molecular physics, here studied in the PDM case for the first time. We have analytically obtained the complete set of eigenstates to this hamiltonian and then shown its full spectrum and eigenfunctions in a case study. We have analytically found confluent-Heun expressions in the general case and compared the PDM eigenfunctions to the constant-mass ones. Heun functions have recently been receiving increasing attention and have been found in a wide variety of contexts, see e.g. [83–88]. PDM particles tend to be more likely tunneling than the ordinary ones. Next, we have addressed the PDM version of the sixth power hyperbolic potential \( V(x) = -A \text{sech}^6 x - B \text{sech}^4 x \) and obtained exact expressions for the zero-modes in the \( A \) and

Table IV. Full list of the energy eigenvalues of the PDM and constant-mass triple-well hamiltonians for \( A = 800 \), \( C = 449 \), and \( B = -\sqrt{4AC} \approx -1198.67 \). The \( s \) and \( a \) subindexes at left indicate symmetric and antisymmetric states.

|      | Constant mass | PDM |
|------|---------------|-----|
| \( E_1^0 \) | -40.0750771677640 | -31.3132652539 |
| \( E_2^0 \) | -40.0731076274700 | -27.0691086460 |
| \( E_3^0 \) | -31.8627686815140 | -26.8175802300 |
| \( E_4^0 \) | -23.0630939687000 | -2.05157297020 |
| \( E_5^0 \) | -23.0065594776400 | |
| \( E_6^0 \) | -10.6509913784700 | |
| \( E_7^0 \) | -10.3287500184298 | |
| \( E_8^0 \) | -3.9363371967000 | |
| \( E_9^0 \) | -2.361296623000 | |
| \( E_{10}^0 \) | -0.782147401000 | |
\( A = -B \) cases belonging to a discrete set of parameters. All such eigenstates have been found proportional to triconfluent forms of the Heun functions. Interestingly, we have met with no zero-modes for any value of the parameter in the ordinary constant-mass counterpart of this potential. In both the Manning and sixth-order hyperbolic potentials we have also analyzed the consequences of considering a complementary three-term potential by comparing their eigenfunctions. The analysis of these and others three-terms cases has been performed for constant-mass and PDM hamiltonians and has shown interesting differences between their spectra, particularly a reduction of eigenstates in the PDM circumstance. Finally, we have discussed the triple-well phase of the potential class and focused especially in a \( V_T(x) = -A \text{sech}^6 x + \sqrt{4AC} \text{sech}^4 x - C \text{sech}^2 x \) case showing the full set of PDM eigenfunctions and probability densities. This triple-well also exposes the phenomenon of merging of the ordinary spectrum when the mass turns nonuniform. It seems to be a general property of this class of hamiltonians.
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