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De la Peña approach for Position-dependent Masses

Luis Canderle[1]*, Angelo Plastino

[1] *Department of Physics, National University La Pampa, Argentina.*
[2] *National University La Plata and IFLP-CCT-CONICET, C. C. 727, 1900 La Plata, Argentina.*
***Corresponding author**: g.kamuntavicius@gmf.vdu.lt

Abstract:
Schrödinger's equation for a position-dependent effective mass is successfully tackled using the De la Peña's factorization technique.

Keywords:
Schrödinger equation; Position-dependent mass; Factorization approach

1. INTRODUCTION

Many physical problems can be treated via a model employing a Schrödinger equation with a position-dependent mass (SEPDM) [0,1,2]. Such an approximation is useful for determining electronic properties of semiconductors [1] and quantum-dots [2]. The concept of effective mass is also relevant in connection with the energy density functional (EDF) approach to the quantum many-body problem. The EDF formalism has provided reasonable theoretical predictions of many experimental properties for several quantum many-body systems. Within the EDF approach, the nonlocal terms of the associated potential can be often interpreted as a position dependence on an appropriate, position dependent effective mass. This has been used for nuclei [3], quantum liquids [4], ^{3}He clusters [5], and metallic clusters [6]. There also exist exactly solvable models with smooth potentials and abrupt mass-jumps [7,8].

In another vein, one encounters interesting activity regarding the application of the so-called super-symmetric quantum mechanics (SUSY) [9,10,11] to SEPDM with $m = m(x)$. For any such system, a super-symmetric partner exists with the same mass-dependence [12]. The pertinent wave equation and eigen-energies of a SEPDM arise form solving an equation of the form

$$\left[-\nabla \frac{\hbar^2}{2m(\mathbf{r})} \nabla + V(\mathbf{r})\right] \psi(\mathbf{r}) = E\psi(\mathbf{r}) \tag{1}$$

We concentrate our efforts here on a SUSY-equivalent formulation advanced by L. de La Peña y R. Montemayor, discussed in reference [14], where it was applied to an important family of potential functions of the form [13] (expressed in Hartree atomic units [144])

$$V = \frac{1}{2}\left[1 - \frac{2}{\cosh^2 x}\right], \tag{2}$$

derived from the general instance

$$V = \frac{1}{2}\left[n^2 - \frac{n(n+1)}{\cosh^2 x}\right] \tag{3}$$

Our present goal is to show the de la Peña-Montemayor - Susy equivalence for SEPDMs.

2. Schrödinger EQUATION FOR A POSITION DEPENDENT EFFECTIVE MASS

The one-dimension SEPDM equation reads [7,8]

$$-\left(\frac{\hbar^2}{2m(x)}\right)\frac{d^2\psi}{dx^2} - \left[\frac{d}{dx}\left(\frac{\hbar^2}{2m(x)}\right)\right]\frac{d\psi}{dx} + V(x)\psi(x) = E\psi(x), \tag{4}$$

with $m(x)$ an effective mass, $V(x)$ the potential function, and E the eigen-energies. We face an eigen-values equation

$$H\psi = E\psi, \tag{5}$$

with a Hamiltonian

$$H = \mathscr{P}\left(\frac{1}{2m}\right)\mathscr{P} + V \tag{6}$$

with $\mathscr{P}$ the impulse. Eq. (4) can be derived from a variational principle similar to the standard one. The energy-expectation value is

$$\begin{gathered}\langle H\rangle = \\ = \int dx \psi(x)\left[-\tfrac{d}{dx}\left(\tfrac{\hbar^2}{2m(x)}\tfrac{d}{dx}\right) + V(x)\right]\psi(x) = \\ = \int dx\left[\tfrac{\hbar^2}{2m(x)}\left(\tfrac{d\psi(x)}{dx}\right)^2 + V(x)\psi^2(x)\right].\end{gathered} \tag{7}$$

It is easily seen that minimization of $\langle H\rangle$ under normalization constraint $\langle\psi \mid \psi\rangle = 1$ leads to Eq. (4). The wave function's ay an abrupt interface originated by a discontinuity of the effective mass, with $V(x)$ finite, are, in self-explanatory notation,

$$\psi_- = \psi_+ \tag{8}$$

plus the continuity of $\frac{1}{m(x)}\frac{d\psi(x)}{dx}$, i.e.,

$$\left(\frac{1}{m(x)}\frac{d\psi(x)}{dx}\right)_- = \left(\frac{1}{m(x)}\frac{d\psi(x)}{dx}\right)_+ \tag{9}$$

Sub-indexes $-$ and $+$ indicate, respectively, the left- and right-hand sides of the mass discontinuity. The last relation is also verified if, at the mass-discontinuity point x_0 the potential V exhibits a finite jump. If V displays a δ-singularity at x_0

$$V \sim V_0\delta(x - x_0), \tag{10}$$

it is possible to replace Eq. (9) by

$$\left(\frac{1}{m(x)}\frac{d\psi(x)}{dx}\right)_+ - \left(\frac{1}{m(x)}\frac{d\psi(x)}{dx}\right)_- = \frac{2V_0}{\hbar^2}\psi(x_0) \tag{11}$$

For more details see reference [15].

3. THE SUPER-SYMMETRIC FORMALISM

3.1 Generalized step operators

In this introductory Section m is constant. Reference [9] is excellent. The formalism is based upon the relations amongst (i) eigen-energies, (ii) eigen-values, and (iii) phase relations between the two partner Hamiltonians

$$H_1 = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V_1, \tag{12}$$

and

$$H_2 = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V_2, \tag{13}$$

associated to potentials that are called super-symmetric, namely, V^1 and V^2. Without loss of generality one can assume that H_1's ground state energy vanishes: $\left(E_0^{(1)} = 0\right)$ and that the associated ψ_0 is known. Then,

$$H_1\psi_0 = \left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V_1(x)\right)\psi_0 = 0. \tag{14}$$

It is clear that

$$V_1(x) = \frac{\hbar^2}{2m}\frac{\psi_0''}{\psi_0}. \tag{15}$$

Accordingly, H_1 adopts the appearance

$$H_1 = -\frac{\hbar^2}{2m}\left(\frac{d^2}{dx^2} - \frac{\psi_0''}{\psi_0}\right), \tag{16}$$

which suggests introducing two operators Q and $Q^\dagger$

$$\begin{aligned} Q &= \frac{\hbar}{\sqrt{2m}}\left[\frac{d}{dx} - \frac{\psi_0'}{\psi_0}\right] \\ Q^\dagger &= \frac{\hbar}{\sqrt{2m}}\left[-\frac{d}{dx} - \frac{\psi_0'}{\psi_0}\right], \end{aligned} \tag{17}$$

so that H_1 becomes

$$H_1 = Q^\dagger Q, \tag{18}$$

and

$$H_2 = QQ^\dagger = -\frac{\hbar^2}{2m}\left(\frac{d^2}{dx^2} + \frac{\psi_0''}{\psi_0} + 2\left[\frac{\psi_0'}{\psi_0}\right]^2\right) = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V_2, \tag{19}$$

where

$$V_2(x) = -V_1(x) - \frac{\hbar^2}{m}\left(\frac{\psi_0'}{\psi_0}\right)^2. \tag{20}$$

It is useful to define a "super-potential" $W(x)$. Given ψ_0, $W(x)$ is

$$W(x) = -\frac{\hbar}{\sqrt{2m}}\left(\frac{1}{\psi_0}\right)\left(\frac{d\psi_0}{dx}\right), \tag{21}$$

and one can cast V_1 - V_2 in $W-$terms

$$V_1 = W^2 - \frac{\hbar W'}{\sqrt{2m}}, \tag{22}$$

$$V_2 = W^2 + \frac{\hbar W'}{\sqrt{2m}}. \tag{23}$$

Also, we can write Q - $Q^\dagger$ in terms of $W(x)$:

$$Q = \frac{\hbar}{\sqrt{2m}} \frac{d}{dx} + W(x), \tag{24}$$

$$Q^\dagger = -\frac{\hbar}{\sqrt{2m}} \frac{d}{dx} + W(x). \tag{25}$$

With the knowledge of W one finds ψ_0

$$\psi_0(x) = \exp\left(-\frac{\sqrt{2m}}{\hbar}\int^x W(x)dx\right). \tag{26}$$

3.2 Identities

The first one is:

$$Q\psi_0 = 0 \tag{27}$$

Since $H^1\psi_0 = 0$ and using (17)

$$Q^\dagger Q\psi_0 = 0,$$

entailing

$$\langle\psi_0|Q^\dagger Q|\psi_0\rangle = 0. \tag{28}$$

Then, the norm of $Q|\psi_0\rangle$ vanishes as well. One also has

$$Q^\dagger H_2 - QH_1 = 0, \tag{29}$$

$$QH_1 - H_2 Q = 0. \tag{30}$$

Given the eigen-state ψ_n^1 of H_1 with energy E_n^1, one has

$$H_1\psi_n^1 = Q^\dagger Q\psi_n^1 = E_n^1\psi_n^1, \tag{31}$$

and applying Q on the left

$$QH_1\psi_n^1 = QQ^\dagger\left(Q\psi_n^1\right) = H_2\left(Q\psi_n^1\right) = E_n^1\left(Q\psi_n^1\right), \tag{32}$$

it is clear that $Q\psi_n^1$ is an eigen-state of H_2 with energy E_n^1, save for the ground state ψ_0^1 on account of (25). Analogously, starting from an eigen-state ψ_n^2 of H_2 of energy E_n^2 we find

$$H_2\psi_n^2 = QQ^\dagger\psi_n^2 = E_n^2\psi_n^2, \tag{33}$$

and applying on the left $Q^\dagger$ to (32):

$$Q^\dagger Q\left(Q^\dagger\psi_n^2\right) = H^1\left(Q^\dagger\psi_n^2\right) = E_n^2\left(Q^\dagger\psi_n^2\right), \tag{34}$$

is it obvious that $Q^\dagger\psi_n^2$ is an eigen-state of H_1 with energy E_n^2. Accordingly, the spectra of our two Hamiltonians can be derived one from the other. The relation between the respective eigen-values becomes:

$$E_n^2 = E_{n+1}^1 \quad n = 0,1,2,... \tag{35}$$

As for normalization, start from $\left\langle\psi_n^2\right|QQ^\dagger\left|\psi_n^2\right\rangle = E_n^2\left\langle\psi_n^2\right|\left.\psi_n^2\right\rangle$. If $\left|\psi_n^2\right\rangle$ is normalized, then

$$\left|\psi_n^1\right\rangle = \frac{1}{\sqrt{E_n^2}}Q^\dagger\left|\psi_n^2\right\rangle, \tag{36}$$

is normalized as well. A similar relation holds for $\left|\psi_n^2\right\rangle$:

$$\left|\psi_n^2\right\rangle = \frac{1}{\sqrt{E_n^1}}Q^\dagger\left|\psi_n^1\right\rangle. \tag{37}$$

4. de La Peña's FORMALISM

This is an alternative treatment which can be matched to that of SUSY [13,14] and we will call the de La Peña one. It is based upon a sort of universal operator for each system that we call here P. Let $\{|n\rangle\}$ stand for a Hilbert-basis, characterized by the set of quantum numbers n. Sea $\{p_n\}$ its eigen-value spectrum

$$P\,|n\rangle = p_n\,|n\rangle \tag{38}$$

The creation-destruction operators associated to P will be called $\eta^\dagger$ and η:

$$\eta^\dagger = \sum_n C_n\,|n+1\rangle\,\langle n|\,; \quad \eta = \sum_n C_{n-1}\,|n-1\rangle\,\langle n|\,, \tag{39}$$

the C_n being appropriate coefficients to be specified later. Rebaptize $|n\rangle \equiv |k\rangle$,

$$\eta^\dagger\,|k\rangle = C_k\,|k+1\rangle\,, \tag{40}$$

$$\eta\,|k\rangle = C_{k-1}\,|k-1\rangle\,. \tag{41}$$

The C_n are related to the bilinear operators $\eta\eta^\dagger$ - $\eta^\dagger\eta$, as from (39),

$$\eta\eta^\dagger\,|k\rangle = |C_k|^2\,|k\rangle \tag{42}$$

$$\eta^{\dagger}\eta\,|k\rangle = |C_{k-1}|^{2}\,|k\rangle \tag{43}$$

As customary, we assume that our spectra are bounded by below, linked to $n=0$, which entails (see (39.b))

$$\eta^{\dagger}\,|0\rangle = 0; \quad \Rightarrow\; C_{-1} = 0. \tag{44}$$

If an upper bound to the spectra also exists, say $n=N$, then

$$\eta^{\dagger}\,|N\rangle = 0; \quad \Rightarrow\; C_{N} = 0. \tag{45}$$

If not, this last restriction does not exist, of course. We are now in a condition to conjecture the form

$$P = a_{00} + a_{10}\eta\eta^{\dagger} + a_{01}\eta^{\dagger}\eta \tag{46}$$

and evaluate the p_m in the fashion

$$p_m = a_{00} + a_{10}\,|C_m|^{2} + a_{01}\,|C_{m-1}|^{2}, \tag{47}$$

ending up with $N+3$ unknowns, in particular, a_{00}, a_{10}, a_{01}, and $\{|C_n|, n=0,1,2,...,N-1\}$. We also have $N+1$ conditions from (43), with $n=0,1,2,...,N$, plus normalization, i.e., scale-fixing and origin-selection. This suffices for a complete determination of P´s spectrum. This line of reasoning makes it evident the convenience of working with the products of η an $\eta^{\dagger}$. We choose:

$$A = \left[\eta,\eta^{\dagger}\right] = \eta\eta^{\dagger} - \eta^{\dagger}\eta; \quad entailing\; S = \left\{\eta,\eta^{\dagger}\right\} = \eta\eta^{\dagger} + \eta^{\dagger}\eta, \tag{48}$$

so that

$$P = q_0 + q_a A + q_s S \tag{49}$$

where the constants will be conveniently adjusted. The eigen-values of A and S will be called, respectively, a_k and s_k. One has, via (39.a), (39.b), and (44):

$$\begin{gathered} A\,|k\rangle = a_k\,|k\rangle = \left(|C_k|^{2} - |C_{k-1}|^{2}\right)|k\rangle; \\ \text{entailing } S\,|k\rangle = s_k\,|k\rangle = \left(|C_k|^{2} + |C_{k-1}|^{2}\right)|k\rangle, \end{gathered} \tag{50}$$

where

$$a_k = |C_k|^{2} - |C_{k-1}|^{2};\ \text{entailing } s_k = |C_k|^{2} + |C_{k-1}|^{2}. \tag{51}$$

A little algebra shows that

$$|C_k|^{2} = \frac{1}{2}\left(s_k + a_k\right) = \frac{1}{2}\left(s_{k+1} - a_{k+1}\right). \tag{52}$$

The spectra of A and S satisfy a series of consistency relations.

(i) From (47) and (48)

$$s_k \geq 0; \quad s_k + a_k \geq 0; \quad s_k - a_k \geq 0. \tag{53}$$

(ii) From (48)

$$s_k + a_k = s_{k+1} - a_{k+1}, \tag{54}$$

and (iii), from (47) and (41.b):

$$s_0 = a_0; \quad s_N = -a_N. \tag{55}$$

Eq. (49) shows that S' spectrum is nonnegative and has a lower limit a_0. Eq. (50) fixes the $P-$spectrum structure. Lower and (possibly) upper bounds are determined by Eq. (51). If applying this equation leads to a contradiction, no upper bound exists. Consistency relations (49), (50), and (51) contain all available information regarding P.

5. POSITION-DEPENDENT MASS

Our original contribution enters here. Schrödinger's equation for $m = m(x)$ is

$$\left[-\nabla \frac{\hbar^2}{2m(x)} \nabla + V(x)\right] \psi(x) = E\psi(x), \tag{56}$$

i.e.,

$$-\left(\frac{\hbar^2}{2m(x)}\right)\frac{d^2\psi}{dx^2} - \left[\frac{d}{dx}\left(\frac{\hbar^2}{2m(x)}\right)\right]\frac{d\psi}{dx} + V(x)\psi(x) = E\psi(x) \tag{57}$$

Super-symmetric operators Q and $Q^\dagger$ are given in $W(x)$-terms as

$$Q\psi = \frac{\hbar\psi}{\sqrt{2m}}\frac{d\psi}{dx} + W\psi, \tag{58}$$

$$Q^\dagger\psi = -\frac{d}{dx}\left(\frac{\hbar\psi}{\sqrt{2m}}\right) + W\psi. \tag{59}$$

so that

$$H_1 = Q^\dagger Q = -\left(\frac{\hbar^2}{2m}\right)\frac{d^2}{dx^2} - \left(\frac{\hbar^2}{2m}\right)'\frac{d}{dx} - \left(\frac{\hbar W}{\sqrt{2m}}\right)' + W^2, \tag{60}$$

corresponding to an effective mass $m(x)$ moving in a potential

$$V_1 = -\left(\frac{\hbar W}{\sqrt{2m}}\right)' + W^2, \tag{61}$$

with

$$H_2 = QQ^\dagger = -\left(\frac{\hbar^2}{2m}\right)\frac{d^2}{dx^2} - \left(\frac{\hbar^2}{2m}\right)'\frac{d}{dx} - \left(\frac{\hbar W}{\sqrt{2m}}\right)' + W^2 + \frac{2\hbar(W)'}{\sqrt{2m}} - \left(\frac{\hbar}{\sqrt{2m}}\right)\left(\frac{\hbar}{\sqrt{2m}}\right)'' \tag{62}$$

$$= H_1 + \frac{2\hbar(W)'}{\sqrt{2m}} - \left(\frac{\hbar}{\sqrt{2m}}\right)\left(\frac{\hbar}{\sqrt{2m}}\right)''. \tag{63}$$

H_1 and H_2 describe particles of mass $m(x)$ moving in different potentials. One has

$$V_2 = V_1 + \frac{2\hbar (W)'}{\sqrt{2m}} - \left(\frac{\hbar}{\sqrt{2m}}\right)\left(\frac{\hbar}{\sqrt{2m}}\right)'' \tag{64}$$

The relation between the de La Peña's A and the SUSY-operators $Q^\dagger$ and Q for a position-dependent mass becomes

$$A\psi = QQ^\dagger\psi - Q^\dagger Q\psi = V_2 - V_1 = H_2 - H_1 = \frac{2\hbar (W)'}{\sqrt{2m}} - \left(\frac{\hbar}{\sqrt{2m}}\right)\left(\frac{\hbar}{\sqrt{2m}}\right)''. \tag{65}$$

If m does not depend upon x the above equation reduces to (taking $\hbar = m = 1$)

$$A = \sqrt{2}W'I \tag{66}$$

with I the identity operator, a relation that coincides with Eq. (4.3) of reference [14]. For de De La Peña's S one has

$$S\psi(x) = QQ^\dagger\psi + Q^\dagger Q\psi = H_2 + H_1 \tag{67}$$

$$= 2H_1 + \frac{2\hbar(W)'}{\sqrt{2m}} - \left(\frac{\hbar}{\sqrt{2m}}\right)\left(\frac{\hbar}{\sqrt{2m}}\right)'' \tag{68}$$

$$= 2\left[-\left(\frac{\hbar^2}{2m}\right)\frac{d^2}{dx^2} - \left(\frac{\hbar^2}{2m}\right)'\frac{d}{dx} - \left(\frac{\hbar W}{\sqrt{2m}}\right)' + W^2\right] + 2\frac{\hbar W'}{\sqrt{2m}} - \left(\frac{\hbar}{\sqrt{2m}}\right)\left(\frac{\hbar}{\sqrt{2m}}\right)''. \tag{69}$$

If m is independent of x, the above expression reduces to (taking $\hbar = m = 1$) to

$$S = 2\left[-\frac{1}{2}\frac{d^2}{dx^2} + W^2\right], \tag{70}$$

i.e., to Eq. (4.4) of reference [14]. One finds

$$P = q_0 + q_a A + q_s S \tag{71}$$

$$= q_0 + q_a\left[\frac{2\hbar(W)'}{\sqrt{2m}} - \left(\frac{\hbar}{\sqrt{2m}}\right)\left(\frac{\hbar}{\sqrt{2m}}\right)''\right] \tag{72}$$

$$+q_s\left(2\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} - \left(\frac{\hbar^2}{2m}\right)'\frac{d}{dx} - \left(\frac{\hbar W}{\sqrt{2m}}\right)' + W^2\right] + \frac{2\hbar W'}{\sqrt{2m}} - \left(\frac{\hbar}{\sqrt{2m}}\right)\left(\frac{\hbar}{\sqrt{2m}}\right)''\right). \tag{73}$$

Given that q_0, q_a, q_s are adjustable parameters, if we take $q_0 = 0$, $q_a = -\frac{1}{2}$, $q_s = \frac{1}{2}$, we can identify P with H_1 and the S-eigen-values are energy ones:

$$s_k = E_k \tag{74}$$

which reconfirms that we are working with the correct spectrum.

6. CONCLUSIONS

Eqs. (61) and (63) are De La Peña's expressions for A and S in the case of a position-dependent effective mass $m(x)$, whose obtention was the goal of this paper. These equation correctly reduced to the known forms for these operators when the mass is constant (see [14]). The all important adjustable parameters q_0, q_a, q_s have here the same form that they had acquired for reflection-less potentials in these operators when the mass is constant [14].This suggests that these forms for q_0, q_a, q_s might be universal.

7. References

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