Quantum mechanics of singular inverse square potentials under usual boundary conditions

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The quantum mechanics of inverse square potentials in one dimension is usually studied through renormalization, self-adjoint extension and WKB approximation. This paper shows that such potentials may be investigated within the framework of the position-dependent mass quantum mechanics formalism under the usual boundary conditions. As a result, exact discrete bound state solutions are expressed in terms of associated Laguerre polynomials with negative energy spectrum using the Nikiforov-Uvarov method for the repulsive inverse square potential.

Keywords: Singular repulsive potentials, Schrödinger equation, position-dependent mass, bound state solutions, quantum mechanics, Nikiforov-Uvarov method.

1 Introduction

The problem of exact discrete bound states for strongly singular potentials has been a subject of intensive analytic studies in the research field of mathematical physics. In particular, the one-dimensional Schrödinger equation for the singular inverse square potential is well known to require a special mathematical treatment. In [1] for example, the renormalization technique has been used to study the one-dimensional attractive inverse square potential. Recently, this potential has been analyzed in [2] in the context of renormalization and self-adjoint extension of the Hamiltonian operator. In [3] WKB approximation with special mathematical treatments are used to solve the Schrödinger wave problem for the strongly repulsive potentials. Such inverse square potentials are known to be used for modeling many practical problems in modern engineering studies. The question of discrete bound state solutions for repulsive potentials is not yet completely resolved [2, 4, 5]. In such a situation, there appears logic to investigate the quantum mechanics of strongly repulsive singular inverse square potentials under usual boundary conditions. In this work, the position-dependent mass formalism is shown to have the ability to remedy some inherent difficultes related to the naturel domain of this potential. Due to its applications for the quantum control [6] the Schrödinger equation with position-dependent mass has fast become an important research field from mathematical as well as physical point of view. Many problems have been solved in various areas of science on the basis of

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quantum harmonic oscillators with position-dependent mass approach [7]. To apply this approach to the singular repulsive inverse square potential, there appears convenient to consider the oscillator equation

$$\ddot{x}+\frac{l-2\gamma}{x}\dot{x}^2+\frac{\omega^2}{l+1}x^{4\gamma+1}=0 \tag{1.1}$$

where the dot over a symbol denotes the time derivative, and l, γ and $\omega>0$, are arbitrary parameters. The equation (1.1) belongs to the class of quadratic Liénard type differential equation recently introduced by some authors of this work [8]. The parametric choice $l=2\gamma\neq 0$, reduces this equation for $l\neq -1$, to the free particle Duffing equation

$$\ddot{x}+\frac{\omega^2}{l+1}x^{2l+1}=0$$

which has been intensively studied in the literature [9] for $l\neq -1$. For $\gamma=l=0$, the equation (1.1) reduces to the linear harmonic oscillator equation with well known exact trigonometric solution. According to [8], the equation (1.1) may be mapped into the linear harmonic oscillator equation so that exact periodic solutions may be exhibited for the equation (1.1). Using the non-local transformation introduced by some authors of the present paper in [8].

$$y(\tau)=\frac{1}{l+1}x^{l+1},\quad d\tau=x^{2\gamma}dt,\quad l\neq -1 \tag{1.2}$$

the equation (1.1) reduces to the linear oscillator equation

$$y''(\tau)+\omega^2 y(\tau)=0$$

where the prime denotes the differentiation with respect to τ. On making $y(\tau)=A_0 sin(\omega\tau+\alpha)$, where A_0 and α are arbitrary parameters, the exact analytical solution to (1.1) reads

$$x(t)=[(l+1)A_0]^{\frac{1}{l+1}}[sin(\omega\phi(t)+\alpha)]^{\frac{1}{l+1}} \tag{1.3}$$

where the function $\tau=\phi(t)$ satisfies

$$\frac{d\tau}{dt}=[(l+1)A_0 sin(\omega\phi(t)+\alpha)]^{\frac{2\gamma}{l+1}}$$

that is

$$[(l+1)A_0]^{\frac{2\gamma}{l+1}}(t-t_0)=\int\frac{d\phi(t)}{[sin(\omega\phi(t)+\alpha)]^{\frac{2\gamma}{l+1}}} \tag{1.4}$$

where t_0 is a constant of integration. The integral from the right hand side may be explicitly computed once the parametric choice is defined. Having demonstrated that the equation (1.1) under consideration admits exact analytical periodic solution [8], the problem to be investigated in this work is to know whether this equation may exhibit an exact solvable position-dependent mass Schrödinger equation with a singular repulsive inverse square potential. More precisely the question to be addressed is: Is the quantization of (1.1) leads to an exact solvable Schrödinger wave equation with a repulsive inverse square potential in terms of discrete bound states under the position-dependent mass approach? The present research contribution predicts that the quantization of (1.1) yields exact discrete bound state solutions to the Schrödinger equation for the repulsive inverse square potential and negative energy spectrum under the context of usual boundary conditions. This prediction is physically interesting since it allows the investigation not only under usual boundary conditions of quantum features of singular potentials but also in terms of exact eigensolutions which are quite suitable for engineering calculations. In this perspective, to demonstrate the preceding prediction, there is convenient to first establish the Schrödinger wave equation associated to the equation (1.1) and secondary to transform the obtained equation to apply the Nikiforov-Uvarov method [10] well known to yield eigenvalue problem solutions in terms of classical orthogonal polynomials.The predicted results are finally discussed and a conclusion is drawn for the paper.

2 Schrödinger eigenvalue problem

The one-dimensional Schrödinger wave equation is an eigenvalue problem that requires the mathematical formulation of the Hamiltonian operator associated to the classical oscillator differential equation under study. By defining the mass function

$$M(x) = e^{2\int^x f(s)ds}$$

According to (1.1), $f(s) = \frac{l-2\gamma}{s}$, thus the function $M(x)$ takes the form

$$M(x) = e^{2\int^x \frac{l-2\gamma}{s}ds}$$

or

$$M(x) = m_0 x^{2(l-2\gamma)} \tag{2.1}$$

where m_0 is the integration constant, and the potential energy

$$V(x) = \int^x g(s)M(s)ds,$$

where $M(s) = m_0 s^{2(l-2\gamma)}$ and $g(s) = \frac{\omega^2}{l+1}s^{4\gamma+1}$ after (1.1) takes the following form

$$V(x) = \frac{m_0}{l+1}\omega^2 \int^x s^{2l+1}ds.$$

Thus, one obtains

$$V(x) = \frac{m_0\omega^2}{2(l+1)^2}x^{2l+2} \tag{2.2}$$

and the classical Hamiltonian

$$H(x,p) = \frac{p^2}{2M(x)} + V(x)$$

associated to (1.1) reads

$$H(x,p) = \frac{1}{2m_0}p^2x^{2(2\gamma-l)} + \frac{m_0\omega^2}{2(l+1)^2}x^{2l+2} \tag{2.3}$$

In this work, the von Roos expression of quantum Hamiltonian [11] associated to (2.3) for harmonic oscillator with position-dependent mass may be suitably used.

2.1 Schrödinger equation

The Schrödinger equation for bound states $\psi(x)$ with the energy eigenvalue E and potential $V(x)$, according to [12, 13], may read

$$\psi''(x) - \frac{M'(x)}{M(x)}\psi'(x) + 2M(x)\left[E - V(x)\right]\psi(x) = 0 \tag{2.4}$$

which becomes in the context of equations (2.1) and (2.2)

$$\psi''(x) - \frac{2(l-2\gamma)}{x}\psi'(x) + \left[2Ex^{2l-4\gamma} - \frac{\omega^2}{(l+1)^2}x^{4l-4\gamma+2}\right]\psi(x) = 0 \tag{2.5}$$

where $m_0 = \hbar = 1$, and the prime means differentiation with respect to x. Now, it becomes possible to clearly state the Schrödinger eigenvalue problem to solve.

2.2 Mathematical problem

Let us consider the parametric choice $l = -2$, and $\gamma = -\frac{3}{2}$. The potential energy (2.2) becomes

$$V(x) = \frac{m_0\omega^2}{2}\frac{1}{x^2} \tag{2.6}$$

with $m_0 = 1$, which is a singular repulsive inverse square potential, as $\omega^2 > 0$, such that (2.5) becomes

$$\frac{d^2\psi(x)}{dx^2} - \frac{2}{x}\frac{d\psi(x)}{dx} + [2Ex^2 - \omega^2]\psi(x) = 0$$

that is in the self-adjoint form

$$\frac{d}{dx}\left(\frac{\psi'(x)}{x^2}\right) + \left(2E - \frac{\omega^2}{x^2}\right) = 0 \tag{2.7}$$

The equation (2.7) may then read as a Schrödinger equation for repulsive inverse square potential under the formalism of position-dependent mass. Therefore, the mathematical eigenvalue problem to be solved may read: Find the discrete bound state solutions to (2.7) over the semi-infinite interval $[0, +\infty[$ with the requirement that $\psi(x) \longrightarrow 0$ as $x \longrightarrow 0$ and $x \longrightarrow +\infty$, that is $\psi(x) \in L^2([0, +\infty[)$. The solution to this problem needs to perform coordinate transformation to apply the Nikiforov-Uvarov method [10].

3 Exact discrete bound state solutions

The NU method applies to the generalized hypergeometric type equation of the form

$$Z''(s) + \frac{\tilde{\tau}(s)}{\sigma(s)}Z'(s) + \frac{\tilde{\sigma}(s)}{\sigma(s)^2}Z(s) = 0 \tag{3.1}$$

where

$$Z(s) = \phi(s)y_n(s) \tag{3.2}$$

the prime means differentiation with respect to s, such that the hypergeometric type function $y_n(s)$ satisfies

$$\sigma(s)y_n''(s) + \tau(s)y_n'(s) + \lambda y_n(s) \tag{3.3}$$

with

$$\frac{\phi'(s)}{\phi(s)} = \frac{\pi(s)}{\sigma(s)} \tag{3.4}$$

The coefficients $\sigma(s)$ and $\tilde{\sigma}(s)$ are polynomials at most of second degree whereas the parameters $\tau(s)$ and $\tilde{\tau}(s)$ are polynomials at most of first degree. λ is a constant. The function

$$\pi(s) = \left(\frac{\sigma'(s) - \tilde{\tau}(s)}{2}\right) \pm \sqrt{\left(\frac{\sigma'(s) - \tilde{\tau}(s)}{2}\right)^2 - \tilde{\sigma}(s) + k\sigma(s)} \tag{3.5}$$

is a polynomial at most of first degree that obeys

$$\tau(s) = \tilde{\tau}(s) + 2\pi(s) \tag{3.6}$$

The coefficient k satisfies

$$\lambda = k + \pi'(s) \tag{3.7}$$

so that

$$\lambda = \lambda_n = -n\tau'(s) - \frac{n(n-1)}{2}\sigma''(s), \quad n = 0, 1, 2, 3, ... \tag{3.8}$$

According to (3.3) the expression of the hypergeometric type function $y_n(s)$ which is a polynomial of degree n may be given by the Rodrigues formula

$$y_n(s) = \frac{A_n}{\rho(s)}\frac{d^n}{ds^n}\left[\sigma(s)^n\rho(s)\right] \tag{3.9}$$

and the weight function $\rho(s)$ should satisfy

$$\frac{d}{ds}\left[\sigma(s)\rho(s)\right] = \tau(s)\rho(s) \tag{3.10}$$

where A_n designates a normalization constant. In this perspective the application of these calculations to (2.7) requires its transformation into the form (3.1).

3.1 Mapping of the Schrödinger wave equation into the hypergeometric type equation

The application of the variable transformation

$$\psi(x) = xZ(x) \tag{3.11}$$

maps the equation (2.7), after a few mathematical manipulations

$$\frac{d\psi(x)}{dx} = Z(x) + x\frac{dZ(x)}{dx}$$

and

$$\frac{d^2\psi(x)}{dx^2} = 2\frac{dZ(x)}{dx} + x\frac{d^2Z(x)}{dx^2},$$

into the differential equation

$$\frac{d^2Z}{dx^2} + \left[2Ex^2 - \frac{2}{x^2} - \omega^2\right] Z = 0 \tag{3.12}$$

Now, consider the coordinate transformation

$$s = x^2 \tag{3.13}$$

with $0 \leqslant s \leqslant \infty$. Using (3.13), one may compute

$$\frac{dZ(x)}{dx} = 2s^{\frac{1}{2}}\frac{dZ(s)}{ds}$$

from which it follows after a few algebraic manipulations

$$\frac{d^2Z(x)}{dx^2} = 2\frac{dZ(s)}{ds} + 4s\frac{d^2Z(s)}{ds^2}$$

The substitution of the above expression into (3.12) yields

$$\frac{d^2Z(s)}{ds^2} + \frac{1}{2s}\frac{dZ(s)}{ds} + \left[\frac{(\frac{E}{2})s^2 - (\frac{\omega^2}{4})s - \frac{1}{2}}{s^2}\right] Z(s) = 0 \tag{3.14}$$

at which the preceding calculations may immediately be applied to compute the discrete bound state solutions under consideration.

3.2 Exact discrete bound state energy spectrum

The comparison of (3.14) with (3.1) gives $\tilde{\tau}(s)=\frac{1}{2}$, $\tilde{\sigma}(s)=(\frac{E}{2})s^2 - (\frac{\omega^2}{4})s - \frac{1}{2}$ and $\sigma(s) = s$, so that the requirement that the derivative of $\tau(s)$ must be negative imposes to choose

$$\pi(s) = \frac{1}{4} - \sqrt{-\frac{E}{2}s^2 + (k + \frac{\omega^2}{4})s + \frac{9}{16}} \tag{3.15}$$

The requirement that the expression under the square root sign must be the square of a polynomial yields

$$k = -\frac{\omega^2}{4} + \frac{3}{2}\sqrt{-\frac{E}{2}} \tag{3.16}$$

so that $\pi(s)$ becomes

$$\pi(s) = 1 - s\sqrt{-\frac{E}{2}} \tag{3.17}$$

with $E \leqslant 0$ and

$$\tau(s) = \frac{5}{2} - 2s\sqrt{-\frac{E}{2}} \tag{3.18}$$

The comparison of (3.7) with (3.8) gives

$$k = (2n+1)\sqrt{-\frac{E}{2}} \tag{3.19}$$

so that by taking into account (3.16) one may obtain the discrete bound state energy spectrum

$$E_n = -\frac{\omega^4}{2(4n-1)^2} \quad , n = 0, 1, 2, 3, ... \tag{3.20}$$

So with that, one may deduce the discrete bound state wave functions $\psi_n(x)$.

3.3 Exact discrete bound state wave functions

Using the functions $\sigma(s)$ and $\tau(s)$ previously defined, the function $\phi(s)$ becomes

$$\phi(s) = s \exp\left(-\frac{\omega^2}{2(4n-1)}s\right) \tag{3.21}$$

and $\rho(s)$ reads

$$\rho(s) = s^{\frac{3}{2}} \exp\left(-\frac{\omega^2}{(4n-1)}s\right) \tag{3.22}$$

such that

$$y_n(s) = \frac{A_n}{s^{\frac{3}{2}} \exp\left(-\frac{\omega^2}{(4n-1)}s\right)} \frac{d^n}{ds^n}\left(s^{n+\frac{3}{2}} \exp\left(-\frac{\omega^2}{(4n-1)}s\right)\right) \tag{3.23}$$

Therefore, the function $Z(s)$ may be written as

$$Z_n(s) = s \exp\left(-\frac{\omega^2}{2(4n-1)}s\right) \frac{A_n}{s^{\frac{3}{2}} \exp\left(-\frac{\omega^2}{(4n-1)}s\right)} \frac{d^n}{ds^n}\left(s^{n+\frac{3}{2}} \exp\left(-\frac{\omega^2}{(4n-1)}s\right)\right) \tag{3.24}$$

Using the identity $s = x^2$, one may obtain

$$Z_n(x^2) = A_n x^{-1} \exp\left(\frac{\omega^2}{2(4n-1)}x^2\right) \frac{d^n}{d(x^2)^n}\left(x^{2n+3} \exp\left(-\frac{\omega^2}{(4n-1)}x^2\right)\right) \tag{3.25}$$

so that the variable transformation (3.11) yields immediately the desired wave functions

$$\psi_n(x) = A_n \exp\left(\frac{\omega^2}{2(4n-1)}x^2\right) \frac{d^n}{d(x^2)^n}\left(x^{2n+3} \exp\left(-\frac{\omega^2}{(4n-1)}x^2\right)\right) \tag{3.26}$$

which may be written in terms of associated Laguerre polynomials as

$$\psi_n(x) = C_n x^3 \exp\left(-\frac{\omega^2}{2(4n-1)}x^2\right) L_n^{\frac{3}{2}}\left(\frac{\omega^2}{(4n-1)}x^2\right) \tag{3.27}$$

where C_n is the new normalization constant which must satisfy the normalization condition.

$$C_n^2 \int_0^{+\infty} x^6 e^{-\varepsilon x^2} \left(L_n^{\frac{3}{2}}(\varepsilon x^2)\right)^2 dx = 1 \tag{3.28}$$

where

$$\varepsilon = \frac{\omega^2}{4n-1}$$

That being so a discussion of the developed singular inverse square potential theory may be performed.

4 Discussion

The problem of singular inverse square potentials in one dimension has been in general studied using the self-adjoint extension and renormalization or WKB approximation technique due to problem related to is natural domain. The discrete negative energy states for the repulsive potentials are still a question under discussion in the fields of quantum mechanics and mathematical physics. In this work the study of the repulsive inverse square potential in the framework of the position-dependent mass formalism has been proposed. Under this formalism it has been possible to predict discrete negative energy eigensolutions to the Schrödinger equation for the singular repulsive square potential. A major advantage is that the integration of the Schrödinger wave equation has been effected under the usual boundary conditions. Another interesting advantage results from the application of the Nikiforov-Uvarov method which led to express the discrete bound state eigenfunctions in terms of associated Laguerre polynomials which are intensively investigated in the literature. The Nikiforov-Uvarov method shows also that the repulsive inverse square potential may exhibit discrete bound state negative energy eigenvalues with zero as upper value in the usual boundary conditions. In this regard the ground state energy is found to be finite and different from zero.

5 Conclusion

The investigation of the inverse square potentials is usually effected by means of renormalization, self-adjointness and WKB approximation. The repulsive inverse square potential is shown in this work to exhibit exact discrete bound state solutions within the framework of position-dependent mass quantum mechanics under usual boundary conditions. The discrete bound state energy eigenvalues showed that the ground state energy is finite with a non-zero value and eigenfunctions were expressed in terms of associated Laguerre polynomials using the Nikiforov-Uvarov method.

References

[1] K. S. Gupta and S. G. Rajeev, Renormalization in quantum mechanics, arXiv.org/9305052v2 [math-phy]. pdf (1993).

[2] A. M. Essin, D. J. Griffiths, Quantum mechanics of the $\frac{1}{x^2}$ potential, Am. J .Phys. 74 (2) (2006).

[3] S. A. Sofianos, S.A. Rakityansky and S.E. Massen, Jost Function for Singular potentials, arXiv.org/9901023v1 [math-phy]. pdf (1999).

[4] H. Brysk and P. F. Zweifel, Possible bound states of repulsive potentials, Physical Review C, 23 (1981) 968-972.

[5] T. Fülöp, Singular potentials in quantum mechanics and ambiguity in the sel-adjoint Hamiltonian, Symmetry, Integrability and Geometry: Methods and Applications, 3: 1-12 (2007).

[6] A. G. M. Schmidt, Time evolution for harmonic oscillators with position-dependent mass, Phys. Scr. 75 (2007) 480-483.

[7] J. Förster, A. Saenz, U. Wolff, Matrix algorithm for solving Schrödinger equations with position-dependent mass or complex optical potentials, Physical Review E, 86 (2012).

[8] J. Akande , D. K. K. Adjaï, L. H. Koudahoun, Y. J. F. Kpomahou, M. D. Monsia, Theory of exact trigonometric periodic solutions to quadratic Liénard type equations, Journal of Mathematics and Statistics, 14 (1): 232-240, DOI: 10.3844/jmssp.2018.232.240 (2018).

[9] Y. J. F. Kpomahou, L. H. Koudahoun, D. K. K. Adjaï, J. Akande, M. D. Monsia, Exact harmonic periodic solution of a Class of Liénard-Type position-dependent mass oscillator equations and exact periodic solution of a class of Duffing equations, Math.Phys.,viXra.org/1609.0037v1.pdf (2016).

[10] A. F. Nikiforov and V. B. Uvarov, Special Functions of Mathematical Physics, ed. Mir, Moscou, 1983.

[11] O. von Roos, Position-dependent effective masses in semiconductor theory, Physical Review, B 27 (1983) 7547.

[12] Jean Akande, Damien K. K. Adjaï, Lucas H. Koudahoun, Biswanath Rath, Pravanjan Mallick, Rati Ranjan Sahoo, Fernando Y. J. Kpomahou , Marc D. Monsia, Exact quantum mechanics of quadratic Liénard type oscillator equations with bound states energy spectrum, Math.Phys.,viXra.org/1702.0242v1.pdf (2017).

[13] J. Akande, D. K. K. Adjaï, L. H. Koudahoun, Y. J. F. Kpomahou, M. D. Monsia, Prolate spheroidal wave function as exact solution of the Schrödinger equation, Math.Phys.,viXra.org/1701.0166v1.pdf (2017).