Analytical simulations of double-well, triple-well and multi-well dynamics via rationally extended Harmonic oscillator

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Abstract. Quantum tunnelling in two-well, triple-well and multi-well potentials is studied analytically with the aid of exact propagators $K^{\sigma}(x,y;t)$ corresponding to rational extensions $H^{\sigma}=H_{\rm osc}+\Delta V^{\sigma}$ of the Harmonic oscillator.

Introduction

One of the main reason to develop new sophisticated analytical models is to use them as tests for the various approximations or as the starting point for perturbation methods. Due to the tunnelling, quantum evolution in the multi-well potentials becomes very complicated. Moreover, it is difficult to use perturbation theory or WKB approach. For instance, calculating path integral for a symmetric two-well potential one has to take into account instanton contributions [1].

The aim of this paper is to present the well-known rationally extended Harmonic oscillators as suitable analytical models for the description of quantum evolution in multi-well potentials. In this respect we follow the idea of works [2, 3], where wave packet dynamics and tunnelling for the oscillator's polynomial SUSY partners were studied with the aid of SUSY QM relations between propagators. We will show that propagators of monodromy free rational extensions of the Harmonic oscillator are expressed in the elementary functions only.

An important property of rational extensions is related with the analytical structure of wave-functions in the complex plane. There is a fundamental theorem which states that all monodromy free rational extensions of the Harmonic oscillator are constructed by a finite chain of level-removing Darboux transformations [4]. Hence, the general form of the corresponding Hamiltonian reads

$$H^{\sigma}=-\partial^2_{xx}+\frac{x^2}{4}-2\partial^2_{xx}(\ln \mathrm{Wr}[\mathrm{He}_{\sigma}(x),x])+2M\,, \tag{1}$$

where σ is a string of increasing integers which label removed energy levels and

$$\mathrm{He}_{\sigma}(x)=\mathrm{He}_{\{n_1,n_2,\ldots,n_{2M}\}}(x)=\{\mathrm{He}_{n_1}(x),\mathrm{He}_{n_2}(x),\ldots,\mathrm{He}_{n_{2M}}(x)\}\,.$$

Our suggestion is based on the following analytical structure of the corresponding propagators

$$K^\sigma(x,y;t) = K_{\rm osc}(x,y;t)\frac{\sum\limits_{k=0}^{\sigma[[-1]]+1} Q_k^\sigma(x,y)\mathrm{e}^{-\mathrm{i}kt}}{\sum\limits_{k=0}^{\sigma[[-1]]+1} Q_k^\sigma(x,y)} \tag{2}$$

where symmetric polynomials $Q_k^\sigma(x,y) = Q_k^\sigma(y,x)$ can be determined iteratively by a finite number of steps. These polynomials provide a non-linear connection between Hermite and exceptional Hermite polynomials.

Despite to the fact that rational extensions of harmonic oscillator are well studied, some important questions still wait an answers. For instance, it worth to know how the shape of a potential (the number and the structure of wells and barriers) depends on the parameters of extension (i.e. on the sequence σ of deleted levels). Regarding the shape of potentials V^σ, it is known that $V^{\{k,k+1\}}$ is a k-well potential [5]. This "landscape" problem for the rational extensions of the Harmonic oscillator is closely related to the pole configurations of the corresponding potentials, which are defined by zeros of wronskians $\mathrm{Wr}[\mathrm{He}_\sigma(x),x]$. As it was shown in [6] these zeros obey the Calogero relations. Some recent advantages in this direction come from studies of "locus" (the term introduced by Airault, McKean and Moser) [7, 8]. In particular, for a certain class of sequences σ, a simple qualitative relation is observed between the shape of the corresponding Young diagram and the pattern of zeros of the Wronskian of the corresponding Hermite polynomials. It is interesting that zeros of exceptional Hermite polynomials define vortex configurations for quadrupole background flow [8].

The paper is organized as follows. In the first section we present a non-linear connection formula between eigen-projectors of the Harmonic oscillator and its rational extensions. Applying this formula to the propagator expansion we obtain analytical expressions for propagators K^σ. In the next sections we will analyse two-well and triple-well potentials as well the corresponding propagators. In a conclusion possible applications are discussed.

1. Rationally extended propagators

1.1. Non-linear connection coefficients

Consider Harmonic oscillator and its (monodromy free) rational extension

$$H_{\rm osc}\psi_n(x) = \left(n+\frac{1}{2}\right)\psi_n(x)\,, \qquad H^\sigma\psi_n^\sigma(x) = \left(n+\frac{1}{2}\right)\psi_n^\sigma(x)\,. \tag{3}$$

First of all, two Hamiltonians are almost isospectral, that is $\mathrm{spec}H^\sigma \subset \mathrm{spec}H_{\rm osc}$ and $\mathrm{spec}H_{\rm osc}\setminus\mathrm{spec}H^\sigma = \sigma$.

It is well known that bound state wave functions for the rationally extended Harmonic oscillator

$$\psi_n^\sigma(x) = \frac{N_n\mathrm{He}_n^\sigma(x)}{W(x)}\mathrm{e}^{\frac{-x^2}{4}} = \frac{h_n^\sigma(x)}{W(x)}\mathrm{e}^{\frac{-x^2}{4}}\,, \tag{4}$$

are related with the oscillator bound state wave functions

$$\psi_n(x) = p_n\mathrm{He}_n(x)\mathrm{e}^{-\frac{x^2}{4}}\,, \qquad p_n = \left(n!\sqrt{2\pi}\right)^{-\frac{1}{2}}\,, \tag{5}$$

by a Darboux transformation. Here and in what follows, together with standard (probabilistic) Hermite polynomials $\mathrm{He}_n(x)$ and exceptional Hermite polynomials

$$\mathrm{He}_n^\sigma(x) = \mathrm{Wr}[\mathrm{He}_{\sigma\cup\{n\}}(x),x]\,, \tag{6}$$

we will use their normalized versions $h_n(x)$ and $h_n\sigma(x)$

$$\begin{aligned} h_n(x) &= p_n \mathrm{He}_n(x)\,, & (7) \\ h_n^\sigma(x) &= N_n \mathrm{Wr}[h_{\sigma\cup\{n\}}(x), x] & (8) \end{aligned}$$

where a normalization factor reads

$$N_n = \begin{cases} \left(\prod_{j=1}^{2M} (n - \sigma[[j]])\right)^{-\frac{1}{2}}, & n \notin \sigma\,, \\ 0\,, & n \in \sigma\,. \end{cases} \tag{9}$$

Finally, the compact notations for the following Wronskians are in order

$$W(x) = \mathrm{Wr}[\mathrm{He}_\sigma(x), x]\,, \qquad w(x) = \mathrm{Wr}[\mathrm{h}_\sigma(x), x]\,. \tag{10}$$

Recently we discovered an alternative possibility to express exceptional Hermite polynomials from standard ones using

Non-linear connection Lemma [9]. Given a Krein-Adler sequence $\sigma = \{k_1, k_1{+}1 \ldots, k_M, k_M{+}1\}$, the corresponding family of (formally normalized) exceptional Hermite polynomials $h_n^\sigma(x)$ obeys the following relation

$$\sum_{k=0}^{\sigma[[-1]]+1} h_{m-k}(x) h_{m-k}(y) Q_k^\sigma(x,y) = h_m^\sigma(x) h_m^\sigma(y)\,, \tag{11}$$

where symmetric connection polynomials Q_k^σ are given by

$$Q_k^\sigma(x,y) = \frac{1}{h_0(x)h_0(y)} \left(h_k^\sigma(x) h_k^\sigma(y) - \sum_{j=1}^{k} Q_{k-j}^\sigma(x,y) h_j(x) h_j(y) \right), \\ 0 \le k \le \sigma[[-1]] + 1\,, \tag{12}$$

and sum of connection polynomials is equal to product of Wronskians $w(x)w(y)$ defined above in (10)

$$\sum_{k=0}^{\sigma[[-1]]+1} Q_k^\sigma(x,y) = w(x)w(y)\,. \tag{13}$$

The proof of this lemma was given in [9].

It is also convenient to rewrite these relations in terms of the corresponding wave functions. Introducing projectors

$$\Pi_n(x,y) = \psi_n(x)\psi_n(y)\,, \qquad \Pi_n^\sigma(x,y) = \psi_n^\sigma(x)\psi_n^\sigma(y)\,, \tag{14}$$

we write (11) as follows

$$\frac{\sum_{k=0}^{\sigma[[-1]]+1} \Pi_{m-k}(x,y) Q_k^\sigma(x,y)}{w(x)w(y)} = \Pi_m^\sigma(x,y)\,. \tag{15}$$

There are also several equivalent representations of non-linear connection lemma in a form of some matrix equations. For instance, $\sigma[[-1]]+2$ dimensional vector $\vec{Q}^\sigma$ can be defined as a solution of the following matrix equation

$$\begin{pmatrix} \Pi_0 & 0 & 0 & \dots & 0 \\ \Pi_1 & \Pi_0 & 0 & \dots & 0 \\ \Pi_2 & \Pi_1 & \Pi_0 & 0 & 0 \\ \dots & \dots & \dots & \dots & 0 \\ \Pi_{2M+1} & \Pi_{2M} & \dots & \dots & \Pi_0 \end{pmatrix} \begin{bmatrix} Q_0^\sigma \\ Q_1^\sigma \\ Q_2^\sigma \\ \dots \\ Q_{2M+1}^\sigma \end{bmatrix} = w(x)w(y) \begin{bmatrix} \Pi_0^\sigma \\ \Pi_1^\sigma \\ \Pi_2^\sigma \\ \dots \\ \Pi_{2M+1}^\sigma \end{bmatrix}, \tag{16}$$

defined by a Toeplitz matrix $\hat{\Pi}_t$ and a vector $\vec{\Pi}^\sigma$ with $2M$ vanishing components. That is, the vector $\vec{Q}^\sigma$ yields

$$\vec{Q}^\sigma = w(x)w(y)\hat{\Pi}_t^{-1}\vec{\Pi}^\sigma .$$

From another hand, we have the following (semi-infinite) matrix equation

$$\begin{pmatrix} Q_0^\sigma & 0 & 0 & 0 & 0 & \dots \\ Q_1^\sigma & Q_0^\sigma & 0 & 0 & 0 & \dots \\ Q_2^\sigma & Q_1^\sigma & Q_0^\sigma & 0 & 0 & \dots \\ \dots & \dots & \dots & \dots & 0 & \dots \\ Q_{\sigma[[-1]]+1}^\sigma & Q_{\sigma[[-1]]}^\sigma & \dots & \dots & Q_0^\sigma & \dots \\ 0 & Q_{\sigma[[-1]]+1}^\sigma & Q_{\sigma[[-1]]}^\sigma & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots \end{pmatrix} \begin{bmatrix} \Pi_0 \\ \Pi_1 \\ \Pi_2 \\ \dots \\ \dots \\ \dots \\ \dots \\ \dots \end{bmatrix} = w(x)w(y) \begin{bmatrix} \Pi_0^\sigma \\ \Pi_1^\sigma \\ \Pi_2^\sigma \\ \dots \\ \dots \\ \dots \\ \dots \\ \dots \end{bmatrix}, \tag{17}$$

1.2. Rational ansatz for the propagators

Combining non-linear connection (15) between projectors and expansion of propagators

$$\begin{aligned} K_{\mathrm{osc}}(x,y;t) &= \lambda^{\frac{1}{2}} \sum_{n=0}^{\infty} \lambda^n \Pi_n(x,y)\,, \qquad \lambda = \mathrm{e}^{-\mathrm{i}t}\,, && (18) \\ K^\sigma(x,y;t) &= \lambda^{\frac{1}{2}} \sum_{n\in\mathbb{N}\backslash\sigma} \lambda^n \Pi_n^\sigma(x,y)\,, && (19) \end{aligned}$$

one can obtain closed expression for the propagator K^σ

$$K^\sigma(x,y;t) = K_{\mathrm{osc}}(x,y;t) \frac{\sum\limits_{k=0}^{\sigma[[-1]]+1} Q_k^\sigma(x,y)\mathrm{e}^{-\mathrm{i}kt}}{\sum\limits_{k=0}^{\sigma[[-1]]+1} Q_k^\sigma(x,y)} \tag{20}$$

in terms of elementary functions.

2. Exact propagators for two-well rational extensions of the Harmonic oscillator

The simplest two-well rational extension of the Harmonic oscillator reads (see also Fig. 1)

$$V^{\{2,3\}}(x) = \frac{x^2}{4} + 2\left(1 + 4x^2\frac{x^4-9}{(x^4+3)^2}\right). \tag{21}$$

This is a so-called "shallow" two-well potential since it holds only one pair of bound states below $V^{\{2,3\}}(0)$.

k	$Q_k^{\{2,3\}}(x,y)$
0	$\frac{(1+x^2)(1+y^2)}{4\pi}$
1	$-\frac{xy(-3+x^2y^2)}{6\pi}$
2	$\frac{-3-12x^2y^2+3y^4+3x^4+x^4y^4}{24\pi}$
3	$\frac{xy(-3+x^2y^2)}{6\pi}$
4	$\frac{(x^2-1)(y^2-1)}{4\pi}$

Table 1. Sequence of connection polynomials $Q_k^{\{2,3\}}(x,y)$

Explicit expressions of connection polynomials $Q_k^{\{2,3\}}(x,y)$ are given in Table 2. Hamiltonian $H^{\{2,3\}}$ has the quasi-equidistant spectrum, $E_n = n + \frac{1}{2}$, $n \in \mathbb{N}_0 \setminus \{2,3\}$. That is the ground and the first excited states are separated from the equidistant part of the spectrum by a gap energy $\Delta E_g = 3$. Using connection polynomials we can construct propagator $K^{\{2,3\}}(x,y;t)$ by rational ansatz (20). It reads explicitly

$$K^{\{2,3\}} = \mathrm{e}^{-2\mathrm{i}t} K_{\mathrm{osc}}(x,y;t) \left(1 - \frac{8\mathrm{i}\sin t \left[xy(x^2y^2-3) - 3(x^2+y^2)\cos t - 3\mathrm{i}(x^2y^2+1)\sin t \right]}{(3+x^4)(3+y^4)} \right).$$

Propagator $K^{\{2,3\}}(x,y;t)$ completely describes wave packet dynamics in the potential (21).

In general a wide class of two-well extensions (see Fig. 1) can be classified by two parameters. The first parameter is the splitting $\Delta E_s = 2s+1$, $s = 0,1,\ldots$ of the ground state and the first excited state (it is always an odd integer). The second parameter is the gap energy $\Delta E_g = 2g+1$, $g = 1,2,\ldots$ between the first excited state and the second excited state. For instance, when $\sigma = \{2,3\}$ we have $\Delta E_s = 1$, $s = 0$, and $\Delta E_g = 3$, $g = 1$. Numerical studies suggest that when

$$s \geq 2g\,,$$

two minima will collapse. An example of collapsing wells when g is fixed and s is increased can be seen in the first column of Fig. 1.

A two-well rational extension of the Harmonic oscillator which corresponds to $s = 1$, $g = 1$ gives the following potential

$$V^{\{1,2,4,5\}}(x) = \frac{x^2}{4} + 4 - \frac{80(5+10x^2+7x^4)}{(5+5x^2+5x^4+x^6)^2} + \frac{12(5+x^4)}{5+5x^2+5x^4+x^6}\,. \tag{22}$$

The corresponding connection polynomials which allow to calculate the propagator $K^{\{1,2,4,5\}}$ are listed in the Table 2.

It should be noted that the parametrization of rationally extended Harmonic oscillators by the splitting energy ΔE_s and the gap energy ΔE_g suggests a possible application to an analytical description of flux's qubit time evolution. Indeed, in general a Josephson qubit behaves like a nonlinear resonator formed from the Josephson inductance and its junction capacitance [10]. The system has many energy levels, nevertheless the operating space of the qubit must contain only the two lowest states. As a result, [11] transition frequencies between the qubit ground

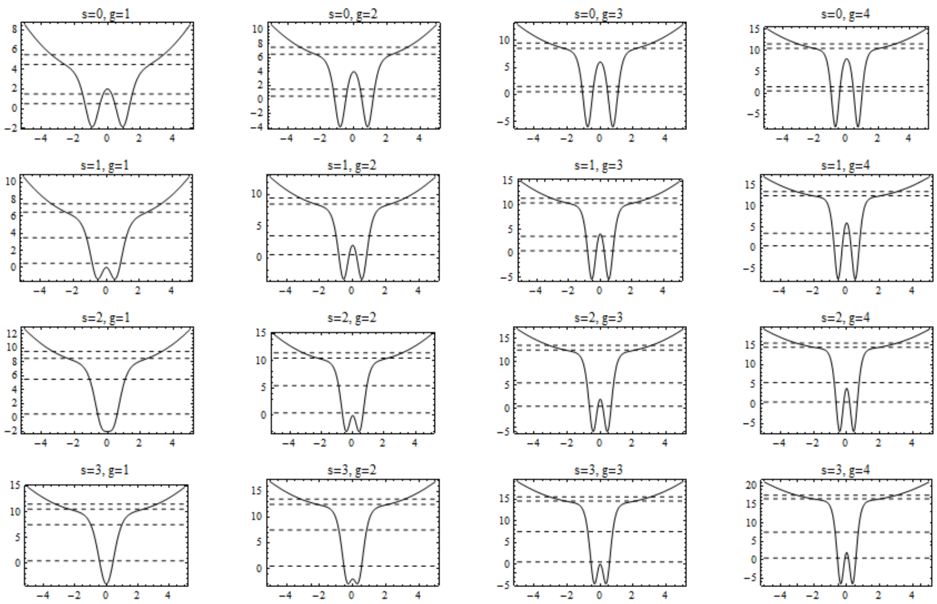

Figure 1. The rationally extended Harmonic oscillators with the splitting energy $\Delta E_s = 2s+1$ and gap energy $\Delta E_g = 2g+1$. Energies of first 4 bound states are plotted by dashed horizontal lines. The spectrum is equidistant starting from the second excited state.

k	$Q_k^{\{1,2,4,5\}}(x,y)$
0	$\frac{9(1+x^2)(1+y^2)}{\pi^2}$
1	$-\frac{9xy(1+x^2)(1+y^2)}{\pi^2}$
2	$-\frac{9(1+x^2)(1+y^2)(y^2+x^2+y^2x^2-1)}{2\pi^2}$
3	$\frac{9xy(-65-30(x^2+y^2)+5(x^4+y^4)+10(x^4y^2+x^2y^4)+3x^4y^4)}{20\pi^2}$
4	$\frac{9(-5+5(x^2+y^2)+15(x^4+y^4)+5(x^6+y^6)-95x^2y^2-35(x^4y^2+x^2y^4)+5(x^6y^2+x^2y^6)-5x^4y^4+5(x^6y^4+x^4y^6)+x^6y^6)}{40\pi^2}$
5	$\frac{9xy(-45-10(x^2+y^2)+5(x^4+y^4)+20x^2y^2+10(x^4y^2+x^2y^4)+3x^4y^4)}{20\pi^2}$
6	$\frac{9(x^4+2x^2-1)(y^4+2y^2-1)}{\pi^2}$

Table 2. Sequence of connection polynomials $Q_k^{\{1,2,4,5\}}(x,y)$

and first excited states should differ from the frequency of transition between the qubit first and second excited states. The Hamiltonian which describes flux qubit reads

$$H_{fq}(p,\delta) = \frac{p^2}{2C} - \frac{I_0\Phi_0}{2\pi}\cos\delta + \frac{1}{2L}\left(\Phi - \frac{\Phi_0}{2\pi}\delta\right)^2, \qquad \Phi_0 = \frac{h}{2e}. \tag{23}$$

The corresponding potential can be fitted at low energies by tuning the splitting and the gap energy of rational extensions of Harmonic oscillator. With the analytical model at hands

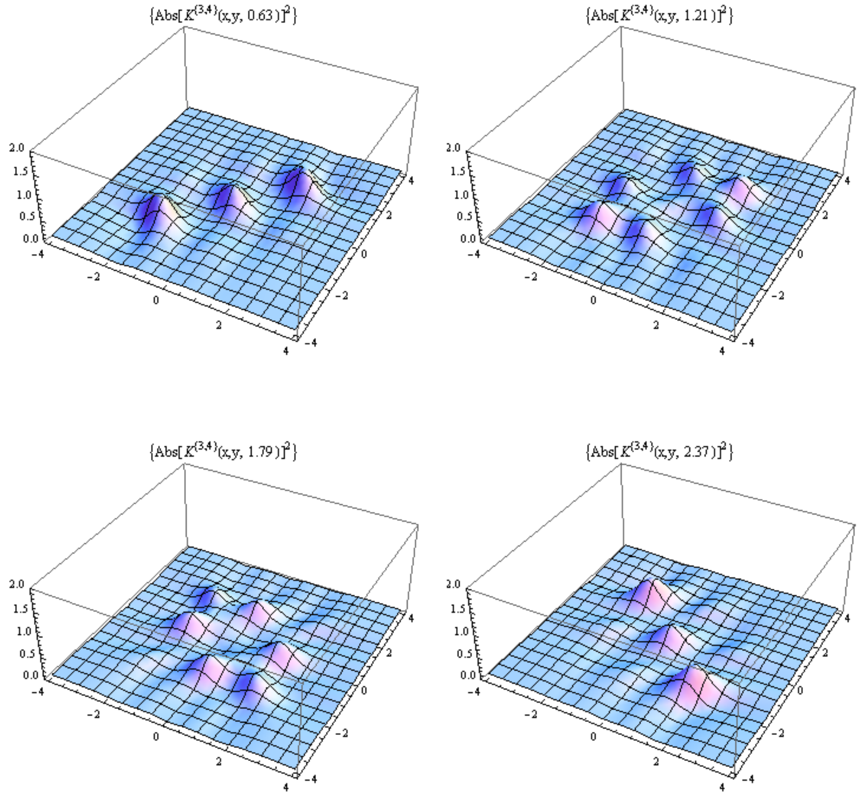

Figure 2. Transition probabilities defined by $|K^{\{3,4\}}(x, y; t)|^2$.

which completely describes all energies and evolution of arbitrary initial state one can optimize efficiency of a flux qubit.

3. Exact propagators for three-well rational extensions of the Harmonic oscillator

The simplest the three-well rational extension of the Harmonic oscillator reads

$$V^{\{3,4\}}(x) = \frac{x^2}{4} + 2 - \frac{1296(x^4 - 2x^2 - 1)}{(9 + 9x^2 - 3x^4 + x^6)^2} + \frac{12(x^4 - 15)}{9 + 9x^2 - 3x^4 + x^6} \tag{24}$$

Explicit expressions of connection polynomials $Q_k^{\{3,4\}}(x, y)$ are given in Table 3. Hamiltonian $H^{\{3,4\}}$ has the quasi-equidistant spectrum, $E_n = n + \frac{1}{2}$, $n \in \mathbb{N}_0 \setminus \{3, 4\}$. That is there exists a group of three levels (ground, first and second excited states) separated from the equidistant part of the spectrum by a gap energy $\Delta E_g = 3$.

Using connection polynomials we can construct propagator $K^{\{3,4\}}(x, y; t)$ by rational ansatz (20). In Fig. 2 we visualize $|K^{\{3,4\}}(x, y; t)|^2$ at different moments of time to show tunnelling pattern.

In general a wide class of three-well extensions (see Fig. 3) can be classified by three parameters. There are two splitting energies $\Delta E_s = E_1^\sigma - E_0^\sigma = 2s + 1$, and $\Delta E_h = E_2^\sigma - E_1^\sigma = 2h+1$ $s, h = 0, 1, \ldots$, and the gap energy $\Delta E_g = E_3^\sigma - E_2^\sigma 2g+1$, $g = 1, 2, \ldots$. For instance, when $\sigma = \{3, 4\}$ we have $\Delta E_s = \Delta E_h = 1$, $s == h = 0$, and $\Delta E_g = 3$, $g = 1$. One can see in Fig. 3 that when g is fixed, wells tend to collapse with increasing parameters s and h. Unfortunately we didn't find any simple criteria to distinguish degenerate and non-degenerate cases.

k	$Q_k^{\{3,4\}}(x,y)$
0	$\frac{(3+x^4)(3+y^4)}{24\pi}$
1	$-\frac{xy(9-6y^2+3y^4+x^4(3-2y^2+y^4)-2x^2(3+2y^2+y^4))}{48\pi}$
2	$\frac{27-27x^2-45x^4+9x^6-27y^2+81x^2y^2+9x^4y^2+9x^6y^2-45y^4+9x^2y^4-21x^4y^4-3x^6y^4+9y^6+9x^2y^6-3x^4y^6+x^6y^6}{288\pi}$
3	$\frac{xy(-27+6x^2+3x^4+6y^2-8x^2y^2-2x^4y^2+3y^4-2x^2y^4+x^4y^4)}{48\pi}$
4	$-\frac{3-6x^2+x^4-6y^2+2x^4y^2+y^4+2x^2y^4-x^4y^4}{16\pi}$
5	$\frac{xy(x^2-3)(y^2-3)}{12\pi}$

Table 3. Sequence of connection polynomials $Q_k^{\{3,4\}}(x,y)$

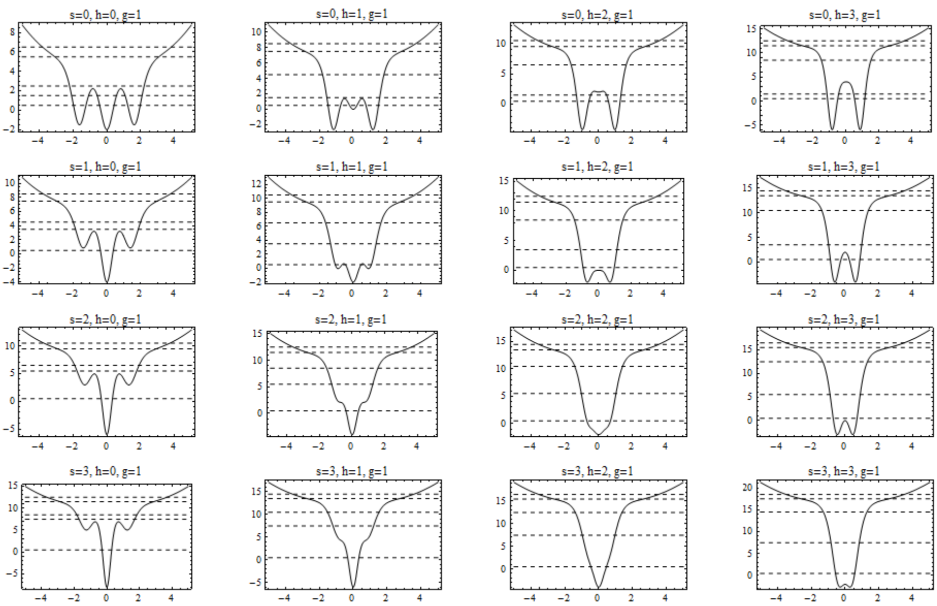

Figure 3. The rationally extended Harmonic oscillators with the splitting energies $\Delta E_s = 2s+1$, $\Delta E_h = 2h+1$, and gap energy $\Delta E_g = 2g+1$, $(g=1)$. Energies of first 5 bound states are plotted by dashed horizontal lines. The spectrum is equidistant starting from the third excited state.

4. Conclusions

Using the rational form of the propagators

$$K^\sigma(x,y;t) = K_{\text{osc}}(x,y;t)\frac{\sum_{k=0}^{\sigma[[-1]]+1} Q_k^\sigma(x,y)\mathrm{e}^{-\mathrm{i}kt}}{\sum_{k=0}^{\sigma[[-1]]+1} Q_k^\sigma(x,y)} \tag{25}$$

we present a new example of Feynman path integrals that can be calculated analytically [12].

Given a sequence σ of levels deleted by Darboux transformation, the rationally extended oscillator potential V^σ appears to be a multi-well potential with N_w minima, where

$$N_w \leq \sigma[[-1]] + 1 - |\sigma| \,. \tag{26}$$

The number N_w of classical vacua (stable equilibrium of V^σ) is related with the structure of non-equidistant part of the spectrum. We established that two-level non-equidistant part of spectrum corresponds to the two well potential when the splitting parameter s, $\Delta E_s = 2s = 1$ is smaller than the doubled gap parameter g, $\Delta E_g = 2g + 1$, that is when $s < 2g$. The resulting two-well potentials and corresponding propagators can be used to model dynamics of a flux qubit [13].

Analytical propagators for the two-well and triple-well potentials may be applied also to studies of oscillations and self-trapping of BEC or to dynamics of a single trapped ion [14, 15, 16, 17, 18].

Acknowledgements

AMPM thanks Brazilian foundation FAPEMIG for the financial support.

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