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ANALYTICAL SOLUTION OF THE POSITION DEPENDENT MASS SCHRÖDINGER EQUATION WITH A HYPERBOLIC TANGENT POTENTIAL

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Abstract: An analytical solution of the position dependent mass Schrödinger equation with a hyperbolic tangent potential is presented. The state energy and the corresponding wave function are obtained using the Nikiforov-Uvarov method. The energy eigenvalues and eigenfunctions are discussed and results are presented for some values of potential parameters.

AMS Subject Classification: 31L40, 81Q80, 81Q05
Key Words: Nikiforov-Uvarov method, Schrödinger equation, wave equation, energy, potential

1. Introduction

The Schrödinger equation is the fundamental equation describing the dynamics in microscopical systems (see [20]). In particular, in molecular and atom physics it is applied to determine the electronic structures and the energy distributions. The associated wavefunction is commonly used to explain the behavior of mi-

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coscopic systems. The exact solutions of the Schrödinger equation are limited to some few particular cases (see [22], [26], [21], [12], [11], [14], [2], and [6]). It is often that we use to approximate complicated potentials with simple known potential in order to catch the main physical proprieties of the system. Furthermore approximate methods were developed to solve the Schrödinger equation such as WKB, variations methods and ERS method (see [17], [27], [8], [18], [5], [9], [4], [3], [16], and [7]). Nikiforov-Uvarov has developed a powerful method to determine energies from potential verifying some particular conditions. With this technique the energies of several potentials are analytically determined. This method is also extend to mass-variable Schrödinger equation (see [1], [10], [25], [24]) and [19]). This equation is used to describe for example the dynamics of semiconductor systems where the effective mass of the electrons and holes vary with the position (see [15] and [23]).

In this work, we consider the case of a mass and a potential having hyperbolic tangent position variation. Analytical exact expressions of the energy and the wavefunction are derived.

2. Review of Nikiforov-Uvarov method

The Nikiforov-Uvarov (NU) method is a technique that takes advantages from orthogonal functions to solve second order differential equations (see [13]). In particular, it can be applied to the Schrödinger equation. We consider

$$\frac{d^2\psi(x)}{dx^2} + [E - V(x)]\psi(x) = 0, \tag{1}$$

where $\hbar = 2m_0 = 1$.

The Schrödinger equation can be transformed into a hypergeometric form by using an appropriate transformation $s = s(x)$

$$\Psi''(s) + \frac{\tilde{\tau}(s)}{\sigma(s)}\Psi'(s) + \frac{\tilde{\sigma}(s)}{\sigma^2(s)}\Psi(s) = 0, \tag{2}$$

where $\sigma(s)$ and $\tilde{\sigma}(s)$ are polynomials at most of second degree, and $\tilde{\tau}(s)$ is polynomial at most of first degree. To solve (2) explicitly, one can use change of variables by means of the wave functions

$$\Psi(s) = \phi(s)\chi(s), \tag{3}$$

to get after substituting (3) into (2)

$$\sigma(s)\chi''(s) + \tau(s)\chi'(s) + \lambda\chi(s) = 0, \tag{4}$$

where $\phi(s)$ is defined by

$$\frac{\phi'(s)}{\phi(s)} = \frac{\pi(s)}{\sigma(s)} \tag{5}$$

and $\pi(s)$ is a polynomial of degree less or equal to one.

The hypergeometric function $\chi(s)$ in (4) satisfies the Rodrigues relation

$$\chi(s) = \frac{B_n}{\rho(s)} \frac{d^n}{ds^n} \left[\sigma^n(s)\rho(s)\right], \tag{6}$$

where B_n is the normalization constant, n is a fixed given number, and $\rho(s)$ is the weight function that satisfies the differential equation

$$\frac{d}{ds}\left[\sigma(s)\rho(s)\right] = \tau(s)\rho(s) \tag{7}$$

with

$$\tau(s) = \tilde{\tau}(s) + 2\pi(s). \tag{8}$$

Condition (7) is satisfied if one imposes a condition on the polynomial function $\tau(s)$ and its derivative, that is, $\tau(s)$ to be zero at some point in some interval I and

$$\tau'(s) < 0. \tag{9}$$

So, the function $\pi(s)$ and the parameter λ required for the Nikiforov-Uvarov method are defined as:

$$\pi(s) = \left(\frac{\sigma' - \tilde{\tau}}{2}\right) \pm \sqrt{\left(\frac{\sigma' - \tilde{\tau}}{2}\right)^2 - \tilde{\sigma} + k\sigma}, \tag{10}$$

$$\lambda = k + \pi'(s). \tag{11}$$

To determine $\pi(s)$ in (10) one need another condition, that is we assume that the discriminant of the expression under the square root be set to zero. With this, the new eigenvalues in equation (11) become

$$\lambda = \lambda_n = -n\tau'(s) - \frac{n(n-1)}{2}\sigma''(s), \quad n = 0, 1, 2, ... \tag{12}$$

The energy eigenvalues are then obtained from (12) and (11).

3. Mass dependent Schrödinger equation

The Schrödinger equation with position dependent mass $m(z) = m_0\tilde{\rho}(z)$ is given by

$$-\frac{d}{dz}\left[\frac{1}{\tilde{\rho}(z)}\frac{d\psi(z)}{dz}\right] + V(z)\psi(z) = E\psi(z).$$

The parametric generalization of the NU method is given by the generalized hypergeometric-type equation as

$$-\frac{d^2\psi(x)}{dx^2} - (2v-1)\frac{m'(x)}{m(x)}\frac{d\psi(x)}{dx} \tag{13}$$

$$+\left\{\begin{array}{c} -[v(v-2)+\alpha(\alpha+\beta+1)+\beta+1]\dfrac{m'^2(x)}{m^2(x)}+ \\ \left[\dfrac{1}{2}(\beta+1)\right]\dfrac{m''(x)}{m(x)}+m(x)(V(x)-E) \end{array}\right\}\psi(x) = 0,$$

where V_0 is the potential depth and the $m(x)$ is the mass distribution to be taken as

$$m(x) = \tanh(\lambda x) + 1. \tag{14}$$

A plot of the mass distribution and the potential are shown in Figures 1 and 2.

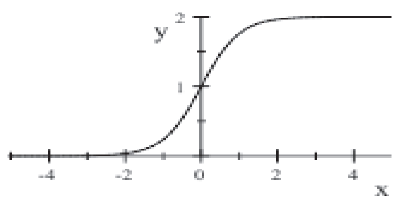

Figure 1: Mass distribution with $\lambda = 1$.

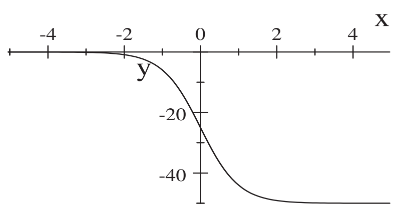

Figure 2: Potential depth with $V_0 = 50,\ \lambda = 1$.

To change Eq. (13) to NU equation form, we define the transformation $s(x) = \tanh(\lambda x)$, $-1 < s < 1$.

We have

$$\begin{aligned} \frac{m'(x)}{m(x)} &= \lambda(1-s) \\ \frac{m''(x)}{m(x)} &= 2\lambda^2 s(s-1) \end{aligned} \tag{15}$$

Using this transformation, we get

$$\begin{aligned} &\frac{d^2\Psi}{ds^2} + \frac{(1+2v)s-2v+1}{s^2-1}\frac{d\Psi}{ds} \\ &+\frac{1}{(s^2-1)^2}\left[A(1-s)^2 - 2Bs(s-1) - \frac{1}{\lambda^2}(s+1)(V(x)-E)\right]\Psi = 0, \end{aligned} \tag{16}$$

where

$$\begin{aligned} A &= v(v-2)+\alpha(\alpha+\beta+1)+\beta+1, \\ B &= \frac{1}{2}(\beta+1)+v, \\ \zeta &= \frac{1}{2}-v. \end{aligned}$$

Rearranging the terms inside the brackets in (14) we obtain the parametric generalization of the NU method, given by the generalized hypergeometric-type equation,

$$\begin{aligned} &\frac{d^2\Psi}{ds^2} + \frac{(1+2v)s-2v+1}{s^2-1}\frac{d\Psi}{ds} + \\ &\frac{1}{(s^2-1)^2}\left[\begin{array}{c} \left(\frac{V_0}{2\lambda^2}+A-2B\right)s^2 \\ +\left(\frac{E+V_0}{\lambda^2}-2A+2B\right)s+\left(\frac{2E+V_0}{2\lambda^2}+A\right) \end{array}\right]\Psi = 0, \end{aligned}$$

or

$$\frac{d^2\Psi}{ds^2} + \frac{(1+2v)s-2v+1}{s^2-1}\frac{d\Psi}{ds} + \frac{1}{(s^2-1)^2}\left[\begin{array}{c} \left(\zeta^2-c_1\right)s^2+ \\ \left(c_2-2\zeta^2\right)s+ \\ \left(\zeta^2-c_3\right) \end{array}\right]\Psi = 0, \tag{17}$$

where

$$c_1-\zeta^2 = 2B-A-\frac{V_0}{2\lambda^2}$$

$$\begin{aligned} c_2 - 2\zeta^2 &= 2B - 2A + \frac{E+V_0}{\lambda^2} \\ c_3 - \zeta^2 &= -A - \frac{2E+V_0}{2\lambda^2} \\ c_1 - c_2 + c_3 &= \varepsilon^2 = -\frac{2}{\lambda^2}(E+V_0). \end{aligned}$$

To get the energy we have from Eqn. (17)

$$\begin{aligned} \sigma(s) &= s^2 - 1 && (18) \\ \tilde{\sigma}(s) &= \left(\zeta^2 - c_1\right)s^2 + \left(c_2 - 2\zeta^2\right)s + \left(\zeta^2 - c_3\right) && (19) \\ \tilde{\tau}(s) &= (1+2v)s + 1 - 2v, && (20) \end{aligned}$$

$\pi(s)$ is given by (10), substituting the above polynomials we get

$$\pi(s) = \zeta(s-1) \pm \sqrt{(k+c_1)s^2 - c_2 s + c_3 - k}. \tag{21}$$

We use the condition that the discriminant of the quadratic expression under the square root in (21) must be zero, that is

$$k = \frac{1}{2}c_3 - \frac{1}{2}c_1 \pm \frac{1}{2}\varepsilon\sqrt{2c_2 + \varepsilon^2}. \tag{22}$$

Therefore $\pi(x)$ can be written as

$$\begin{aligned} \pi(x) &= \zeta(s-1) - \frac{1}{2}(\sqrt{\varepsilon^2 + 2c_2} + \varepsilon) + \frac{1}{2}s(\sqrt{\varepsilon^2 + 2c_2} - \varepsilon) && (23) \\ &= \zeta(s-1) - \frac{1}{2}(\sqrt{\zeta^2 - A + B} + \varepsilon) + \frac{1}{2}s(\sqrt{\zeta^2 - A + B} - \varepsilon) \\ \text{if} \quad k &= \frac{1}{2}c_3 - \frac{1}{2}c_1 - \frac{1}{2}\varepsilon\sqrt{2c_2 + \varepsilon^2}. \end{aligned}$$

So to obtain the energy E we need to find ε.
We have

$$\begin{aligned} \lambda &= k + \pi'(s) && (24) \\ \lambda &= \lambda_n = -n\tau'(s) - \frac{n(n-1)}{2}\sigma''(s) = -n\tau'(s) - n(n-1) && (25) \\ \tau(s) &= \tilde{\tau}(s) + 2\pi(s) = (2 - \varepsilon + \sqrt{\varepsilon^2 + 2c_2})s - (\sqrt{\varepsilon^2 + 2c_2} + \varepsilon) \\ \tau'(s) &= 2 - \varepsilon + M \\ M &= \sqrt{\varepsilon^2 + 2c_2}. && (26) \end{aligned}$$

Combining Eqns (24) and (25) we get

$$\begin{aligned}\varepsilon &= 2n+1+M+2\sqrt{c_1+v-\frac{1}{4}}\\ \text{where } M &= 2\sqrt{2v-\alpha-\frac{\beta}{2}-\alpha^2-\alpha\beta-\frac{1}{4}}.\end{aligned}$$

Combining (23), (24) and (25) we obtain

$$E_n = -2\lambda^2\left(\begin{array}{c} n+\frac{1}{2}+\sqrt{2v-\alpha-\frac{\beta}{2}-\alpha^2-\alpha\beta-\frac{1}{4}+} \\ \sqrt{4v-\alpha-\alpha^2-\alpha\beta-\frac{1}{2\lambda^2}V_0} \end{array}\right)^2 - V_0. \tag{27}$$

To derive the approximation of the wave function $\Psi(s)$ in (3) we need to determine $\phi(s)$ and $\chi(s)$. By using Eqns (7), (8) and (18) we get

$$\rho(s) = (s-1)^{-\varepsilon}(s+1)^{\sqrt{\varepsilon^2+2c_2}}. \tag{28}$$

Similarly using (5), (18) and (23) we get

$$\phi(s) = (s-1)^{\frac{1}{2}-v-\frac{1}{2}\varepsilon}(s+1)^{\frac{\sqrt{\varepsilon^2+2c_2}}{2}} \tag{29}$$

The wave equation which is given by (3)

$$\Psi_n(s) = \phi(s)\frac{B_n}{\rho(s)}\frac{d^n}{ds^n}\left[\sigma^n(s)\rho(s)\right]. \tag{30}$$

From Eqns (28) and (29) we obtain

$$\begin{aligned}\Psi_n(s) &= (-1)^n(-1)^{\frac{1}{2}-v-\varepsilon/2}(1-s)^{\frac{1}{2}-v+\varepsilon/2}(1+s)^{-\frac{1}{2}\sqrt{\varepsilon^2+2c_2}}\\ &\quad\times B_n\frac{d^n}{ds^n}\left[(1-s)^{n-\varepsilon}(1+s)^{n+\sqrt{\varepsilon^2+2c_2}}\right].\end{aligned} \tag{31}$$

By introducing the Jacobi polynomial given by

$$P_n^{(\mu,\theta)}(x) = \frac{(-1)^n(1-x)^{-\mu}(1+x)^{-\theta}}{2^n n!}\times\frac{d^n}{dx^n}\left[(1-x)^{n+\mu}(1+x)^{n+\theta}\right], \tag{32}$$

the wave equation takes the form

$$\Psi_n(s) = 2^n n!(-1)^{1/2-v-\varepsilon/2}(1-s)^{1/2-v-\varepsilon/2}(1+s)^{\frac{1}{2}\sqrt{\varepsilon^2+2c_2}}B_n P_n^{(\mu,\theta)}(s) \tag{33}$$

with $\mu = -\varepsilon, \quad \theta = \sqrt{\varepsilon^2 + 2c_2}$.

There B_n is the normalized constant that can be obtained using the relation

$$\int_0^1 |\Psi_n(s)|^2 \, ds = 1.$$

The graph of the wave function $\Psi_n(s)$ and the energy E_n are shown in Figures 3 and 4, respectively.

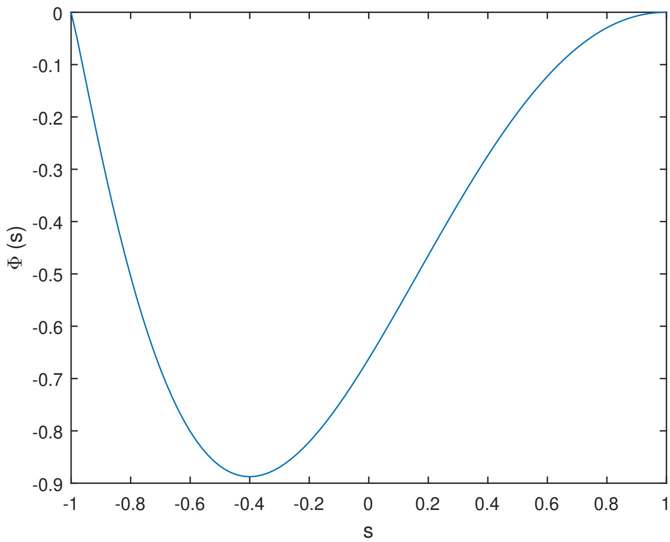

Figure 3: Wave equation for $\alpha = 0$, $\beta = -1$, $\upsilon = 1/2$, $n = 1$, $\lambda = 1$ and $V_0 = 4$.

4. Conclusion

In this paper the Nikiforov-Uvarov method is used to derive the solution of the mass variable Schrödinger equation with a hyperbolic tangent potential. The wave function is expressed in terms of the Jacobi polynomials and the energy eigenvalues are analytically determined. The hyberbolic tangent potential is one of the toy models that can be used in several fields of physics such as solid states physics and quantum field theories, where the supersymmetry can be associated to such a hyperbolic potential.

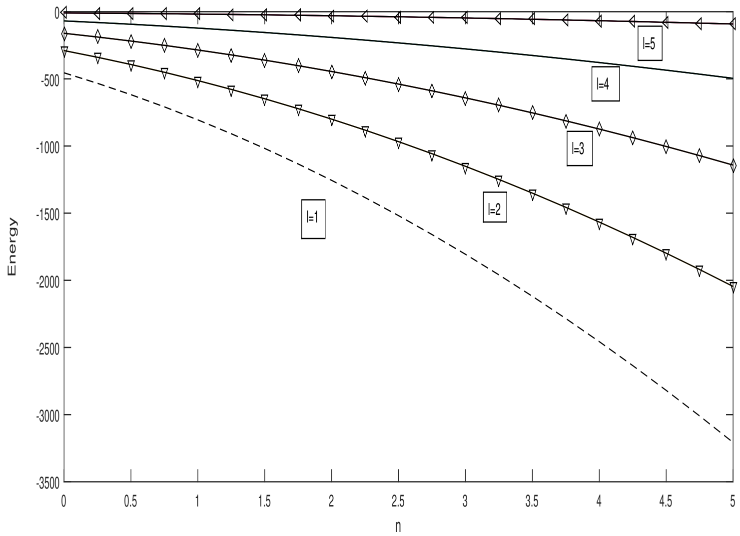

Figure 4: Energy E_n for different values of $\lambda = 1$.

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