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M. Razavy

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An exactly soluble Schrödinger equation with a bistable potential

M. Razavy
Theoretical Physics Institute, Department of Physics, University of Alberta, Edmonton, Alberta, Canada T6G 2J1
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For a bistable potential which is the sum of two hyperbolic cosine functions, the Schrödinger equation for the low-lying states of a homonuclear diatomic molecule can be solved analytically. In this model the potential and the energy eigenvalues depend on three parameters, and the resulting wave functions are continuous and have continuous derivatives everywhere. This last property of the wave functions enables one to generate a family of soluble bistable potentials by applying the theorem of Darboux to the discrete eigenfunctions of the Schrödinger equation.

I. INTRODUCTION

Double-well potentials have been used in the quantum theory of molecules as a crude model to describe the motion of a particle in the presence of two centers of force. Recently solutions of the Schrödinger equation with these potentials have found applications in the classical theory of diffusion in a bistable potential field,[1] and also in the quantum theory of instantons.[2] Because of the rather complicated form of the force law, only a few exactly soluble models have been discussed in the literature. The examples most often cited are the double square-well,[3] the double oscillator,[3] the Manning potential,[4] and two square-wells separated by a delta function.[3] For these potentials the Schrödinger equation is soluble for all eigenfunctions, and the eigenvalues are the roots of transcendental equations. But in most of the problems the complete solvability (i.e., the determination of all eigenfunctions) is not important, since the distinctive features of the motion in a double-well potential are reflected in the properties of the low-lying quantum states of the system.

An interesting example of a bistable potential for which the wave equation is partially soluble (i.e., few of the lowest eigenfunctions are known analytically) is the sum of two hyperbolic cosine functions. The Schrödinger equation in this case is identical with the equation of wave motion describing the normal modes of vibration of a stretched membrane of variable density.[5] The advantages of this model over most of the other models are: (i) the wave function and the eigenvalues are simple functions, and (ii) the eigenfunctions and their derivatives are continuous everywhere. This latter property enables one to construct other soluble potentials, some having the form of a double well. In Sec. II the solution of the Schrödinger equation is obtained by Sommerfeld's technique,[6] and in Sec. III, it is shown that by utilizing Darboux's theorem,[7] other potentials can be found for which the lowest eigenfunctions are expressible in terms of elementary functions.

II. EIGENFUNCTIONS OF THE BISTABLE POTENTIAL

Let us consider the one-dimensional Schrödinger equation

$$\psi'' + (2m/\hbar^2)[E - V(x)]\psi = 0 \qquad (2.1)$$

which describes the motion of a single particle of mass m in the bistable potential

$$V(x) = (\hbar^2\beta^2/2m)[(1/8)\xi^2 \cosh 4\beta x - (n+1)\xi \cosh 2\beta x - (1/8)\xi^2]. \qquad (2.2)$$

This potential depends on three parameters, β, ξ, and a positive integer n. The wave equation (2.1) admits an infinite number of bound states, and the wave function is localized in space; i.e., the solution satisfies the boundary condition

$$\psi(x) \to 0, \qquad x \to \pm\infty. \qquad (2.3)$$

In Eqs. (2.2) and (2.3), we choose

$$V(x) = (\hbar^2\beta^2/2m)v(x) \qquad (2.4)$$

and

$$E = (\hbar^2\beta^2/2m)\epsilon, \qquad (2.5)$$

and also measure the distance in units of β^{-1}; i.e., set $\beta = 1$. Thus the wave equation will be transformed to the equation

$$\psi'' + [\epsilon + (1/8)\xi^2 + (n+1)\xi \cosh 2x - (1/8)\xi^2 \cosh 4x]\psi = 0. \qquad (2.6)$$

To solve Eq. (2.6), we use the "polynomial method" of Sommerfeld, and first determine the asymptotic solution of Eq. (2.6) by considering the differential equation

$$\psi_a'' - [(1/8)\xi^2(\cosh 4x - 1) - \xi \cosh 2x]\psi_a = 0, \qquad (2.7)$$

which has the same asymptotic form as Eq. (2.6). The acceptable solution of Eq. (2.7) which vanishes for $x = \pm\infty$ is given by

$$\psi_a(x) = \exp[(-1/4)\xi \cosh 2x]. \qquad (2.8)$$

Therefore, following Sommerfeld, we write the wave function $\psi(x)$ as

$$\psi(x) = \exp[(-1/4)\xi \cosh 2x]\phi(x), \qquad (2.9)$$

where $\phi(x)$ satisfies the following differential equation which is obtained by substituting Eq. (2.9) in (2.6):

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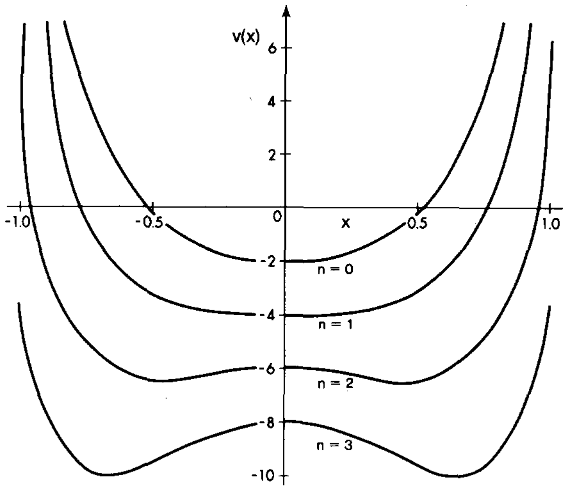

Fig. 1. Plot of the potential described by Eq. (2.2) for $\beta = 1$ and $\xi = 4$. When $n = 1$, the potential has a "flat bottom," but for $n > 1$ it takes the form of a double well.

$$\phi''(x) - \xi \sinh(2x)\phi'(x) + (\epsilon + n\xi \cosh 2x)\phi(x) = 0. \quad (2.10)$$

Now let us consider those solutions of Eq. (2.6) that are expressible in terms of a finite sum involving cosine or sine hyperbolic of jx, where j is an integer. These solutions can be divided into groups of even and odd parities, each group having two different states. Thus we have

$$\phi(x) = \sum_{j=0}^{k} C_{2j+1} \cosh(2j+1)x \quad (n = 2k+1), \quad (2.11)$$

$$\phi(x) = \sum_{j=0}^{k} C_{2j} \cosh(2jx) \quad (n = 2k), \quad (2.12)$$

for even states, and

$$\phi(x) = \sum_{j=0}^{k} S_{2j+1} \sinh(2j+1)x \quad (n = 2k+1), \quad (2.13)$$

$$\phi(x) = \sum_{j=0}^{k} S_{2j} \sinh(2jx) \quad (n = 2k), \quad (2.14)$$

for odd states.

By substituting Eqs. (2.11)–(2.14) in Eq. (2.10), we find three term recurrence relations for the coefficients C_{2j+1}, C_{2j}, S_{2j+1}, and S_{2j}. For instance, for even states we obtain

$$[(2j+1)^2 + \epsilon]C_{2j+1} + (\tfrac{1}{2})\xi(n+1-2j)C_{2j-1} + (\tfrac{1}{2})\xi(n+3+2j)C_{2j+3} = 0 \quad (2.15)$$

and

$$[(2j)^2 + \epsilon]C_{2j} + \xi[(\tfrac{1}{2})n + 1 + \delta_{j1} - j]C_{2j-2} + \xi[(\tfrac{1}{2})n + 1 + j]C_{2j+2} = 0 \quad (2.16)$$

with similar relations for S_{2j+1} and S_{2j}. Since we are interested in the solution of Eq. (2.10) with a finite number of terms, the coefficients C_{2j+1} and C_{2j} have to satisfy the conditions

$$C_{-2} = C_{n+2} = 0 \quad (n \text{ even}) \quad (2.17)$$

and

$$C_{-1} = C_{n+2} = 0 \quad (n \text{ odd}). \quad (2.18)$$

Thus each of the Eqs. (2.15) or (2.16) may be regarded as a homogeneous difference equation with ϵ as the eigenvalue. We observe that for even n and for states of even parity there are $[(\frac{1}{2})n + 1]$ nonzero terms in Eq. (2.12) and therefore $[(\frac{1}{2})n + 1]$ eigenvalues, whereas for even n, but for states of odd parity, there are $(\frac{1}{2})n$ nonzero terms in Eq. (2.14) and hence $(\frac{1}{2})n$ eigenvalues. For odd n values we have $(\frac{1}{2})(n+1)$ nonzero terms for either even or odd parity states and therefore $n+1$ eigenvalues for states of even and odd parities. Thus for a given integer n, we have $(n+1)$ eigenvalues that can be obtained from the finite expansion of $\phi(x)$. These states are the $(n+1)$ low-lying states of the system. This conclusion follows from the observation that the number of nodes of ϕ for states of even parity is

$$N = (\tfrac{1}{8})n(n+2) \quad (n \text{ even}), \quad (2.19)$$

$$N = (\tfrac{1}{8})(n^2 - 1) \quad (n \text{ odd}), \quad (2.20)$$

and for states of odd parity (excluding the node at the origin) is

$$N = (\tfrac{1}{8})n(n-2) \quad (n \text{ even}), \quad (2.21)$$

$$N = (\tfrac{1}{8})(n^2 - 1) \quad (n \text{ odd}), \quad (2.22)$$

and these are exactly the number of nodes associated with the lowest levels of the system for a given n. A different method of obtaining the eigenvalues and eigenfunctions of Eq. (2.10) is by series solution which is discussed in the Appendix.

In Table I the eigenfunctions ϕ_k and their corresponding eigenvalues ϵ_k are given for $n = 0$, 1, 2, and 3.

III. METHOD FOR GENERATING OTHER SOLUBLE POTENTIALS

From the solution of the eigenvalue equation (2.6), we can construct other soluble potentials. These potentials may be mono- or bistable depending on the integer n that appears in the original force law [Eq. (2.2)]. The method of construction is the direct application of Darboux's theorem to the solution of the eigenvalue problem.[7] A version of this theorem that is applicable to the present problem can be stated in the following way:

If the solution of

$$\psi_k'' + [\epsilon_k - v(x)]\psi_k = 0 \quad (k = 0, \ldots, n) \quad (3.1)$$

is known for the set of $(n+1)$ lowest eigenvalues $\epsilon_0, \epsilon_1, \ldots, \epsilon_n$, then the set of lowest n eigenvalues of the differential equation

$$u_{k-1}'' + \left[\epsilon_k - \epsilon_0 - \psi_0 \left(\frac{1}{\psi_0}\right)''\right] u_{k-1} = 0, \quad (k = 1, \ldots, n) \quad (3.2)$$

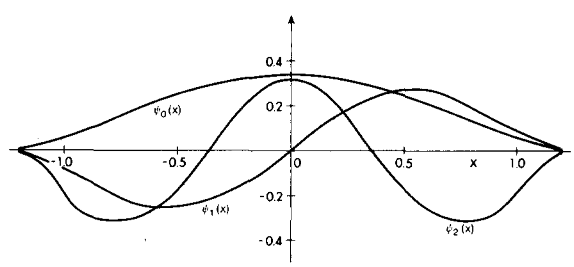

Fig. 2. Wave functions corresponding to the first three levels of the double-well potential ($n = 2$).

Table I. First few polynomial solutions of the eigenvalue Eq. (2.10).

$n = 0$	$\phi_0(x) = 1$	$\epsilon_0 = 0$
$n = 1$	$\phi_0(x) = \cosh x$	$\epsilon_0 = -(1+\xi)$
	$\phi_1(x) = \sinh x$	$\epsilon_1 = \xi - 1$
$n = 2$	$\phi_0(x) = \xi + [1 + (1+\xi^2)^{1/2}]\cosh 2x$	$\epsilon_0 = -2[1 + (1+\xi^2)^{1/2}]$
	$\phi_1(x) = \sinh 2x$	$\epsilon_1 = -4$
	$\phi_2(x) = \xi - [(1+\xi^2)^{1/2} - 1]\cosh 2x$	$\epsilon_2 = 2[(1+\xi^2)^{1/2} - 1]$
$n = 3$	$\phi_0(x) = 3\xi\cosh x + [4 - \xi + 2(4 - 2\xi + \xi^2)^{1/2}]\cosh 3x$	$\epsilon_0 = -[5 + \xi + 2(4 - 2\xi + \xi^2)^{1/2}]$
	$\phi_1(x) = 3\xi\sinh x + [4 + \xi + 2(4 + 2\xi + \xi^2)^{1/2}]\sinh 3x$	$\epsilon_1 = \xi - 5 - 2(4 + 2\xi + \xi^2)^{1/2}$
	$\phi_2(x) = 3\xi\cosh x + [4 - \xi - 2(4 - 2\xi + \xi^2)^{1/2}]\cosh 3x$	$\epsilon_2 = 2(4 - 2\xi + \xi^2)^{1/2} - 5 - \xi$
	$\phi_3(x) = 3\xi\sinh x + [4 + \xi - 2(4 + 2\xi + \xi^2)^{1/2}]\sinh 3x$	$\epsilon_3 = 2(4 + 2\xi + \xi^2)^{1/2} + \xi - 5$

are given by

$$u_{k-1} = \psi_0(\psi_k/\psi_0)', \tag{3.3}$$

where $\psi_0(x)$ is the ground-state wave function. Thus for a new potential

$$v^{(1)} = \psi_0(1/\psi_0)'', \tag{3.4}$$

the wave equation (3.2) is exactly soluble with the wave functions given by Eq. (3.3). We note that for all finite values of x, $v^{(1)}(x)$ is a well-behaved potential since $\psi_0(x)$ has no nodes.

This process of generating new potentials from the old wave functions can be continued n times, each time reducing the number of the wave functions determinable by this method by one. As an example, let us consider the case where $n = 1$ in the potential $V(x)$ [Eq. (2.2)]. The ground-state wave function for this potential is given by

$$\psi_0 = \cosh x \exp[-(1/4)\xi\cosh 2x]. \tag{3.5}$$

Substituting $\psi_0(x)$ in Eq. (3.4), we find the new potential

$$v^{(1)}(x) = \frac{1}{8}\xi^2(\cosh 4x - 1) + \xi + 1 - \frac{2}{\cosh^2 x}. \tag{3.6}$$

With this potential the Schrödinger equation (3.2) can be solved for the new ground-state wave function $u_0(x)$,

$$u_0(x) = (\cosh x)^{-1}\exp[-(1/4)\xi\cosh 2x], \tag{3.7}$$

a result which follows from Eq. (3.3), and can be verified by substituting Eq. (3.7) in (3.2). For this new potential the ground-state eigenvalue is given by

$$\epsilon_1 - \epsilon_0 = 2\xi. \tag{3.8}$$

Now let us consider the same problem when $n = 3$. For $\xi < 1$, the eigenvalues of Eq. (3.2) are given by

$$\begin{aligned} \lambda_0 &= \epsilon_1 - \epsilon_0 \simeq O(\xi^2), \\ \lambda_1 &= \epsilon_2 - \epsilon_0 \simeq 8 - 2\xi + O(\xi^2), \\ \lambda_3 &= \epsilon_3 - \epsilon_0 \simeq 8 + 2\xi + O(\xi^2). \end{aligned} \tag{3.9}$$

Here we observe that for the potential $v^{(1)}(x)$ the first and the second excited states are closely spaced, but both are far from the ground state. Thus the spectrum of $v^{(1)}(x)$ is different from that of $v(x)$, since for the latter $\epsilon_1 - \epsilon_0$ and $\epsilon_3 - \epsilon_2$ are both small but the spacing between ϵ_1 and ϵ_2 is large. To find a potential where only the two lowest eigenvalues are closely spaced, we can apply Darboux's theorem for the second time and obtain the potential

$$v^{(2)}(x) = u_0(1/u_0)''. \tag{3.10}$$

For this potential which is again bistable, the two lowest eigenvalues are given by $\lambda_1 - \lambda_0$ and $\lambda_2 - \lambda_0$. Now from Eq. (3.9) it is clear that the separation between these eigenvalues is of the order ξ^2 when $\xi \ll 1$, and hence this potential has a spectrum similar to $v(x)$ (when $n = 1$). For values of n larger than 3, this process can generate a number of bistable potentials.

IV. CONCLUSION

While the solution of the eigenvalue equation (2.6) predates the formulation of wave mechanics, the bistable potential function (2.2) does not seem to have been used previously. Yet the simplicity of the analytic form of the wave function for the low-lying states makes the wave equation (2.6) an interesting soluble bound-state problem in quantum mechanics. Let us summarize some of the interesting features of this eigenvalue problem:

(a) The potential depends on three parameters, and hence one can fit different spectra by adjusting these parameters. Also, for the same potential function, one finds both monostable and bistable quantal systems. The former property makes Eq. (2.2) a convenient force law for the description of a homonuclear molecule.

(b) This eigenvalue problem, like many other exactly soluble problems, can be solved by Sommerfeld's polynomial method. Thus the solution of Eq. (2.10) for $\phi(x)$ admits polnomials of $\cosh x$ and $\sinh x$ for even and odd parity states, respectively.

(c) Higher eigenvalues may be obtained in terms of elliptic integrals by using the WKB approximation.

(d) Finally, one can use these solutions to test approximate schemes carried out for complex systems, or to solve other problems such as the solution of the Fokker–Planck equation.[8]

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APPENDIX

In this appendix we consider an alternative way of solving the eigenvalue equation (2.10) using power series method. This is done by introducing a new variable z defined by

$$z = \cosh 2x - 1 \quad 0 \le z < \infty. \tag{A1}$$

Now, by changing the variable x in Eq. (2.10) to z, we find the differential equation

$$z(z+2)\phi'' + [1 + z - (1/2)\xi z(z+2)]\phi' + (1/4)(\epsilon + n\xi + n\xi z)\phi = 0, \tag{A2}$$

where primes indicate derivatives with respect to z. This equation has a regular singular point at $z = 0$, therefore we seek a solution of the form

$$\phi(z) = z^s f(z). \tag{A3}$$

By substituting Eq. (A3) in (A2) and putting the coefficients of the term $z^{s-1}f(z)$ equal to zero, we obtain the indicial equation for s and the differential equation for

$$2s^2 = s, \tag{A4}$$

$$z(z+2)f'' + [(2s + 1 - (1/2)\xi z)(z+2) - 1]f' + [s^2 - (1/2)\xi s(z+2) + (1/4)(\epsilon + n\xi + n\xi z)]f = 0 \tag{A5}$$

From Eq. (A4) it follows that we have two sets of independent solutions: the even states for $s = 0$, and the odd states for $s = 1/2$. Let us write $f(z)$ as a power series in $z + 2 = 2\cosh^2 x$:

$$f(z) = \sum_{j=0} (z+2)^{j+\sigma}. \tag{A6}$$

Substituting Eq. (A6) in (A5), we find

$$\sum_{j=0} a_j \Big[(z+2)^{j+\sigma+1}\xi\left(-\frac{1}{2}s + \frac{1}{4}n - \frac{1}{2}(j+\sigma)\right) + (z+2)^{j+\sigma}\left[(j+\sigma)(j+\sigma-1) + s^2 + \frac{1}{4}(\epsilon + n\xi) - \frac{1}{2}n\xi + (2s+1+\xi)(j+\sigma)\right] + (z+2)^{j+\sigma-1}(j+\sigma)[1 - 2(j+\sigma)]\Big] = 0. \tag{A7}$$

For polynomial solutions of Eq. (A2), the series in Eq. (A7) has to terminate and hence the coefficient of $(z+2)^{j+\sigma+1}$ for some integer $j = k$ must vanish. This condition gives a relation for σ:

$$n = 2(k + \sigma + s). \tag{A8}$$

One can verify that Eqs. (A3) and (A7) yield the same results as Eqs. (2.15) and (2.16).

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