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Solutions of the time-independent Schrödinger equation by uniformization on the unit circle

Abstract. The idea presented here of a general quantization rule for bound states is mainly based on the Riccati equation which is a result of the transformed, time-independent, one-dimensional Schrödinger equation. The condition imposed on the logarithmic derivative of the ground state function W_0 allows to present the Riccati equation as the unit circle equation with winding number equal to one which, by appropriately chosen transformations, can be converted into the unit circle equation with multiple winding number. As a consequence, a completely new quantization condition, which gives exact results for any quantum number, is obtained.

1. Introduction

The most basic problem in quantum mechanics is to solve stationary, one-dimensional Schrödinger equation with bound state spectrum

$$-\frac{\hbar^2}{2m}\psi_n''(x) + V(x)\psi_n(x) = E_n\psi_n(x), \tag{1}$$

where $V(x)$ is real-valued function, for the energy eigenvalues E_n and the associated energy eigenfunctions $\psi_n(x)$. Some general considerations regarding integrability of equation (1) are presented in paper [3]. There are a few important potentials for which the stationary Schroedinger equation can be solved analytically, like the harmonic oscillator, the Coulomb potential and the Morse potential [2]. However, in most cases of the practical interest approximate methods must be employed. Among them, the semiclassical WKB method and the Bohr-Sommerfeld quantization rule are used [5].

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2. The Schrödinger and the Ricatti equations

Basing on the ideas presented in the articles [6, 7] we are able to transform the Schrödinger equation (1), where $\hbar = 2m = 1$, into the Ricatti equation

$$W_n'(x) - W_n^2(x) = E_n - V(x) \tag{2}$$

by use of the logarithmic derivative

$$W_n(x) = -\frac{\psi_n'(x)}{\psi_n(x)}. \tag{3}$$

For the ground state we assume that the logarithmic derivative $W_0(x)$ has a zero on interval I, where we look for the solutions of (2), and

$$W_0'(x) > 0 \qquad \text{for all } x \in I \subset \mathbb{R}. \tag{4}$$

The last assumption, which is concerned with normalizability of the ground wavefunction ψ_0, results in reversibility of the function $W_0(x)$ on interval I. This condition has its equivalents in article [3].

Condition (4) leads us to the equations

$$W_0'(x) = W_0^2 + f(W_0), \tag{5}$$

where

$$E_0 - V(x) = f(W_0).$$

An arbitrary function $f(W_0)$ has to satisfy only condition (4). Thus, we have an opportunity to choose an appropriate potential by means of the function $f(W_0)$, as it has been done in the paper [7] and, where (5) takes the form

$$W_0' = AW_0^2 + BW_0 + C. \tag{6}$$

The solution of this equation is

$$W_0(x) = -\frac{B}{2A} + \frac{\sqrt{-B^2+4AC}}{2A}\tan\Big(\frac{1}{2}\sqrt{-B^2+4AC}(x-x_0)\Big), \tag{7}$$

where the interval I, which satisfy condition (4), is given by

$$x_0 - \frac{\pi}{\sqrt{-B^2+4AC}} \le x \le x_0 + \frac{\pi}{\sqrt{-B^2+4AC}}.$$

It is worth to notice that different values of A, B, C parameters lead us to different sets of the orthogonal polynomials, as it was shown in [7].

3. The Ricatti [8] equation as the unit circle equation

Dividing (6) by W_0' and introducing

$$q_0^2 = \frac{W_0^2}{AW_0^2 + BW_0 + C} \quad \text{and} \quad p_0^2 = 1 - q_0^2 = \frac{(A-1)W_0^2 + BW_0 + C}{AW_0^2 + BW_0 + C}$$

we obtain the unit circle equation

$$q_0^2 + p_0^2 = 1 \qquad \text{for } t_{0,0} \leq W_0 \leq t_{0,1}. \tag{8}$$

Classical turning points

$$t_{0,0} = \frac{B - \sqrt{B^2 + 4(1-A)C}}{2(1-A)}$$

and

$$t_{0,1} = \frac{B + \sqrt{B^2 + 4(1-A)C}}{2(1-A)},$$

are the solution of the equation $q_0^2 = 1$. Parameters A, B and C should have properly chosen values ($t_{0,0}$ and $t_{0,1}$ must exist and have opposite signs) to make calculations reasonable.
Typical graph of the function q_0^2 in the variable W_0 is illustrated in Figure 1.

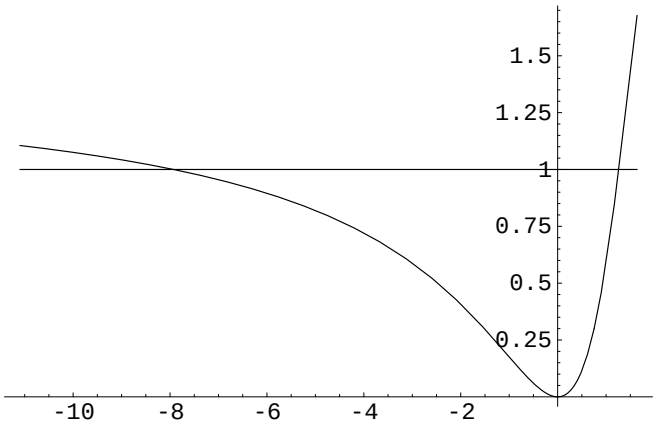


Fig. 1: The graph of the function q_0^2 for $A = 0.7$, $B = -2$, $C = 3$, where W_0 is on the horizontal axis and q_0^2 on the vertical one. Classical turning points are determined by the condition $q_0^2(t_{0,0}) = q_0^2(t_{0,1}) = 1$.

Thus, the area of the circle (equation (8)) can be calculated by the integral

$$\oint p_0 dq_0 = 2 \int_{t_{0,0}}^{t_{0,1}} p_0 dq_0 = \pi.$$

The bound state function W_1 can be easily obtained in terms of the ground state function W_0, see [7]. Substituting

$$W_1 = W_0 - \frac{a_{11}}{b_{11} W_0 - c_{11}} \tag{9}$$

and taking (6) into account we obtain

$$a_{11} = (A+2)C - \frac{B^2(A+2)^2}{4(A+1)^2},$$

$$b_{11} = A + 2,$$
$$c_{11} = -\frac{B(A+2)}{2(A+1)}.$$

Hence, the Riccati equation for the first excited state has the following form

$$W_1' = W_1^2 + (A-1)W_0^2 + BW_0 + C + a_{11}$$

or, dividing the last equation by W_1' we have

$$q_1^2 + p_1^2 = 1, \tag{10}$$

where

$$q_1^2 = \frac{W_1^2}{W_1'} \quad \text{and} \quad p_1^2 = 1 - q_1^2.$$

In analogy to eq.(8), classical (external) turning points

$$t_{1,0} = \frac{(A+1)B - \sqrt{A+3}\sqrt{(A^2+A-1)B^2 + 4(1-A)(1+A)^2C}}{2(1-A^2)}$$

and

$$t_{1,1} = \frac{(A+1)B + \sqrt{A+3}\sqrt{(A^2+A-1)B^2 + 4(1-A)(1+A)^2C}}{2(1-A^2)}$$

are obtained from the equation $q_1^2 = 1$. In addition, the function q_1^2 has a removable singularity (internal turning point) at

$$W_0 = \frac{c_{11}}{b_{11}} = -\frac{B}{2(A+1)},$$

where

$$q_1^2\Big(-\frac{B}{2(A+1)}\Big) = 1,$$

although W_1 is singular at this point. The results are illustrated in Figure 2.

It shows that, in this case, the multiple of winding number is 2 and thus, the area of the circle (10) can be calculated by the integral

$$\oint p_1 dq_1 = 2\int_{t_{1,0}}^{t_{1,1}} p_1 dq_1 = 2\pi,$$

where the value 2π arises from the double rotation of this circle around the origin. Repeating the procedure outlined above [7] for the $n-th$ excited state function

$$W_n = W_0 - \cfrac{a_{n1}}{b_{n1}W_0 - \cfrac{c_{n1}}{b_{n2}W_0 - \cdots}} \tag{11}$$

we get

$$q_n^2 + p_n^2 = 1 \qquad \text{for } t_{n,0} \le W_0 \le t_{n,1}, \tag{12}$$

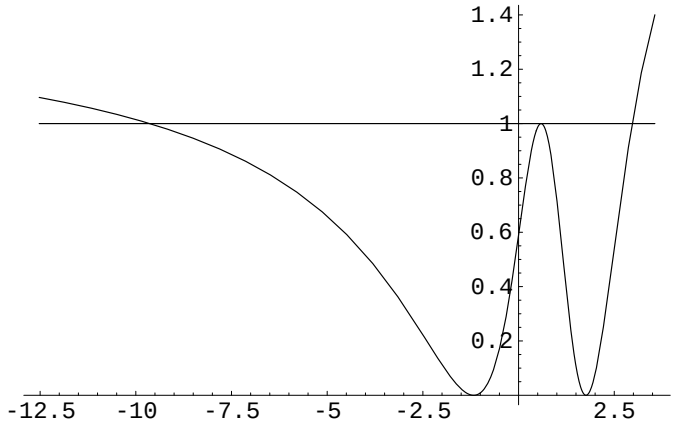


Fig. 2: The graph of the function q_1^2 for $A = 0.7$, $B = -2$, $C = 3$, where W_0 is on the horizontal axis and q_1^2 on the vertical one. Classical (external and internal) turning points can be seen.

where

$$q_n^2 = \frac{W_n^2}{W_n'}.$$

Thus, we construct the circle (12) with winding number equal to $n+1$ (see [4]), where external turning points $t_{n,0}$ and $t_{n,1}$ are solutions of the equation $q_n^2 = 1$. Finally, the area of this circle provides the strict quntization condition (see [1]) of the form

$$\oint p_n dq_n = 2\int_{t_{n,0}}^{t_{n,1}} p_n dq_n = (n+1)\pi. \tag{13}$$

In addition, the function q_n^2 has n removable singular points (internal turning points) which are strictly connected with the multiple of the winding number equal to $n+1$. Therefore, they are important and have influence on the final results of the above calculations.

4. Application to the classic potentials

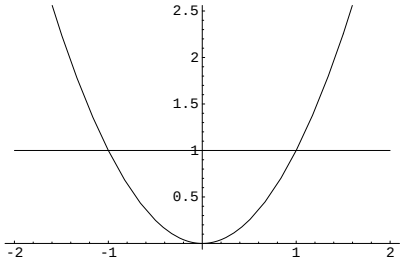
Equation (7) offers a convenient way to link this simple method with well known solutions of the Schrödinger equation.
For instance, choosing $B = 0$, $C = 1$ we get the following results

$$W_0' = AW_0^2 + 1 \quad \text{and} \quad W_1 = W_0 - \frac{1}{W_0},$$

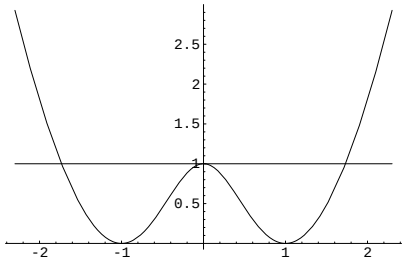
where

$$W_1' = W_1^2 + (A-1)W_0^2 + A + 3.$$

Limits of the functions considered above as $A \to 0$ give solutions of the quantum oscillator in variable W_0. Corresponding functions can be seen in Figure 3.



(a) Graph of the function q_0^2. Classical turning points: $t_{0,0} = -1, t_{0,1} = 1$ as $A \to 0$.



(b) Graph of the function q_1^2. Classical turning points: $t_{1,0} = -\sqrt{3}, t_{1,1} = \sqrt{3}$ as $A \to 0$.

Fig. 3: Graphs of the functions q_0^2 (left) and q_1^2 (right) in variable W_0 (horizontal axis) for the quantum harmonic oscillator.

Another example, where $C = \frac{B^2}{4}$, $B = -1$, leads to well known solution of the Schrödinger equation with the Coulomb potential (without angular momentum). In this case we have

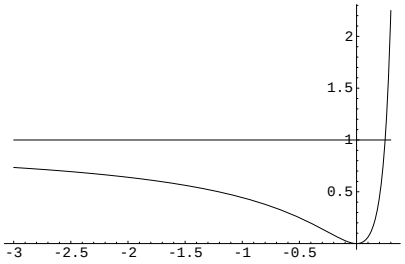
$$W_0' = AW_0^2 - W_0 + \frac{1}{4} \quad \text{and} \quad W_1 = W_0 - \frac{A^2 + A - 1}{2(A+1)} \frac{1}{2(A+1)W_0 - 1},$$

where

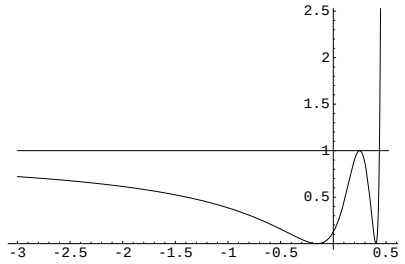
$$W_1' = W_1^2 + (A-1)W_0^2 - W_0 + \frac{A^3 + 4A^2 + 3A - 1}{4(A+1)^2}.$$

As in the previous case, we evaluate limits of the functions q_0^2 and q_1^2 but this time for $A \to 1$. Results of this evaluation can be seen in Figure 4.

As we see the results are valuable and consistent with our earlier considerations.



(a) Graph of the function q_0^2. Classical turning points: $t_{0,0} = -\infty, t_{0,1} = \frac{1}{4}$ as $A \to 1$.



(b) Graph of the function q_1^2. Classical turning points: $t_{1,0} = -\infty, t_{1,1} = \frac{7}{16}$ as $A \to 1$.

Fig. 4: Graphs of the functions q_0^2 (left) and q_1^2 (right) in variable W_0 (horizontal axis) for the quantum Coulomb potential.

5. The general quantization condition in variable x

All previous calculations can be presented in variable x. It is sufficient to express $W_0 = W_0(x)$ (see (7)) and repeat earlier considerations. In particular

$$q_n^2(x) = \frac{W_n^2(x)}{W_n'(x)}, \qquad p_n^2(x) = \frac{E_n - V(x)}{W_n'(x)}, \tag{14}$$

where (11) remains valid. Thus, the quantization condition (13) takes the form

$$\begin{aligned} \oint p_n dq_n &= 2\int_{x_{n,0}}^{x_{n,1}} p_n(x) dq_n(x) \\ &= 2\int_{x_{n,0}}^{x_{n,1}} \sqrt{E_n - V(x)}\Big(1 - \frac{1}{2}\frac{W_n(x)W_n''(x)}{(W_n'(x))^2}\Big)dx \\ &= (n+1)\pi, \end{aligned} \tag{15}$$

where external classical turning points $x_{n,0}, x_{n,1}$ satisfy the following equation $E_n - V(x) = 0$.

By direct calculations we can see, that (15) is fulfilled not only for all analytically solvable potentials but also for those which need numerical calculations to solve the Schrödinger equation.

6. Application to the new analytically solvable potential

In paper [7] we considered a more general form of (6),

$$W_0' = AW_0^2 + \frac{P_{l+1}(W_0)}{Q_l(W_0)} = R_{l+2,l}(W_0),$$

which leads to a new class of the solvable potentials. In this equation $P_{l+1}(W_0)$ is a polynomial in W_0 with degree no greater than $l+1$, $Q_l(W_0)$ is a polynomial in W_0 with degree equal to l. $R_{l+2,l}(W_0)$ is a rational function. Taking

$$W_0' = W_0^2 + \frac{3W_0 - 1}{W_0 - 3} = \frac{(W_0 - 1)^3}{W_0 - 3},$$

as the example, we get

$$W_0(x) = \frac{2\sqrt{x + \frac{1}{4}} - 3}{2\sqrt{x + \frac{1}{4}} - 1},$$

where the potential is

$$V(x) = -\frac{2}{\sqrt{x + \frac{1}{4}}} \qquad \text{for } x \geq 0 \tag{16}$$

and the corresponding eigenvalue $E_0 = -1$. Thus the ground state function, without normalization constant, has the form

$$\psi_0(x) = e^{-x+2\sqrt{x+\frac{1}{4}}}\left(2\sqrt{x + \frac{1}{4}} - 1\right).$$

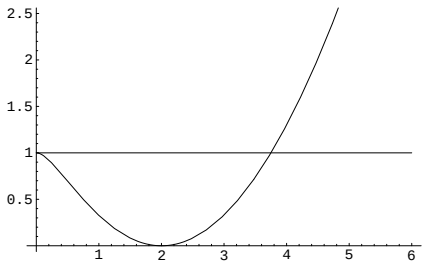
Substituting

$$W_1 = \frac{P_2(W_0)}{Q_1(W_0)},$$

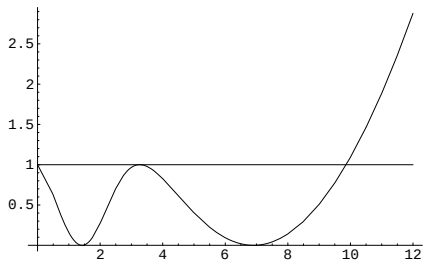
which is more general form then (9), in equation (2) and taking into account (16) we obtain the unnormalized wavefunction of the first excited state

$$\psi_1(x) = e^{-0.79x+2.52\sqrt{x+\frac{1}{4}}}\left(2\sqrt{x+\frac{1}{4}}-1\right)\left(2\sqrt{x+\frac{1}{4}}-3.74\right), \qquad (17)$$

where all decimal numbers are approximated and $E_1 \approx -0.63$.
As a consequence, the corresponding functions $q_0^2(x), q_1^2(x)$ are easily determined by use of (3) and (14). These functions are illustrated in Figure 5.



(a) Graph of the function $q_0^2(x)$. Classical turning points: $x_{0,0} = 0, x_{0,1} = 15/4$.



(b) Graph of the function $q_1^2(x)$. Classical turning points: $x_{1,0} = 0, x_{1,1} \approx 9.86$.

Fig. 5: Graphs of the functions $q_0^2(x)$ (left) and $q_1^2(x)$ (right) for the potential $V(x) = -\frac{2}{\sqrt{x+1/4}}$, where variable x is on the horizontal axis.

The results are in accordance with our considerations and they confirm the correctness of (15) and, what should be emphasized, these equation is fulfilled regardless of the value of quantum number.

7. Conclusions

The form of Riccati equation and features of its solutions play basic role in the method, considered in this paper, which leads to the new form of the quantization condition. As a result we get the formula where the energy eigenvalues and the associated energy eigenfunctions are involved. Equation (15) gives exact results not only for potentials which are explicitly known in the closed form in terms of simple functions, but also for other potentials which are only known formally. It has been confirmed in many numerical calculations. Moreover, this quantization condition can be understood in terms of a few basic ideas which include Pythagorean theorem and the area of the unit circle. These considerations may serve as an aid for further investigations concerning the relationship between geometry and quantization conditions.

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