Elementary functions and Schrödinger equations

Y. J. F. Kpomahou[a*], J. Akande[b], D. K. K. Adjaï [b], L. H. Koudahoun[b], M. D. Monsia[b]

a- Department of Industrial and Technical Sciences, ENSET-LOKOSSA, University of Abomey, Abomey, BENIN.

b- Department of Physics, University of Abomey-Calavi, Abomey-Calavi, 01. BP. 526, Cotonou, BENIN.

Abstract

The Schrödinger eigenvalue problem with diverse potentials is investigated in this work. It is shown that exact and explicit discrete bound state solutions may be computed in terms of elementary functions.

Introduction

The solution of the Schrödinger eigenvalue problem plays a fundamental role in description of quantum properties of dynamical systems. The Schrödinger equation with the purely exponential potential [1, 2]

$$V(x) = ae^{bx} \tag{1}$$

where $b \neq 0$, is, since many decades, the object of interesting mathematical and physical studies. This potential has been examined as a model of attractive potentials [3] for $a \prec 0$, and $b \prec 0$, and as a representation of repulsive potentials [4] where $a \succ 0$, and $b \prec 0$, for molecular physics. The complex eigenvalues of the Schrödinger equation with the repulsive potential have been explored recently [2]. Also the interest to study the discrete bound states defined by $a \succ 0$, and $b \succ 0$, has been underlined in the literature from the mathematical viewpoint as well as physical standpoint [1]. It is important to notice that the general solution to the Schrödinger equation with the exponential potential seems to be only computed in terms of various kinds of Bessel functions. More recently, scattering and bound states have been computed, within the framework of position- dependent mass Schrödinger equation with the exponential potential, in terms of elementary functions [5]. Therefore the investigation of exact and explicit integration of the Schrödinger equation with the purely exponential potential in terms of other types of functions rather than Bessel functions, precisely in terms of elementary functions, may be an interesting research problem in mathematical physics, for comparison objective. This may only be achieved under the condition that the Schrödinger equation with the exponential potential [1, 2]

* Corresponding author. fkpomahou@gmail.com

$$\psi''(x)+\left(E-a\,e^{bx}\right)\psi(x)=0 \tag{2}$$

where prime stands for differentiation with respect to the argument, is transformed into other types of exactly solvable differential equations, rather than in Bessel equation. In this context the fundamental problem in this work reduces to find such an appropriate transformation of variables. The present work assumes the existence of such a transformation so that the objective is to calculate the exact discrete bound state solutions of (2) in terms of elementary functions, for the first time, for the purely attractive exponential potentials. Thus using the point canonical transformation the Schrödinger equation (2) is mapped into an adequate differential equation which may be exactly solved in terms of elementary functions (section 2). Finally a discussion of results and a conclusion are drawn for the work.

2. Mathematical problem and solutions

In this part the Schrödinger eigenvalue problem is formulated and explicitly solved in terms of elementary functions for the attractive exponential potentials.

2.1 Schrödinger eigenvalue problem

Consider the Schrödinger equation (2), where a and b are constants. Then the following Schrödinger eigenvalue problem may be stated:

Determine the condition under which the Schrödinger equation (2) may exhibit exact discrete bound state solutions in terms of elementary functions.

To do so equation (2) needs to be transformed into an appropriate form.

2.2 Mapping of (2) under canonical transformation

Consider as a general expression for the point canonical transformation

$$\psi(x)=y(\tau)e^{-l\varphi(x)},\quad \tau=\beta e^{\gamma\varphi(x)} \tag{3}$$

As a consequence the following result may be formulated.

Theorem 1. Let $l=\dfrac{b}{4}$, $\beta=\dfrac{2}{b}$, $\gamma=\dfrac{b}{2}$, *and* $\varphi(x)=x$. *Then by the transformation (3), equation (2) reduces to the differential equation*

$$y''(\tau)+\left[\frac{1}{\tau^2}\left(\frac{1}{4}+\frac{4E}{b^2}\right)-a\right]y(\tau)=0 \tag{4}$$

Proof. By application of $l=\dfrac{b}{4}$, $\beta=\dfrac{2}{b}$, $\gamma=\dfrac{b}{2}$, and $\varphi(x)=x$, the point canonical transformation (3) becomes

$$\psi(x) = y(\tau)e^{-\frac{b}{4}x} \quad , \quad \tau = \frac{2}{b}e^{\frac{b}{2}x} \tag{5}$$

Using (5) one may obtain

$$\frac{d\psi}{dx} = \left(\frac{b}{2}\right)^{\frac{1}{2}}\left[y'(\tau)\tau^{\frac{1}{2}} - \frac{1}{2}y(\tau)\tau^{-\frac{1}{2}}\right]$$

which leads to

$$\frac{d^2\psi}{dx^2} = \left(\frac{b}{2}\right)^{\frac{3}{2}}\left[y''(\tau)\tau^{\frac{3}{2}} + \frac{1}{4}\tau^{-\frac{1}{2}}y(\tau)\right] \tag{6}$$

Substituting (6) into (2), equation (4) may be obtained, where $\left[E - ae^{bx}\right]\psi(x) = \left[E - a\left(\frac{b}{2}\right)^2\tau^2\right]\left(\frac{b\tau}{2}\right)^{-\frac{1}{2}}y(\tau)$.

In this way the equations (2) and (4) are mathematically equivalent. Therefore, to find the exact eigensolutions of (2), it suffices to solve (4).

2.3 Bound state solutions for the attractive exponential potential

This part is devoted to compute the exact discrete bound state solutions in terms of elementary functions to the Schrödinger eigenvalue problem under consideration. In this situation the condition to achieve this goal must first be determined. It suffices to notice that, as $\tau \neq 0$, it is always possible to set the condition

$$\frac{1}{4} + \frac{4E}{b^2} = 0$$

that is

$$E = -\frac{b^2}{16} \tag{7}$$

to obtain the desired bound state solutions in terms of elementary functions. The above shows the following theorem.

Theorem 2. Let $E = -\frac{b^2}{16}$. *Then equation (4) reduces to*

$$y''(\tau) - ay(\tau) = 0 \tag{8}$$

The general solution of (8) depends on the sign of the parameter a.

In this case, $a \prec 0,\; b \prec 0,$ and $0 \le x \prec +\infty.$ The general solution to (8) with the condition $a \prec 0$ may read

$$y(\tau) = A\cos\left(\sqrt{-a}\,\tau\right) + B\sin\left(\sqrt{-a}\,\tau\right) \tag{9}$$

where A and B are arbitrary constants to be determined by boundary conditions. In this way the following theorem may be considered.

Theorem 3. Let $a \prec 0, b \prec 0,$ *and* $0 \le x \prec +\infty.$ *If (9) is the general solution of (8), then the bound state solutions of (2) are given by*

$$\psi_n(x) = B_n\, e^{\frac{\sqrt{-a}}{2n\pi}x} \sin\left(n\pi e^{-\frac{\sqrt{-a}}{n\pi}x} \right) \tag{10}$$

where B_n *is the normalization constant defined by*

$$B_n^2 = \frac{1}{\int_0^{+\infty} e^{\frac{\sqrt{-a}}{n\pi}x} \sin^2\left(n\pi e^{-\frac{\sqrt{-a}}{n\pi}x} \right) dx} \tag{11}$$

and n *is an integer.*

Proof. From (9) and (5), it follows

$$\psi(x) = \left[A\cos\left(\frac{2}{b}\sqrt{-a}\, e^{\frac{b}{2}x} \right) + B\sin\left(\frac{2}{b} e^{\frac{b}{2}x} \right) \right] e^{-\frac{b}{4}x} \tag{12}$$

As the wave functions $\psi_n(x)$ must be zero as $x \to +\infty,$ then the constant A is required to be zero, that is $A = 0$, so that

$$\psi(x) = B e^{-\frac{b}{4}x} \sin\left(\frac{2}{b}\sqrt{-a}\, e^{\frac{b}{2}x} \right) \tag{13}$$

From (7), one may find $b = -4\sqrt{-E}$. Substituting this value of b into (13) leads to

$$\psi(x) = B e^{x\sqrt{-E}} \sin\left(\frac{\sqrt{aE}}{2E} e^{-2\sqrt{-E}\,x} \right) \tag{14}$$

On the other hand, the boundary condition $\psi(0) = 0$, may be satisfied by requiring $\sin\left(\frac{\sqrt{aE}}{2E} \right) = 0$, and $B \ne 0$, which leads to

$$E = E_n = \frac{a}{4\pi^2}\frac{1}{n^2} \tag{15}$$

Introducing (15) into (14) gives the desired bound state solutions (10).

Therefore the normalization condition may read

$$B_n^2 \int_0^\infty e^{\frac{\sqrt{-a}}{n\pi}x} \sin^2\left(n\pi e^{-\frac{\sqrt{-a}}{n\pi}x} \right) dx = 1 \tag{16}$$

References

[1] Miloslav Znojil, Symmetrized exponential oscillator, arXiv: 1609.00166v1 (2016).

[2] Paolo Amore, Accurate calculation of the complex eigenvalues of the Schrödinger equation with an exponential potential, arXiv: 0712.3375v1 (2007).

[3] S. T. Ma, Redundant zeros in the discrete energy spectra in Heisenberg's theory of characteristic matrix, Phys. Rev. 69 (1946) 668.

[4] O. Atabek, R. Lefebvre and M. Jacon, Poles of the scattering amplitude for the repulsive exponential: analytic and complex rotation studies, J. Phys. B: At. Mol. Phys. 15 (1982) 2689-2701.

[5] M. Sebawe Abdalla and H. Eleuch, Exact solutions of the position-dependent-effective mass Schrödinger equation, AIP ADVANCES 6, 055011-1-055011-7 (2016).