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ANALYTICAL SOLUTION OF THE SCHRÖDINGER EQUATION WITH THE QUASI-HARMONIC POTENTIAL AND CENTRIFUGAL TYPE TERM VIA LAPLACE TRANSFORM

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Abstract. We consider the Schrödinger equation (*SE*) with the potential: $V_q(r) = \delta r^2 + \frac{A}{r} + \frac{B}{r^2}$ defined by us as the quasi-harmonic potential with $\frac{B}{r^2}$ the centrifugal type term, $\delta, A, B > 0$ and $0 < \mu\delta \ll 1$. Applying Laplace transform method (*LTM*), we obtain a new analytical solution in the V_q- potential problem. Using directly and inverse Laplace transforms, we give the complete forms of the energy eigenvalues and the wave functions. Furthermore, introducing the potentials family $\left\{\lambda V_q\right\}_{\lambda>0}$, we outline a path for deriving the critical value of the angular momentum ℓ_c depending on the scalar minimum value λ_c chosen such that bound states exist. For this family of potentials, we obtain a useful approximation of upper bound ℓ_c^+ to ℓ_c .

Key words: Schrödinger equation, Laplace transform, analytical eigenfunctions, quasi-harmonic potential with centrifugal term

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1. INTRODUCTION

In quantum mechanics, several authors have solved the Schrödinger equation [1] for potentials, such as pseudo harmonic, Mie type, Coulomb-like potentials [2–4], and Halton, Manning Rosen [5,6], Pöshel-Teller [7] and Wood-Saxon potential at the nuclear scale [8, 9].

There are several methods for solving the *SE* such as Laplace transform [10], Nikiforov-Uvarov [6], homotopy perturbation [11], series solution [12], Fourier transform [13], asymptotic iteration methods [14], super-symmetric approach [15], variational method [16] and others.

In this paper, we note that the Laplace transform leads to the analytical and exact forms of eigenfunctions for the potential:

$$V_q(r) = \delta r^2 + \frac{A}{r} + \frac{B}{r^2}, \tag{1}$$

which is a special quasi-harmonic type potential containing a centrifugal type term.

The V_q potential at the nuclear scale implies a short range behaviour of the potential. For this reason, there is a finite number of bound states beyond which the ℓ -state is unbounded [17]. It is important to obtain the critical value of angular momentum ℓ_c, defined indirectly by $\lambda > 0$, a scalar chosen to ensure $V_{eff} < 0$ (see to Sect. 3.2), which gives rise to bound states for the short-range potential. Therefore, the second aim of this paper is to obtain an approximation for ℓ_c. More exactly, in the case of V_q potential, we find an upper bound ℓ_c^+ to ℓ_c .

The present paper gives an analytical solution to the V_q- potential problem by *LTM* to solve SE. In Section 2, we find the proper Laplace transform to solve *SE*. In Section 3, we give two categories of results: in subsection 3.1, the energy and eigenfunctions, and in subsection 3.2, the assessment of ℓ_c^+; we also introduce a family of V_q potentials, determined by some values of scalar λ to ensure the bound states.

Conclusions close our paper.

2. THE PROPER LAPLACE TRANSFORM FOR BOUND STATES SPECTRUM

In the natural units $c = \hbar = 1$, assuming spherical symmetry of the potential, the time-independent Schrödinger equation in the spherical coordinates (r, θ, φ) is given by [6, 18]:

$$\left[-\frac{1}{2\mu}\nabla^2 + V(r)\right]\Psi_{n\ell m}(r, \theta, \varphi) = E_{n\ell}\Psi_{n\ell m}(r, \theta, \varphi), \tag{2}$$

where $E_{n\ell}$ and $V(r)$ denote the energy eigenvalues, the potential and μ the reduced mass, respectively, for a certain physical system.

The $\Psi_{n\ell m}(r, \theta, \varphi)$ denotes the n-th state of eigenfunctions. We choose the bound state eigenfunctions $\Psi_{n\ell m}(r, \theta, \varphi)$ such that wave functions are vanishing for $r \longrightarrow 0$, $r \longrightarrow \infty$. We look for separable solutions form of *SE*:

$$\Psi_{n\ell m}(r, \theta, \varphi) = \Re_{n\ell}(r)Y_\ell^m(\theta, \varphi), \tag{3}$$

where $\Re_{n\ell}(r)$ are the radial functions and $Y_\ell^m(\theta, \varphi)$ the angular functions, respectively.

Equation (2) provides two separated equations: one is known as the spherical harmonics equation and the other is known as the radial equation, which generally takes the following form in a *D*- dimensional space with the hyper-sphere $\Sigma_D = \Sigma_D(r, \varphi, \theta_1, .., \theta_{D-2})$:

$$\Re''(r) + \frac{2}{r}\Re'(r) + \left[-\frac{\ell(\ell + D - 2)}{r^2} + 2\mu(E_{n\ell} - V(r))\right]\Re(r) = 0, \tag{4}$$

where $\ell(\ell + D - 2)$ is the separation constant with $D > 1$ and $\ell = 0, 1, 2, 3, ..., n - 1$.

In this paper, because we consider the stationary case of *SE* with the potential V_q, we work in three spatial dimensions $D = 3$. So, eq. (4) becomes:

$$\Re''(r) + \frac{2}{r}\Re'(r) + \left[-\frac{\ell(\ell + 1)}{r^2} + 2\mu\left(E_{n\ell} - \delta r^2 - \frac{A}{r} - \frac{B}{r^2}\right)\right]\Re(r) = 0. \tag{5}$$

In the eq. (5), for $r \to \infty$, we consider the following asymptotic form: [19]

$$\begin{aligned} &\Re''(r) - 4d^2r^2\Re(r) = 0, \\ &d = \sqrt{\frac{\mu\delta}{2}},\ \delta > 0, \end{aligned} \tag{6}$$

and consequently, we propose to find the solution in the following form:

$$\Re(r) = r^k e^{-dr^2} f(r),\ k > 0. \tag{7}$$

Further, we solve the following *SE* form with *k*-value and $f(r)$ function as unknowns:

$$r^2 f''(r) + r(\eta_k + 2r - 2dr^2)f'(r) + \left[Q_{n\ell} - 2\mu Ar + \in_k r^2 + dkr^3 - 2\mu\delta r^4 + 4d^2r^4\right] f(r) = 0, \tag{8}$$

where the prime over $f(r)$ denotes the derivative with respect to r; also, we introduce the following notations:

$$Q_{n\ell} = k(k+3) - \ell(\ell+1) - 2\mu B,$$
$$\in_k = 2\mu E_{n\ell} - 4dk - 6d, \eta_k = 2k. \tag{9}$$

Starting from this point, we impose several parametric restrictions.

Firstly, we aim to obtain:

$$Q_{n\ell} = 0. \tag{10}$$

For that, we consider the following correlation $\mu B = \ell$, which is possible physical speaking, because both $\mu > 0$ (as a mass) and $B > 0$, with μB taking an integer value like ℓ; also, it is useful from a mathematical point of view, because it simplifies the $Q_{n\ell}$ expression; after that, the eq.(10) implies two values for k:

$$k_+ = \ell,$$
$$k_- = -(\ell+3). \tag{11}$$

The acceptable physical value remains $k_+ = \ell$.

For $r > 0$, the equation (8) becomes:

$$rf"(r) + (\eta_\ell + 2r - 2dr^2)f'(r) + [4d^2r^3 - 2\mu\delta r^3 + d\ell r^2 + \in_\ell r - 2\mu A]f(r) = 0. \tag{12}$$

In eq. (12), in order to reduce the complexity of its polynomis coefficients, we simultaneously consider two restrictions: a) a parametric restriction $\mu\delta \ll 1$ and b) a scale restriction $r \ll 1$, making d and r small enough (e.g. $1 \sim a_0$ - the first Bohr radius at the atomic scale, or $1 \sim$ the nucleus radius at the nuclear scale, depending on the considered physical conditions).

Hence, the following differential equation in the unknown function $f(r)$ remains unsolved:

$$rf"(r) + (\eta_\ell + 2r - 2dr^2)f'(r) + (d\ell r^2 + \in_\ell r - 2\mu A)f(r) = 0. \tag{13}$$

So, in eq. (8), before working in the transform space by applying Laplace transform, we reduce the differential equation from third to the second order by using $Q_{n\ell} = 0$ with the above restrictions.

Therefore, we apply the Laplace transform $\Phi(s) = L\{f(r)\}(s)$, with $Re(s) > 0$ [10], and eq. (13) becomes:

$$d(2s-\ell)\Phi"(s) + (s^2 + 2s + \tilde{\in})\Phi'(s) + (\gamma s + \alpha)\Phi(s) = 0, \tag{14}$$

where :

$$\gamma = 2 - 2\ell,$$
$$\alpha = 2\mu A + 2, \tag{15}$$
$$\tilde{\in} = \in + 4d.$$

We observe that $s_0 = \frac{\ell}{2}$ is a singular point, suggesting the following form of the Laplace transform:

$$\Phi(s) = \frac{C_{n\ell}}{\left(s - \frac{\ell}{2}\right)^{n+1}}. \tag{16}$$

The inverse Laplace transform $f(r) = L^{-1}\{\Phi(s)\}(r)$ leads to the following expression:

$$f(r) = \frac{C_{n\ell}}{n!} r^n e^{\frac{\ell r}{2}}. \tag{17}$$

3. RESULTS

3.1. The energy eigenvalues and wave functions

Using the form (16) in eq.(14), we obtain the system of conditions:

$$\begin{aligned} &\gamma = n+1, \\ &\alpha = 2(n+1) + d\ell\gamma, \\ &\tilde{N} - \ell\alpha = 2(n+1)\tilde{\in}, \end{aligned} \tag{18}$$

where $\tilde{N} = 4d(n+1)(n+2)$.

Solving the third equation from (18), we obtain the energy eigenvalues:

$$E_{n\ell} = \frac{d}{\mu}\left[n + 2\ell + 3 - \frac{\alpha\ell}{4d(n+1)}\right] = \sqrt{\frac{\delta}{2\mu}}\left[n + 2\ell + 3 - \ell\frac{(4+\ell)}{8d}\right]. \tag{19}$$

We remark that in the case of harmonic oscillator $V(r) = \frac{1}{2}\mu\omega^2 r^2$, the energy expression leads to the eigenvalue $E_{00} = \frac{3}{2}\omega$ which is the well known ground state energy.

A complete solution of *SE* implies the computation of normalization constant $C_{n\ell}$ from the condition:

$$\int_0^\infty [\Re(r)]^2 r^2 \mathrm{d}r = 1. \tag{20}$$

In order to calculate elegantly the normalization constant, we propose to use a special and remarkable integral; but for that, it is necessary to take in account the approximation $r - \frac{\ell}{4d} \approx r$ which occurs in the exponential part of the integral by the above condition (20).

The remarkable integral is:

$$\int_0^\infty x^p e^{-ax^q} \mathrm{d}x = \frac{1}{q}\frac{\Gamma\left(\frac{p+1}{q}\right)}{a^{\frac{p+1}{q}}}, p, q, a > 0, \tag{21}$$

where $\Gamma(\cdot)$ is the gamma function.

Thus, we obtain the normalization constant:

$$C_{n\ell} = n!\left\{\frac{2(2d)^{\ell+n+\frac{3}{2}}}{\Gamma(\ell+n+\frac{3}{2})}e^{-\frac{\ell^2}{8d}}\right\}^{\frac{1}{2}}. \tag{22}$$

Finally, using the relations (11), (17), (22) in the radial function (7), we find the complete analytical form of the eigenfunctions:

$$\Re_{n\ell}(r) = r^{n+\ell}\frac{C_{n\ell}}{n!}e^{-dr^2 + \frac{\ell}{2}r}. \tag{23}$$

Further, we compute the r_{rms} radius:

$$r_{rms} = \sqrt{< r^2 >}, \tag{24}$$

where

$$< r^2 > = \int_0^\infty r^2 [\Re(r)]^2 r^2 \mathrm{d}r, \tag{25}$$

and obtain :

$$r_{rms} = \sqrt{\frac{\ell + n + \frac{3}{2}}{2d}} = \sqrt{\frac{\ell + n + \frac{3}{2}}{\sqrt{2\mu\delta}}}, \delta \neq 0. \tag{26}$$

3.2. The upper bound approximation of angular momentum

The methodology for the *SE* via *LTM* is also useful in the short range potential case [20]. At the nuclear scale, we introduce the family of potentials $\left\{\lambda V_q\right\}_{\lambda>0}$ with $\delta, A, B > 0$.

In eq. (4), considering the transformation $\Re(r) = \frac{U(r))}{r}$ and unit $2\mu = 1$, we obtain a *SE* form [21]:

$$\left[-\frac{\mathrm{d}^2}{\mathrm{d}r^2} - \lambda V_q(r) + \frac{\ell(\ell+1)}{r^2}\right] U_{n\ell}(r) = \tilde{E}_{n\ell} U_{n\ell}(r). \tag{27}$$

Combining $\lambda > 0$ and V_q at nuclear scale, the $-\lambda V_q$ term is an attractive potential with λ as a measure of the V_q- family's strength.

We consider the effective potential: [17]

$$V_{eff}(r) = -\lambda V_q(r) + \frac{\ell(\ell+1)}{r^2}. \tag{28}$$

A possible bound state of positive energy corresponds to the proposed λV_q potentials including quasi-bound states, where λ is relevant in the binding of ℓ-states.

An infinitely small but negative part of V_{eff} would permit a bound state.

So, the critical strength value $\lambda_c(\ell)$ is needed to bind a ℓ-state, thus occurring indirectly the critical value for ℓ.

Regarding the above, we make several computations:

• We define r_0- the radius such that $V'_{eff}(r_0) = 0$ and we obtain:

$$r_0 = \sqrt[3]{\frac{A}{2\delta}} > 0, \delta \neq 0. \tag{29}$$

• The critical strength value of λ_c occurs as the minimum value necessary to get a bound state from the condition:

$$\lambda_c \geq \ell(\ell+1)\frac{2}{-r_0^3 V'_q(r_0)}, V'_q(r_0) < 0. \tag{30}$$

• We obtain the upper bound ℓ_c^+ as:

$$\ell_c^+ \approx \sqrt{\frac{-r_0^3 V'_q(r_0)}{2}}\sqrt{\lambda_c} = \sqrt{\frac{1}{2}(2B + (4^{-\frac{2}{3}} - 1)Ar_0)}\sqrt{\lambda_c}, \tag{31}$$

this upper bound approximation being appropriate for practical work.

4. CONCLUSIONS

In the two body problem, associated with a V_q quasi-harmonic potential having $0 < \mu\delta \ll 1$, and our defined parametric constraints, we solved 3-dimensional Schrödinger equation via Laplace transform method. We obtained a complete analytical solution, namely the energy eigenvalues and eigenfunctions.

In the computation of k positive value, we considered the correlation $\mu B = \ell$ and obtained $k_+ = \ell$. Therefore, the k value, involved in parametric restriction $Q_{n\ell} = 0$, may be a subject of interest in quantum computing.

Using the wave function, we computed the root-mean-square (*rms*) charge radius, which is measured for most stable nuclei by electron scattering form factors and/or from the x-ray transition energies of muonic atoms. It will be interesting to compare our formula of r_{rms} with experimentally-derived values.

Considering at nuclear scale a potentials family $\left\{\lambda V_q\right\}_{\lambda>0}$, such that $-\lambda V_q$ term becomes an attractive potential, we also obtained the analytical solution, which is only valid for well bound states, but not for angular momentum close to or above the critical ℓ_c. We estimated the $\lambda_c(\ell)$, representing the necessary strength of the λV_q potentials, required such that V_{eff} contains a negative part. Therefore, we calculated an upper bound ℓ_c^+ which is a good approximation of ℓ_c and find ℓ_c^+ is proportional to $\sqrt{\lambda_c}$, namely with the strength of the potentials family $\left\{\lambda V_q\right\}_{\lambda>0}$.

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