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# Some properties of double-Morse potentials

Henryk Konwent, Paweł Machnikowski, Piotr Magnuszewski and Andrzej Radosz†

Institute of Physics, Wrocław University of Technology, Wybrzeże Wyspiańskiego 27, 50-370 Wrocław, Poland

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**Abstract.** In the framework of various exact and approximate methods, the properties of the quasi-exactly solvable double-Morse potential are discussed. The relation between the hidden algebraic structure of the model and its geometrical properties is examined. The potential is used as a testing model for a semiclassical approximation which proves to work well both in the symmetric and asymmetric cases. The relation between semiclassical energy-level splitting and perturbation theory is underlined, leading to conclusions on the interpretation of the semiclassical results.

#### 1. Introduction

Recently several new types of *quasi-exactly solvable (QES)* one-dimensional double-well potentials have been proposed [1–7]. Their most important property is that the Schrödinger equation for a particle moving in these potentials can be solved exactly for certain values of the potential parameters. It is well known that the so-called  $\phi^4$  potential

$$V_4(x) = -\frac{A}{2}x^2 + \frac{B}{4}x^4 \tag{1}$$

where A and B are positive constants, commonly used in various branches of physics, does not have this property.

Razavy [1] suggested that the bistable potential

$$V_{\rm R}(x) = \frac{\hbar^2 \beta^2}{2m} \left[ \frac{1}{8} \xi^2 \cosh 4\beta x - (n+1)\xi \cosh 2\beta x - \frac{1}{8} \xi^2 \right]$$
(2)

might be used in many applications. If n is a natural number then the n lowest energy levels for this potential may be found.

Matsushita and Matsubara [2] and Lawrence and Robertson [3, 4] proposed a description of a proton in a hydrogen bond with the potential

$$V_{\rm L}(x) = V_0[\frac{1}{2}A^2 \cosh 2ax - 2A \cosh ax].$$

This potential may be obtained as a sum of two Morse potentials, oriented in opposite directions (back-to-back) and centred at different points. Various estimations (see e.g. [3, 8]) show that this potential is suitable for the description of a hydrogen bond.

A similar potential

$$V_Z(x) = \frac{\hbar^2 a^2}{2m} \left[\frac{1}{4}B^2 \sinh^2 ax - B(S + \frac{1}{2})\cosh ax\right]$$
(3)

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† E-mail address: radosza@rainbow.if.pwr.wroc.pl

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was derived by Zaslavsky and Ulyanov [5, 6] and used, in the latter work, for the description of a spin system—a uniaxial ferromagnet.

It is evident that all these potentials are equivalent to the symmetric double-Morse potential [7],

$$V_{\rm dM}(x) = V_0 (A \cosh ax - 1)^2.$$
(4)

The most comprehensive discussion of the properties of the double-Morse potential was given by Zaslavsky and Ulyanov [6] by using coherent states representation. Special attention was paid to the question of quantum tunnelling considered in terms of the WKB approximation.

Considerable progress in better understanding and a more systematic description of QES models has been made within the last few years due to work by Turbiner [9], González-López *et al* [10], Deenen [11], Ushveridze [12] and others. The interplay between spin and coordinate representations has turned out especially fruitful (see also [13]). In that context the discussion on the properties of the double-Morse potential seems to be worth extending, in particular involving its asymmetric generalization, which also preserves the property of quasi-exact solvability.

Introducing notation that will be useful in what follows, the potential may be written in the form

$$V(x) = \frac{\hbar^2 a^2}{2m} \left[ \frac{1}{4} (2S+1)^2 \left( \frac{B}{2S+1} \cosh ax - 1 \right)^2 + \frac{1}{2} BC \sinh ax \right] = \frac{\hbar^2 a^2}{2m} U(\xi)$$
(5)

where  $\xi = ax$ . One finds that for integer and half-integer values of S,  $S = 0, \frac{1}{2}, 1, \ldots$ , the first 2S + 1 lowest energy levels and corresponding eigenfunctions may be found.

The purpose of this paper is to present a discussion of the following problems.

The first one is associated with the virtually untouched question of the relation between apparent (i.e. geometrical) and hidden (i.e. dynamical) symmetries. We develop here a method proposed previously [13], where the underlying dynamical sl(2) symmetry is involved in an effective way. We show how the whole family of one-dimensional QES models may be generated. The proposed construction explains what is the place of the double-Morse potential and in what sense the member of the family which is the closest to the double-well potential (5) is a periodic potential, with the resulting close relationship between exact eigenvalues and eigenfunctions of these two problems.

We underline the relation between coordinate and spin representations of the sl(2) algebra that allows for a deeper insight revealing interesting spectral properties and their interpretation.

The second problem relates to the semiclassical approximation. The shape of the potential barrier in the model (5) is very flat compared with that of the  $\phi^4$  model (1) (see figure 1); this suggests that the range of applicability of the semiclassical approximation may be much wider here than in the model (1). This can be seen in the considerations of Ulyanov and Zaslavsky [6] which were, however, limited to the symmetric case. We will extend the discussion to the asymmetric potential.

There exists a considerable list of references where the split of energy levels in symmetric double-well potentials due to tunnelling is discussed [14] (see also references therein). On the other hand, accidental degeneration in the asymmetric potential should lead to a 'split' as well. The double-Morse potential enables one to perform an appropriate examination. Its unique feature is that it is composed of two Morse potentials, each of them exactly solvable (bound states are known), the separation between them being a free parameter. Therefore, in this model one may easily study how the levels, that are



**Figure 1.** (*a*) The double-Morse potential has different shapes, depending on the value of A = B/(2S + 1). (*b*)–(*d*) Comparison of the double-Morse potential for  $A = 10^{-2}$ ,  $A = 10^{-3}$  and  $A = 10^{-4}$ , respectively, (full curve) with a fitted  $\phi^4$  potential (broken curve). The potential barrier for the double-Morse potential becomes very flat for small *A*; the separation of wells grows as  $-\ln A$ .

degenerated for infinite separation, are split due to an increasing overlap of eigenstates when the separation becomes finite. We exploit that opportunity finding rather startling behaviour: both in symmetric and asymmetric cases degeneration of the energy levels, accidental in the latter case, is lifted leading to the same split regarded as a perturbative effect (in the small under-barrier penetration limit).

The paper is organized as follows. In section 2 we present the well known solution of the Schrödinger equation by the ansatz method. We point out that the same method may be applied to a related periodic potential. Hidden symmetry and the resulting relation between the models (double-well potential, periodic potential and a wider class of models) is presented in sections 3 and 4. Semiclassical approximation, the *real trajectories in complex time* (RTCT) method is briefly introduced and applied to the symmetric and asymmetric double-Morse potential in sections 5 and 6. It is compared with the exact results and WKB approximation, wherever it applies. Concluding remarks are given in section 7.

## 2. The ansatz method

a)

In this section we summarize the method of using the appropriate ansatz for solving the Schrödinger equation

$$H\Psi = E\Psi$$

with the double-Morse potential (5). A similar method was first given by Razavy [1]. The ansatz method is equivalent to a somewhat different approach involving the use of generating functions which was presented in [6]. Below the solution for the symmetric limit (C = 0) of the potential is presented but it may be easily generalized to the asymmetric case.

The discussed equation has the form

$$\left[-\frac{\mathrm{d}^2}{\mathrm{d}\xi^2} + U(\xi) - \mathcal{E}\right]\Psi(\xi) = 0 \tag{6}$$

where

$$\mathcal{E} = \frac{2m}{\hbar^2 a^2} E.$$

We are interested in square integrable solutions of equation (6). Making the ansatz

$$\Psi(\xi) = \Phi(\xi) \cdot \exp[-\varphi(\xi)] \qquad \varphi(\xi) = \int^{\xi} g(y) dy$$

we obtain the following equation:

$$g'(\xi) - g^{2}(\xi) - \frac{\Phi''(\xi) - 2g(\xi) \cdot \Phi'(\xi)}{\Phi(\xi)} = \mathcal{E} - U(\xi)$$

where the primes denote the derivatives with respect to  $\xi$ . Note that this equation, for given functions  $\Phi(\xi)$  and  $U(\xi)$ , is a Ricatti equation for  $g(\xi)$ . Its solution can be found only in particular cases.

For the ground state the wavefunction  $\Psi(\xi)$  has no nodes in the finite interval,  $\Phi(\xi) \equiv 1$ . After some algebra one gets the ground state eigenfunction for lower values of *S*, e.g.

$$\Psi_0(\xi) = \exp\left[-\frac{B}{2}\cosh\xi\right] \quad \text{for } S = 0$$

and

$$\Psi_0(\xi) = C_0 \cosh\frac{\xi}{2} \exp\left[-\frac{B}{2}\cosh\xi\right] \qquad \text{for } S = \frac{1}{2}.$$

The above results suggest a solution in the form

$$\Psi(\xi) = \Phi(\xi) \exp\left[-\frac{B}{2}\cosh\xi\right].$$
(7)

Then we get from (6)

$$\Phi'' - B\sinh\xi\Phi' + [\varepsilon + B \cdot S\cosh\xi]\Phi = 0$$
(8)

where

$$\varepsilon = \mathcal{E} - \frac{1}{4}[(2S+1)^2 + B^2].$$
 (9)

We look for solutions of this equation having the form of a polynomial in  $\sinh \xi$  or  $\cosh \xi$ . It is convenient to assume that  $\Phi(\xi)$  is a polynomial in  $\exp[m\xi]$ ,

$$\Phi(\xi) = \sum_{m=-m_0}^{+m_0} a_m \exp(m\xi).$$
 (10)

Inserting this expression into equation (8) one obtains

$$\sum_{m} (\varepsilon + m^2) a_m \mathrm{e}^{m\xi} + \frac{B}{2} \sum_{m} (S - m) \mathrm{e}^{(m+1)\xi} + \frac{B}{2} \sum_{m} (S + m) a_m \mathrm{e}^{(m-1)\xi} = 0$$

which leads to the following three-term difference equation for the coefficients  $a_m$ :

$$(\varepsilon + m^2)a_m + \frac{B}{2}[(S+1-m)a_{m-1} + (S+1+m)a_{m+1}] = 0.$$
(11)

**Table 1.** Height of the potential hump  $U_0 = U(0)$ , energy eigenvalues  $\mathcal{E}$  and the pre-exponential part  $\Phi$  (up to a constant) of the corresponding wavefunctions (see (7)) for the symmetric double-well potential. For the parameter  $\varepsilon_i$  see (9).

S	$U_0$	ε	Φ
0	$(\tfrac{B}{2}-\tfrac{1}{2})^2$	$(\frac{B}{2})^2 + \frac{1}{4}$	1
$\frac{1}{2}$	$(\frac{B}{2}-1)^2$	$\frac{(\frac{B}{2})^2 - \frac{B}{2} + \frac{3}{4}}{(\frac{B}{2})^2 + \frac{B}{2} + \frac{3}{4}}$	$\frac{\cosh\frac{\xi}{2}}{\sinh\frac{\xi}{2}}$
1	$(\frac{B}{2}-\frac{3}{2})^2$	$(\frac{B}{2})^2 - \sqrt{B^2 + \frac{1}{4}} + \frac{7}{4}  (\frac{B}{2})^2 + \frac{5}{4}  (\frac{B}{2})^2 + \sqrt{B^2 + \frac{1}{4}} + \frac{7}{4}$	$(B - \varepsilon_0 \cosh \xi)$ sinh $\xi$ $(B - \varepsilon_2 \cosh \xi)$
<u>3</u> 2	$(\frac{B}{2}-2)^2$	$\begin{aligned} & (\frac{B}{2})^2 - \frac{B}{2} - \sqrt{B^2 - B + 1} + \frac{11}{4} \\ & (\frac{B}{2})^2 + \frac{B}{2} - \sqrt{B^2 + B + 1} + \frac{11}{4} \\ & (\frac{B}{2})^2 - \frac{B}{2} + \sqrt{B^2 - B + 1} + \frac{11}{4} \\ & (\frac{B}{2})^2 + \frac{B}{2} + \sqrt{B^2 + B + 1} + \frac{11}{4} \end{aligned}$	$\begin{aligned} \cosh\frac{3}{2}\xi &= \frac{2}{B}(\varepsilon_0 + \frac{9}{4})\cosh\frac{1}{2}\xi\\ \sinh\frac{3}{2}\xi &= \frac{2}{B}(\varepsilon_1 + \frac{9}{4})\sinh\frac{1}{2}\xi\\ \cosh\frac{3}{2}\xi &= \frac{2}{B}(\varepsilon_2 + \frac{9}{4})\cosh\frac{1}{2}\xi\\ \sinh\frac{3}{2}\xi &= \frac{2}{B}(\varepsilon_3 + \frac{9}{4})\sinh\frac{1}{2}\xi \end{aligned}$
2	$(\frac{B}{2}-\frac{5}{2})^2$	$\frac{(\frac{B}{2})^2 - \sqrt{B^2 + \frac{9}{4}} + \frac{15}{4}}{(\frac{B}{2})^2 + \sqrt{B^2 + \frac{9}{4}} + \frac{15}{2}}$	$\sinh 2\xi - \frac{2}{B}(4 + \varepsilon_1)\sinh \xi$ $\sinh 2\xi - \frac{2}{B}(4 + \varepsilon_3)\sinh \xi$

To terminate the series at finite  $m_0$  it is sufficient to assume that

 $a_{S+1} = 0 = a_{-S-1}$ 

with

$$m = -S, -S + 1, -S + 2, \dots, S - 2, S - 1, S.$$

For given S the polynomial (10) contains 2S + 1 terms. The condition of solvability of the system of homogeneous equations (11), i.e. the zeros of the determinant of this system of equations, which is an algebraic equation of the order 2S + 1 with respect to  $\varepsilon$ , allows us to calculate 2S + 1 energy levels.

Table 1 contains the solutions of the Schrödinger equation (6) for particular values of the parameter  $S = 0, \frac{1}{2}, 1, \frac{3}{2}, 2$ , along with the height of the potential hump.

For the first four cases the wavefunctions and corresponding energy levels can be easily found in the analytical form. For S = 2, the odd energy levels may be found from the equation

$$\epsilon^{3} + 5\epsilon^{2} + 4(1 - B^{2})\epsilon - 12B^{2} = 0$$

which may be solved analytically e.g. using the computer symbolic calculation systems (in [7] there are some mistakes in the formulae related to this case). The question of analytical solution of the eigenvalue problem was recently investigated in [15]. It was noted that for  $S = \frac{5}{2}$  the eigenvalue problem is reduced to finding roots of two third-order polynomials. Once the roots are known, the eigenfunctions may be found.

A regular behaviour of the energy spectrum may be observed. Increasing the value of the parameter B ( $B \in (0, 2S + 1)$ ) causes 'movement' of the energy levels upwards: they tend to leave the wells. Note (a property not obvious at first sight) that when only one level is known exactly, S = 0, it lies above the barrier. When two or three levels are known,



**Figure 2.** Various examples of the periodic potential related to the double-Morse potential: (*a*) single-well form (A < 1); (*b*) double-well form (A > 1) (equation (12)); (*c*) asymmetric generalization analogous to (5).

 $S = \frac{1}{2}$  or S = 1, respectively, no more than two of them lie below the barrier; in the case  $S = \frac{3}{2}$ , all four of the levels might be below the potential hump. For sufficiently small values of *B*, out of the exactly known first 2S + 1 levels,  $2[S + \frac{1}{2}]$  are below the potential hump ([x] is the integer part of x). This regularity will become clear when the algebraic approach is developed in section 3.

The method presented above may also be used to find a partial solution to another, related problem. The formal substitution  $x \rightarrow i\phi$  made in the Schrödinger equation with the potential (4) provides us with a related QES model with periodic potential

$$V_{\rm per}(\phi) = -V_0 (A\cos a\phi + 1)^2.$$
(12)

It may describe a one-dimensional periodic lattice or (if *a* is a natural number) a potential in a rotational problem. Using an appropriate shift  $\phi \rightarrow \phi - \phi_0$  we may consider only positive values of *A*.

This potential written in the form analogous to (2) was used by Razavy [16]. A similar periodic potential, having the form related to (3) was proposed by Zaslavsky and Ulyanov [5].

The potential (12) has different form depending on the value of A, as shown in figure 2.

The Schrödinger equation for a molecule moving (or rotating) in the potential (12) reads (in dimensionless units, cf (5))

$$\left[-\frac{\mathrm{d}^2}{\mathrm{d}\xi^2} + U_{\mathrm{per}}(\xi) - \mathcal{E}\right]\Psi(\xi) = 0$$

where  $\xi = a\phi$ , (in a rotational problem the mass should be replaced by the moment of inertia *I*).

Making the corresponding substitution in the ansatz (7),

$$\Psi(\xi) = \Phi(\xi) \exp\left[\frac{B}{2}\cos\xi\right]$$

one reproduces all the results found for the double-well potential.

The obtained solutions fulfil the condition

$$\Psi(\xi + 2\pi) = (-1)^{2S} \Psi(\xi).$$

Therefore, in a rotational problem only the solutions with S being a natural number are correct. On the other hand, interpreted as wavefunctions of a Bloch electron, the solutions correspond to the top or the bottom of the band.

#### 3. Hidden algebraic structure

One may expect that the quasi-exact solvability of the model (5) is a result of some kind of algebraic structure or dynamical symmetry of the model. In this section we discuss this structure as well as the relation between the hidden algebra of the model and its properties.

Zaslavsky and Ulyanov [6, 17] showed that by using an appropriate representation this model may be transformed into an algebraic spin Hamiltonian. They discussed also other models that possess this property. Energy eigenvalues of spin Hamiltonians were associated with the (2S + 1) lowest levels of the original Hamiltonian.

The following questions arise: how are the properties of the coordinate Hamiltonian related to the corresponding spin Hamiltonian and how wide is the class of similar QES models? The answer to the second question is known. The QES Hamiltonians have a hidden algebraic structure related to the sl(2) algebra. All such Hamiltonians may be classified. Some of them yield physically meaningful potentials with corresponding normalizable wavefunctions [10]. A comprehensive review of the subject is contained in [12].

Below, we present a simple, systematic way of deriving coordinate Hamiltonians from the spin ones. This approach allows us to identify QES Hamiltonians as divided into 31 classes. The analysis throws light to a deeper meaning of the relation between the models (4) and (12). We discuss also the relation between the properties of the spectrum and the algebraic structure of the Hamiltonian.

As was noticed by Ulyanov and Zaslavsky [6], both the double-well and the periodic potentials correspond to the spin Hamiltonian

$$H = aS_z^2 - BS_x + CS_z \tag{13}$$

where the case of C = 0 corresponds to symmetric forms of the potentials. The relation between the mechanical problems and the spin Hamiltonians was discussed using the generating function formalism or the coherent states representation. However, since all of the discussed models belong to the sl(2) algebra, the properties of that algebra may be used in a more direct way in order to construct coordinate realizations of spin operators (an alternative construction was proposed by Deenen [11]). Let us consider a realization of the sl(2) algebra in terms of generalized Lie derivatives

$$S_{3} = v(\xi) \frac{d}{d\xi} + u(\xi)$$

$$S_{+} = v_{+}(\xi) \frac{d}{d\xi} + u_{+}(\xi)$$

$$S_{-} = v_{-}(\xi) \frac{d}{d\xi} + u_{-}(\xi)$$
(14)

(throughout this section we use the dimensionless notation introduced in the equation (5)). The generators must satisfy the usual commutation relations

$$[S_3, S_+] = S_+$$
  $[S_3, S_-] = -S_ [S_+, S_-] = 2S_3$ 

The differential equations resulting from these relations determine the functions  $u_{\pm}$ ,  $v_{\pm}$  in terms of u, v. One finds that only one parameter S is left free:

$$v_{\pm}(\xi) = \pm v(\xi) e^{\pm F(\xi)} \qquad u_{\pm}(\xi) = (\pm u(\xi) - S) e^{\pm F(\xi)}$$
(15)

where

$$F(\xi) = \int \frac{\mathrm{d}\xi}{v(\xi)}.$$

Any choice of u, v, S defines one realization of sl(2).

Now, consider the general class of Hamiltonians

$$H = \sum a_{ij} S_i S_j + \sum b_i S_i \qquad i, j = +, -, 3.$$
(16)

Suppose that a specific set of parameters  $a_{ij}$ ,  $b_i$  is selected. Then the requirement that the operator resulting from insertion of (14) into (16) should have a usual Schrödinger form determines the two functions u, v. Thus, the obtained mechanical (coordinate) Hamiltonian, as well as the associated realization (14) is in fact uniquely determined by the set of parameters. In practice one finds that the parameters  $a_{ij}$  are responsible for the general form of the potential (i.e. for the class to which it belongs: polynomial, hyperbolic functions, trigonometric, Jacobi elliptic functions etc), whereas the choice of  $b_i$  allows some freedom within the class. Taking into account commutation relations and constant Casimir operator for the realization (14), one obtains 31 non-equivalent combinations of coefficients  $a_{ij}$  corresponding to 31 classes of potentials, although not all of them are physically interesting.

The Casimir operator for the realization (14, 15) is a multiple of the unit operator,

$$\mathcal{C} = S_{-}S_{+} + S_{3}^{2} + S_{3} = S(S+1) \cdot I$$

therefore such a realization of the sl(2) algebra has got one invariant subspace of dimension 2S + 1 if and only if 2S is a non-negative integer. This subspace is obviously invariant under H and therefore the diagonalization of the original Hamiltonian is partly reduced to a matrix problem and the corresponding (2S + 1) eigenvalues may be found. The known eigenvalues correspond to the lowest energy levels of the coordinate Hamiltonian.

#### 4. Algebraic structure and spectral properties of the double-Morse potential

The class of double-Morse and periodic potentials discussed in this paper corresponds to all  $a_{ij}$  coefficients equal to zero except for  $a_{33} = a$  (cf (13)) [13]. For a > 0 the above procedure leads to a family of periodic potentials containing (12). When a < 0 (it may be assumed without loss of generality that a = -1) one gets the Hamiltonian with a potential which may be written in the following form as a sum of two Morse potentials

$$U(\xi) = U_{+}[e^{2(\xi - \xi_{+})} - 2e^{(\xi - \xi_{+})}] + U_{-}[e^{-2(\xi + \xi_{-})} - 2e^{-(\xi + \xi_{-})}] + \frac{1}{4}b_{3}^{2} - \frac{b_{+}b_{-}}{2}$$
(17)

where

$$U_{\pm} = \frac{1}{4}(2S + 1 \mp b_3)^2 \qquad \xi_{\pm} = \ln \frac{2S + 1 \mp b_3}{b_{\pm}}.$$
 (18)

It is straightforward to verify that the above potential is equal (up to a constant) to (5) when

$$b_{-} = b_{+} = B/2$$
  $b_{3} = C_{-}$ 

As we discuss below, choosing  $b_- \neq b_+$  yields no essential generalization.

We find that the geometrical property of the double-Morse potential, its decomposition into a sum of two Morse potentials, is directly reflected by the hidden algebraic structure of the model. The parameters S and  $b_3$  define the amplitudes,  $U_+$  and  $U_-$ , of the two components of the double-well potential; for  $b_3 = 0$  the two Morse potentals have equal amplitudes and the resulting double-well potential is symmetric. The Morse wells are separated by the distance  $d = \xi_+ + \xi_-$  which, for given amplitudes, depends only upon the product  $p = b_+b_-$ . For a given value of p, changes in the ratio  $r = b_-/b_+$  correspond only to translating the whole potential along the X axis. The infinite separation corresponds to  $p \rightarrow 0$ . This may be achieved by decreasing one of the parameters  $b_+$ ,  $b_-$  while the other one is kept constant. It corresponds to moving one of the Morse potential by keeping r = 1. Therefore the geometry of the potential is directly governed by the parameters of its spin counterpart:  $p = b_+b_-$  related to the separation of the wells and  $b_3$  responsible for asymmetry.

From the formulae (17), (18) it is clear that the condition of quasi-exact solvability may be satisfied no matter how far the component potentials are separated, provided that the amplitudes are appropriately selected (2*S* a non-negative integer). In other words, the family of QES potentials for a given value of *S* consists of potentials obtained as a sum of two Morse potentials with fixed amplitudes (parameters *S* and  $b_3$ ). The family of potentials is parametrized by the separation of the wells  $d \sim -\ln(b_+b_-)$ .

Partial algebrization of the problem makes it possible to find several energy levels for small values of S. The results for the symmetric potential are the same as those in table 1 up to the shift by

$$-\frac{B^2}{4} - (S + \frac{1}{2})^2 \tag{19}$$

where  $B = 4b_+b_-$ . For the asymmetric potential one gets the levels

$$S = 0: \qquad \mathcal{E}_0 = \left(\frac{B}{2}\right)^2 - \left(\frac{C}{2}\right)^2 + \frac{1}{4}$$
$$S = \frac{1}{2}: \qquad \mathcal{E}_0 = \left(\frac{B}{2}\right)^2 - \left(\frac{C}{2}\right)^2 - \frac{1}{2}\sqrt{B^2 + C^2} + \frac{3}{4}$$
$$\mathcal{E}_1 = \left(\frac{B}{2}\right)^2 - \left(\frac{C}{2}\right)^2 + \frac{1}{2}\sqrt{B^2 + C^2} + \frac{3}{4}$$

The above energy levels correspond to the potential (5) and are obtained by the shift (19) from the algebraic ones corresponding to (17).

The relation with the spin Hamiltonian allows us to draw some conclusions concerning the spectrum of energy levels. In the limit of infinite separation of the wells,  $d \to \infty$  (i.e.  $b_+b_- \to 0$ ), the spectrum is formed by the energy levels of the two Morse potentials. In the symmetric case ( $b_3 = 0$ ) all these levels are degenerate, except the highest one for integer values of S. The degeneracy is lifted for finite d, resulting in energy levels grouped in pairs. Note that for S integer, the largest diagonal element of the matrix Hamiltonian (13) is equal to 0. Hence, at least one of the exactly known levels must be non-negative. On the other hand, the top of the potential hump lies below 0. Thus we are sure that we know all the under-barrier levels and at least one over-barrier one. At most 2S levels may lie below the barrier. This statement does not hold for asymmetric potentials. The following question remains open: does the spin Hamiltonian spectrum correspond to all under-barrier states in a general case (asymmetric potential, S half-integer) or only to part of them?



**Figure 3.** (*a*) Energy levels in two Morse wells with amplitudes corresponding to an integer value of C are degenerated. (*b*) The degeneracy is lifted when the distance between the wells is decreased. The splitting of energy levels for lower levels is too small to be visible in the graph.

As a final element of our discussion on the algebraic structure of the double-Morse potential, let us mention the possibility of using the usual perturbation theory as an alternative to semiclassical approximations applied in the mechanical picture.

Let us fix  $b_+ = b_- = B/2$ . According to the formulae (18), the separation of the single Morse wells depends (logarithmically) on *B* and is infinite when  $B \rightarrow 0$ . On the other hand, considering (13) as a matrix Hamiltonian in a standard basis [18] we see that it becomes diagonal for B = 0. Hence, the operator  $BS_x$  may be treated as a perturbation. Moreover, it has a special band-diagonal structure with non-zero elements only just above and just below the diagonal.

In the coordinate picture the diagonal Hamiltonian corresponds to a potential with an infinite separation of wells. Its spectrum consists of two interwoven series

$$\{-(S+b_3/2-n)^2\}_{n=0}^{[S+b_3/2]} \qquad \{-(S-b_3/2-n)^2\}_{n=0}^{[S-b_3/2-\frac{1}{2}]}.$$
 (20)

When  $b_3$  is integer the two series overlap resulting in degeneracy of several energy levels (note that this 'accidental degeneracy' always affects a whole series of levels, cf figure 3(*a*)). One expects that this degeneracy should be lifted when the wells are at a finite distance (figure 3(*b*)). Indeed, systematic use of the perturbation theory results in splitting of the levels at a certain order of perturbation. If the highest level is degenerated  $(S+b_3/2 \text{ is half$  $integer})$  then the splitting for this level is proportional to *B*. The *k*th level (counting from the highest one) is split in the order 2k - 1 and the splitting correction  $\Delta E_k$  is proportional to  $B^{2k-1}$ . If the highest level is not degenerated  $(S + b_3/2 \text{ is integer})$  then one finds that  $\Delta E_k \sim B^{2k}$ , where the levels are counted downwards and the highest degenerated one corresponds to k = 1.

In the non-degenerate case the first non-zero correction appears at the second order and is proportional to  $B^2$ .

The perturbative analysis performed on the matrix Hamiltonian is insensible to the location of the energy level under or above the barrier. Within this approach two energy levels may be considered a pair with degeneration lifted by perturbation even though they have already moved over the barrier (an example is shown in figure 3). Moreover, it usually



**Figure 4.** Dependence on *B* of the energy split between the two highest exactly known levels  $\Delta \varepsilon = \varepsilon_{2S+1} - \varepsilon_{2S}$  (-----) compared with the first-order perturbative result (----) and the top of the potential barrier with respect to the position of the lower level of the pair,  $\tilde{U}_0 = U_0 - \varepsilon_{2S}$  (-----) for two classes of potentials: (*a*) S = 4, C = 1 and (*b*) S = 10, C = 1.

turns out that the first-order perturbation splitting (proportional to B for the degenerated upper level) is very close to the exact one until the *lower* of the two levels leaves the wells, i.e. the first-order perturbation theory is valid even when one of the levels is over the barrier (figure 4).

We would like to stress that the above discussion of energy-levels splitting—traditionally belonging to the range of applications of semiclassical methods—was based on a perturbative analysis. In the following section we show that semiclassical approximation yields the same results.

## 5. WKB and RTCT methods

Ulyanov and Zaslavsky [6] widely discussed a semiclassical approximation for the QES model (4). The connection between the mechanical (coordinate) system (6) and its spin counterpart (13) may be exploited in a two-fold way.

While for small values of spin S exact solution of spin Hamiltonian provides analytical formula for 2S + 1 lowest eigenvalues and eigenfunctions, in the case of large S quantum behaviour of the spin system (cf the discussion of spin tunnelling in [6]) may be studied via semiclassical approximation in the corresponding mechanical system.

On the other hand, various semiclassical approximations might be verified in this case since for small values of *S* analytical formulae are known. The behaviour of the energy levels in the vicinity of the potential hump is of particular interest.

Ulyanov and Zaslavsky investigated WKB and its modifications reporting coincidence between the exact and approximate results [6, section 4]. Their analysis was limited, however, to the symmetric double-well potential. In this section we shall discuss the modified version of the WKB approximation obtained in the framework of path integral formalism, the so-called RTCT method [19], which allows for exhaustive discussion, including the general case of the asymmetric potential.

In the quantum mechanical problem with Hamiltonian H, energy levels might be determined as the poles of the Laplace transform of the propagator

$$K(x_2, x_1; T) = \langle x_2 | \mathrm{e}^{-\frac{1}{\hbar}HT} | x_1 \rangle.$$

The semiclassical approximation leads to the simple formulae of summation over closed orbits (see figure 5) of constant energy [19].







Symmetric double-well potentials have been extensively discussed and the standard WKB formula defining energy levels reads

$$(1+a^2)^2 + b^2 = 0 \tag{21}$$

where  $a = a_1 = a_2$  due to symmetry and  $a_i$  relate to the classically allowed regions

$$a_{i} = \exp\left(-\frac{\mathrm{i}}{\hbar}W_{i}\right) = \exp\left(-\frac{\mathrm{i}}{\hbar}\int_{B_{i-1}}^{A_{i}}\sqrt{2m(E-V(x))}\,\mathrm{d}x\right)$$

whereas b is related to the classically forbidden region

$$b = \exp\left(-\frac{1}{\hbar}W'\right) = \exp\left(-\frac{1}{\hbar}\int_{A_1}^{B_1}\sqrt{2m(V(x)-E)}\,\mathrm{d}x\right).$$

Energy eigenvalues are found from (21) by means of the perturbation expansion,

$$E_n = E_n^0 \pm \Delta E_n \tag{22}$$

with *b* regarded as a small parameter:

$$1 + a^{2} = 0 \Rightarrow W(E_{n}^{0}) = (n + \frac{1}{2})\pi\hbar$$
  

$$(1 + a^{2})^{2} = -b^{2} \Rightarrow \Delta E_{n} = \frac{\hbar}{2}\omega_{n}\exp\left(-\frac{1}{\hbar}W'\right)$$
(23)

where

$$\omega_n = \left(\frac{\partial W}{\partial E}\right)_{E_n^0}^{-1}.$$

Modifications of various types used to improve the estimation of the energy-levels split,  $2\Delta E_n$ , were outlined by Ulyanov and Zaslavsky [6], and comparison with the exact result of the mechanical analogue was made. In this way the behaviour of the corresponding spin model was investigated.

Special modifications are necessary in particular while calculating energy levels lying just below the top of the potential barrier where the WKB approximation yields not only quantitatively inaccurate but even qualitatively wrong results.

Moreover, as has been extensively discussed [19], the standard WKB approximation suffers from serious inconsistency: energy levels are not well defined as they are complexvalued and only expansion up to the first order yields the real numbers. Another disadvantage of this approximation is that it might be applied to the symmetric doublewell potential, but not to the asymmetric one. In fact, in this latter instance, the WKB formula for energy levels,

$$(1 + a_1^2)(1 + a_2^2) + b^2 = 0$$

does not provide a reasonable approximation as even first order expansion yields complex numbers. It was also pointed out there that the RTCT method makes remarkable progress in removing the above-mentioned problems. Its predictions seem to work both in symmetric and asymmetric potential as well, providing well defined, real-valued energy eigenvalues. Moreover, the RTCT method has the advantage of accounting also for energy levels close to the top of the potential hump within a single calculation scheme. No additional methods are necessary to obtain these levels.

In the case of general double-well potential, poles of the Green's function are defined (see [19]):

$$(1+a_1^2)(1+a_2^2) + \frac{1}{4}b^2(1-a_1^2)(1-a_2^2) = 0.$$

Now in general  $a_1 \neq a_2$ , leading to the following formula:

$$\cot\left[\frac{1}{\hbar}W_1(E)\right]\cot\left[\frac{1}{\hbar}W_2(E)\right] = \frac{1}{4}b^4.$$

In the symmetric case the above equations take the form

$$(1+a^2)^2 + \frac{1}{4}b^2(1-a^2)^2 = 0$$

and

$$\cot^{2}\left[\frac{1}{\hbar}W(E)\right] = \frac{1}{4}\exp\left(-\frac{1}{\hbar}W'(E)\right)$$

respectively. Resulting energy eigenvalues are obviously real-valued. WKB results are reproduced in the symmetric potential for the deep levels, well below the potential hump, b < 1. Below we examine the RTCT method in the double-Morse potential and these predictions are compared with those of WKB in the symmetric case.

#### 6. Semiclassical results for the double-Morse potential

#### 6.1. Symmetric case

Table 2 contains energy levels for the symmetric potential (4) calculated using the standard WKB method, the RTCT method and exact (numerical or algebraic) results for comparison. For levels lying above the potential hump both semiclassical approximations yield the same Bohr–Sommerfeld formula.

Unlike the WKB method, the RTCT approximation yields energy levels one by one, not binding them into pairs. This becomes important when an odd number of levels lie below the hump. The WKB results may then give an incorrect number of levels. An example appears in the rows 4–6 of table 2, where four levels should be below the barrier. This is reflected by the standard WKB calculation but then one gets another level (row 6) when computing above the barrier. In principle it is not clear which one of the two levels should be chosen. An opposite situation takes place in rows 13, 22 and 28 of table 2, where one level gets lost.

In all these cases the RTCT method provides the correct number of levels without any ambiguities, although in the case of row 5 one of the levels is incorrectly placed above the

Number	S	Α	$U_0$		Exact	WKB	RTCT
1	$\frac{3}{2}$	0.02	3.8416	$\varepsilon_0$	1.749 10	1.74929	1.749 28
2	2			ε1	1.749 29	1.74947	1.749 47
3				$\Delta \varepsilon_{0,1}$	0.00019	0.00018	0.00019
4				ε2	3.674 10	3.66208	3.672 51
5				83	3.833 91	3.81308	_
6				E3		3.91	393
7				$\Delta \varepsilon_{2,3}$	0,15981	0,15100	0.241 42
8				$\varepsilon_4$	4.506 02	4.47	7 74
9				$\varepsilon_5$	5.29073	5.26	5 29
10	$\frac{3}{2}$	0.04	3.6864	$\varepsilon_0$	1.746 02	1.74681	1.74675
11	2			ε1	1.747 55	1.74821	1.748 27
12				$\Delta \varepsilon_{0,1}$	0.001 53	0.001 40	0.001 52
13				$\varepsilon_2$	3.60678		3.597 15
14				83	3.925 25	3.95	625
15				$\Delta \varepsilon_{2,3}$	0.31847	—	0.359 10
16	10	$\frac{2}{21}$	90.25	$\varepsilon_8$	73.177 71	73.19087	73.190 82
17		21		89	73.178 51	73.191 58	73.191 63
18				$\Delta \varepsilon_{8,9}$	0.000 80	0.00071	0.000 81
19				$\varepsilon_{10}$	83.354 81	83.39746	83.393 13
20				$\varepsilon_{11}$	83.44471	83.47988	83.48629
21				$\Delta \varepsilon_{10,11}$	0.089 90	0.09242	0.09316
22				$\varepsilon_{12}$	89.95270		89.934 85
23				$\varepsilon_{13}$	91.732 54	92.02	23 67
24				$\Delta \varepsilon_{12,13}$	1.779 84	—	2.088 82
25	10	$\frac{12}{21}$	20.25	$\varepsilon_0$	8.009 86	8.11447	8.109 36
26		21		$\varepsilon_1$	8.115 57	8.204 99	8.211 87
27				$\Delta \varepsilon_{0,1}$	0.105 71	0.090 52	0.102 51
28				ε2	19.475 06		19.55171
29				83	22.53948	23.12	23 71
30				$\Delta \varepsilon_{2,3}$	3.064 42	_	3.57200

 Table 2. Selected results for the symmetric double-Morse potential compared to exact energy levels.

barrier. Note, however, that the level  $\varepsilon_3$  causing these problems is very close to the top of the barrier and the semiclassical methods cannot yield absolutely correct results in this case.

When the energy-levels splitting is calculated for any levels except the highest one in the wells, the accuracy of the RTCT method is usually better than that of the WKB approximation. For example, in rows 1 and 2 we have 0.5% discrepancy for RTCT versus 7% for WKB. In rows 16–17 the errors are 1.3% and 10%, respectively. For the next pair in the same series they are 4% (RTCT) and 8% (WKB). In the critical case when one of the levels belonging to the WKB pair is above the hump, the RTCT method produces an error up to 20%. This is worse than with the specialized formulae used in [6] but the advantage here is of using one simple scheme for all levels.

**Table 3.** Selected results for the asymmetric double-Morse potential compared to exact energy levels. Here S = 10, A = 0.5, C = 1.4, the potential minima are  $U_1 = -13.396$  and  $U_2 = 12.05792$  and the maximum is  $U_0 = 28.05698$ .

Number		Exact	RTCT
1	$\varepsilon_0$	-3.65632	-3.619 599
2	$\varepsilon_1$	13.55689	13.63341
3	$\varepsilon_2$	19.41916	19.545 75
4	ε3	26.53653	26.769 10
5	$\varepsilon_4$	31.187 23	31.144 48

#### 6.2. Asymmetric case

The RTCT formula, unlike the standard WKB one may be used to generate semiclassical approximation to the energy levels in asymmetric potentials. Table 3 shows an example of energy levels obtained using this method.

The RTCT results are in good agreement with the exact ones, even for the levels closest to the top of the barrier. The error does not exceed 5% of the distance between the levels.

A point that seems especially worthy of investigation is the 'accidental degeneracy' case, where part of the levels of infinitely separated Morse wells  $(B \rightarrow 0)$  coincide although the wells are different. Such a situation corresponds to integer values of *C* in (5) (see the discussion at the end of the section 3). The exact degeneracy is reproduced by the zeroth-order WKB (Bohr–Sommerfeld) approximation since for the Morse potential the WKB method yields exact results.

In this case in the RTCT formulae one has for any energy  $a_1^2 = a_2^2$  (since  $W_1 = W_2 + C\hbar\pi$ ) and  $\partial W_1/\partial E = \partial W_2/\partial E$  (for proof of these equalities see the appendix). Hence, using the expansion (22) one has in the zeroth order

$$(1 + a_1^2)(1 + a_2^2) = 0 \Rightarrow W_i(E_n^{(0)}) = (n + 1/2)\pi\hbar.$$

The solutions for  $W_1$  and  $W_2$  coincide and the levels are degenerated. In the first order

$$(1 - a_1^2)(1 - a_2^2) \approx 4 \Rightarrow b^2 = (1 + a_1^2)(1 + a_2^2) \Rightarrow \Delta E_n = \frac{\hbar}{2}\omega_n \mathrm{e}^{-\frac{1}{\hbar}W'(E_n^{(0)})}$$

where

$$\omega_n = \left(\frac{\partial W_1}{\partial E}\right)_{E_n^{(0)}}^{-1} = \left(\frac{\partial W_2}{\partial E}\right)_{E_n^{(0)}}^{-1}.$$

In this way we come back to the formula (23). There is no difference in the behaviour of the energy levels between the symmetric case and asymmetric degenerated case.

In table 4 several results for an asymmetric potential (5) are shown.

The energy-levels splitting in this case is very close to the exact one for all levels except the one or two just below the barrier. The error for the highest pair is about 15% even when one of the two levels lies over the barrier (rows 12, 13). For lower levels the inaccuracy is 1-2%. Thus, the RTCT method gives qualitatively and usually even quantitatively correct results in the asymmetric case when the standard WKB formulae cannot be used.

Number	S	Α	$U_0$		Exact	RTCT
1	10	0.1	89.3303	ε7	67.08786	67.09777
2				$\varepsilon_8$	67.08795	67.097 86
3				89	78.45085	78.47475
4				$\varepsilon_{10}$	78.46662	78.490 85
5				$\varepsilon_{11}$	86.81996	86.91030
6				$\varepsilon_{12}$	87.54865	87.743 36
7				$\varepsilon_{13}$	92.21151	91.79771
8				$\varepsilon_{14}$	95.827 58	95.79832
9	10	0.5	27.8136	$\varepsilon_0$	0.000 00	0.041 65
10				$\varepsilon_1$	16.44673	16.544 65
11				$\varepsilon_2$	16.58793	16.585 01
12				ε3	27.393 65	27.395 51
13				ε4	30.595 07	31.086 19
14				ε5	38.07686	37.834 22

 Table 4.
 Selected results obtained by the RTCT method for the asymmetric double-Morse potential with degeneracy of energy levels, compared to exact energy levels.

#### 6.3. Semiclassical approximation and energy-levels splitting for small B

If  $B \ll 1$  then the hump is very wide and is flat over most of its width. Therefore it may be approximated by a rectangle and one can write

$$\frac{1}{\hbar}W' \approx \sqrt{\frac{2m}{\hbar^2 a^2} (E_{\rm B} - E_n^{(0)})} \ln \frac{4(2S+1)^2 - 4b_3^2}{B^2}$$

where  $E_{\rm B}$  is the top of the potential barrier. On the other hand, in the limit  $B \rightarrow 0$  one can use the known formulae for energy levels in the Morse potential

$$E_n^{(0)} = E_{\rm B} - \frac{2m}{\hbar^2 a^2} \left( S + \frac{b_3}{2} - n \right)^2 \qquad n = 0, \dots, \left[ S + \frac{b_3}{2} \right]$$

(cf (20)). Hence,

$$\Delta E_n \approx \frac{\hbar \omega_n}{8(2S+1)^2 - 8b_3^2} B^{2(S+\frac{b_3}{2}-n)}.$$

This relation generalizes the result of section 4 to non-QES (2S non-integer) cases.

## 7. Conclusions

The double-well Morse potential is obtained as a sum of two Morse potentials and in a natural way is a promising candidate for the modelling of many physical systems. In this paper we discussed the properties of this model by using various methods. The model is a member of a group of one-dimensional QES models with dynamical sl(2) symmetry. We proposed here a simple method of treatment of that algebra which enabled us to draw up a general framework for the whole family of models divided into 31 classes and to indicate the 'closest' neighbours of the model of interest.

Spectral properties were examined within exact and approximate approaches. Mutual relationship between coordinate and spin representations led to a comprehensive analysis and interpretation of particular features. This model possesses a unique feature: changing the separation between the wells, therefore changing their overlap, does not alter its main

property. The quasi-exact solvability of the model is retained. Thus the influence of the growing interaction between the wells on the split of energy levels might be studied. Some interesting observations can be made. Peculiar distribution of the exactly known energy levels found in the symmetric potential results from original degeneration of levels in infinitely spaced wells. Finite separation lifts degeneration: increasing overlap of the wells leads to the increasing split of the corresponding levels in such a way that for the *k*th level (below the hump) the split is proportional to  $B^{2k}$  or  $B^{2k-1}$ . This is the first-order perturbative expansion obtained in spin representation; interpretation for *B* comes from coordinate representation,  $|\ln B|$  being proportional to the distance between the wells. Rather surprisingly, asymmetric potential with accidental degeneration reveals the same behaviour: the split for the *k*th level below the hump is proportional to  $B^{2k}$  ( $B^{2k-1}$ ). The gap between close but not degenerated levels varies with *B* as well but the first-order perturbative term is always proportional to  $B^2$ .

Another aspect of these considerations relates to the question of interpretation of the split of energy levels—regarded, within semiclassical approximation, as a tunnelling effect. Looking at a bound state which is degenerated for infinite separation of the wells one finds that its splitting may be traced as separation is decreased and, therefore, the two levels may be considered to constitute a pair (they have a 'common origin'). Since no information about the barrier is encoded in the spin representation, this picture is valid even for levels lying above the barrier!

The double-Morse potential is a suitable model for verification of the semiclassical approximations. We applied here an approach previously developed by one of us (AR), the RTCT method, formulated in the framework of path integrals, where the proper way of summation over the orbits was claimed to provide an essential improvement. Indeed, apart from the qualitative advantage over standard WKB approximation (improper summation over the closed orbits in the latter), quantitative predictions are found to be quite satisfactory. The quantitative corrections to WKB results in the symmetric case, although not very impressive in general, are quite substantial in ambiguous situations: WKB may lead to overcounting the levels or underestimation of their number, whereas RTCT is a uniform scheme yielding correct answers. In the asymmetric case, where the standard method does not apply, it proves to be a good approximation of the exact results, even close to the top of the barrier.

## Appendix

Consider an asymmetric double-Morse potential (5) and a certain energy, such that the classical motion may take place in either of the wells. We will show that classical actions calculated for both wells differ by a magnitude  $C\hbar\pi$ .

The period of oscillation of a classical particle in the left  $(T_1)$  and right  $(T_2)$  well is given by

$$T_i(E) = \sqrt{\frac{m}{2}} \int_{B_{i-1}}^{A_i} \frac{\mathrm{d}x}{\sqrt{E - V(x)}}$$

where it is convenient to use the potential in the form (17)

$$V(x) = \frac{\hbar a^2}{2m} \left[ \frac{B^2}{16} e^{2x} - \frac{B}{2} \left( S + \frac{1}{2} - \frac{C}{2} \right) e^x + \frac{B^2}{16} e^{-2x} - \frac{B}{2} \left( S + \frac{1}{2} + \frac{C}{2} \right) e^{-x} \right].$$

(We shifted the energy scale as compared with the previous sections of the paper.) The integration limits are the turning points for the left or right well (see figure 5). Upon

substitution

$$t = \tanh \frac{ax}{2}$$

we get

$$T_1(E) = \frac{m}{\hbar a^2} \int_d^c \frac{\mathrm{d}t}{\sqrt{r(t)}} \qquad T_2(E) = \frac{m}{\hbar a^2} \int_b^a \frac{\mathrm{d}t}{\sqrt{r(t)}}$$

where r(t) is a certain polynomial of fourth order in t having four real roots a > b > c > d

$$r(t) = r_0(t-a)(t-b)(t-c)(t-d).$$

Using the tables of elliptic integrals [20] one finds that

$$T_1 = T_2 = \frac{2m}{\hbar a^2} \frac{2}{\sqrt{r_0}} gK(k) \qquad g = \frac{2}{\sqrt{(a-c)(b-d)}} \qquad k^2 = \frac{(a-b)(c-d)}{(a-c)(b-d)}$$

and K(k) is the complete elliptic integral of the first kind with modulus k. Thus, the periods of oscillations in both wells are equal and depend only on the zeros of r(t) and therefore indirectly on the potential parameters and energy.

Now notice that

$$T_i = 2\pi \frac{\mathrm{d}W_i}{\mathrm{d}E}$$

where  $W_1$ ,  $W_2$  are actions for movement in the left and right well, respectively. Hence

$$\frac{\mathrm{d}W_1}{\mathrm{d}E} = \frac{\mathrm{d}W_2}{\mathrm{d}E}$$

and

$$W_1(E) = W_2(E) + W_0$$

where  $W_0$  is a constant equal to the action corresponding to movement with energy  $E_0$  equal to the local minimum of the potential (see figure 5)

$$W_0 = \int_{B'_0}^{A'_1} \sqrt{2m(E_0 - V(x))} \, \mathrm{d}x.$$

Now we use the substitution  $t = e^{ax}$  which yields

$$W_0 = \hbar \int_{t_1}^{t_2} \frac{\sqrt{q(t)}}{t^2} \,\mathrm{d}t$$

where

$$q(t) = -\frac{B^2}{16}t^4 + \frac{B}{2}\left(S + \frac{1}{2} - \frac{C}{2}\right)t^3 + E_0t^2 + \frac{B}{2}\left(S + \frac{1}{2} + \frac{C}{2}\right)t - \frac{B^2}{16}.$$

Since q(t) must have one double root and two single roots, we may write

$$q(t) = \frac{B^2}{16}(t_3 - t)^2(t_2 - t)(t - t_1).$$

The integral for  $W_0$  is elementary and the result is

$$W_0 = \hbar \frac{B}{4} \left[ \frac{a^2 c + a^2 d + 2acd}{2a\sqrt{cd}} - \frac{1}{2}(2a + c + d) \right] \pi = C\hbar\pi$$

where we made use of the Viete formulae.

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