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Semi-exact Solutions of Konwent Potential*

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Abstract *In this work we study the quantum system with the symmetric Konwent potential and show how to find its exact solutions. We find that the solutions are given by the confluent Heun function. The eigenvalues have to be calculated numerically because series expansion method does not work due to the variable $z \geq 1$. The properties of the wave functions depending on the potential parameter A are illustrated for given potential parameters V_0 and a. The wave functions are shrunk towards the origin with the increasing $|A|$. In particular, the amplitude of wave function of the second excited state moves towards the origin when the positive parameter A decreases. We notice that the energy levels ϵ_i increase with the increasing potential parameter $|A| \geq 1$, but the variation of the energy levels becomes complicated for $|A| \in (0,1)$, which possesses a double well. It is seen that the energy levels ϵ_i increase with $|A|$ for the parameter interval $A \in (-1,0)$, while they decrease with $|A|$ for the parameter interval $A \in (0,1)$.*

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Key words: exact solution, Konwent potential, confluent Heun function, double well potential

1 Introduction

It is well known that the exact solutions of quantum systems play an important role since the early foundation of the quantum mechanics. Generally speaking, two typical examples such as the hydrogen atom and harmonic oscillator have been taken in classical quantum mechanics textbooks.[1−2] Until now, some main methods have been used to solve the quantum soluble systems. First, it is the functional analysis method. That is to say, one solves the second-order differential equation and obtains their solutions[3] given by some well-known special functions. Second, it is called the algebraic method. This method can be realized by studying the Hamiltonian of quantum system and is also related with supersymmetric quantum mechanics (SUSYQM),[4] further closely with the factorization method.[5] Third, it is so-called the exact quantization rule method[6] and proper quantization rule.[7] The latter shows more beauty and symmetry than exact quantization rule. It should be recognized that almost all soluble potentials mentioned above belong to single-well potentials. For example, the classical single-well potential Rosen-Morse potential[8] has been used to treat the vibrations of diatomic molecules such as Na_2 and SiC radical[9−10] and to predict successfully the molar enthalpy values, molar entropy values and Gibbs free energies for molecular NO and P_2 in a wide temperature range.[11−13] Scattering States of l-wave Schrödinger equation with modified Rosen-Morse potential was also studied.[14] This potential can also be used to construct a double-well potential to treat the vibrations of polyatomic molecules such as the ammonia molecule.[8] The double well potentials[15−23] have been studied for a long time due to their complications and they could be used in the quantum theory of molecules to describe the motion of the particle in the presence of two centers of force, the heterostructures, Bose-Einstein condensates, and superconducting circuits, etc.

Thirty years ago, Konwent proposed an interesting potential[24]

$$V(x) = V_0[A\cosh(a\,x) - 1]^2\,, \tag{1}$$

where V_0, A, and a are positive constants. As we will see below, the parameter A can also be taken negative. In Fig. 1, we plot it as the function of the variables x with various A and a, in which we take $V_0 = 5$ and $a = 1$. We see that the potential has a flat bottom in a single well for $A \geq 1$, while it has the form of a double well for $A \in (0,1)$ as shown in Fig. 1(a). The parameter a is related with the width of the potential well, which is inversely proportional to the a as seen in Fig. 1(b). The double-well case is illustrated in Fig. 1(c) for small a and $A = 1$.

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Through the series expansion around the origin, we have

$$V(x) = (A^2V_0 - 2AV_0 + V_0) + x^2(a^2A^2V_0 - a^2AV_0) + x^4\Big(\frac{1}{3}a^4A^2V_0 - \frac{1}{12}a^4AV_0\Big) + O(x^5)\,, \tag{2}$$

which shows that $V(x)$ is symmetric to variable x, i.e., $V(-x) = V(x)$. We find that the minimum value of the potential $V_{\min}(x) = 0$ at minimum values $x = \pm\text{arccosh}(1/A)/a$ for $A \in (0,1)$ and $x = 0$ for $A \geq 1$. Konwent presented the so-called exact solutions by using the "polynomial method" following the Razavy's approach.[17] After studying Konwent's work carefully, we find that the solutions cannot be given exactly due to the complicated three-term recurrence relation. The method presented there[24] is more like the Bethe Ansatz method as summarized in our recent book.[25]

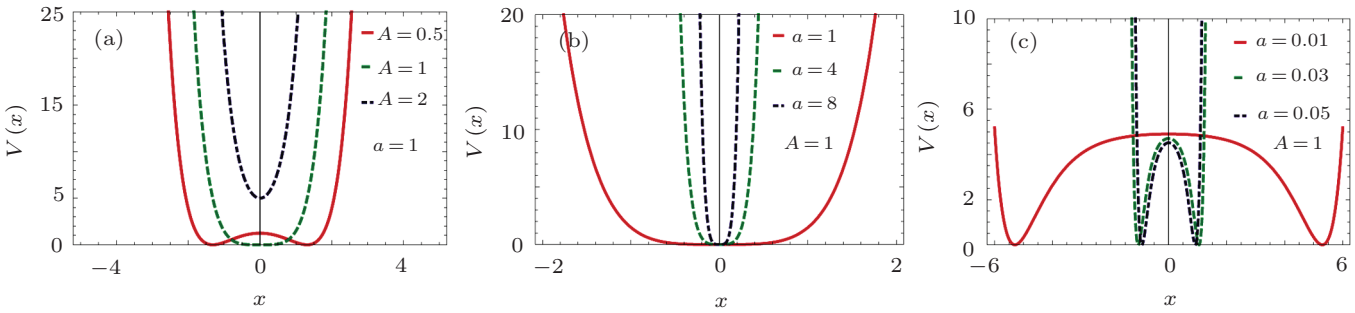

Fig. 1 (Color online) A plot of potential as function of the variables y and A.

That is, the solutions cannot be expressed as one of special functions because of three-term recurrence relations. In order to obtain some so-called exact solutions, the authors have to take some constraints on the coefficients in the recurrence relations as shown in Refs. [17, 24]. As shown in recent study of the hyperbolic type potential well,[26−34] we have found that their solutions can be exactly expressed by the confluent Heun function.[29] In this work we attempt to study the solutions of the Konwent potential. We shall find that the solutions can be written as the confluent Heun function but their energy levels have to be calculated numerically since the energy level term is involved in the parameter η of the confluent Heun function $H_c\,(\alpha,\ \beta,\ \gamma,\ \delta,\ \eta;\ z)$. This constraints us to use the traditional Bathe ansatz method to get the energy levels. It should be pointed out that the Heun function has been studied well, but its main topics are focused in the mathematical area. Only recent connections with the physical problems have been discovered, in particular the quantum systems for those hyperbolic type potential have been studied.[26−34] For this reason, it is not surprising why the authors did not find their solutions related to Heun function.[17,24] The terminology "semi-exact" solutions used in Ref. [27] arise from the fact that the wave functions can be obtained analytically, but the eigenvalues cannot be written out explicitly. The eigenvalues can be calculated by taking the series expansion and then by studying the behaviors of the wave functions at the infinity or by other numerical method.

This paper is organized as follows. In Sec. 2, we present the solutions of the Schrödinger equation with the Konwent potential. It should be recognized that the Konwent potential is single or double well depends on the potential parameter A. In Sec. 3 some fundamental properties of the wave functions are studied. The energy levels for different A are calculated numerically. It is interesting to see that the energy spectra increase with the potential parameter $|A| \geq 1$ and $A \in (-1,0)$, while decrease with $|A|$ for the parameter interval $A \in (0,1)$. Some concluding remarks are given in Sec. 4.

2 Semi-exact Solutions

Let us consider the one-dimensional Schrödinger equation,

$$-\frac{\hbar^2}{2\mu}\frac{\mathrm{d}^2}{\mathrm{d}x^2}\psi(x) + V(x)\psi(x) = E\psi(x)\,. \tag{3}$$

Substituting potential (1) into (3), we have

$$\frac{\mathrm{d}^2}{\mathrm{d}y^2}\psi(y) + [\epsilon - m^2(A\cosh y - 1)^2]\psi(y) = 0\,, \tag{4}$$

where

$$y = ax\,, \quad \epsilon = \frac{2\mu E}{\hbar^2a^2}\,, \quad m^2 = \frac{2\mu V_0}{\hbar^2a^2}\,, \quad \frac{\epsilon}{E} = \frac{m^2}{V_0}\,. \tag{5}$$

How to solve Eq. (4) becomes our main task. Take the wave functions of the form

$$\psi(y) = \mathrm{e}^{mA\cosh(y)}f(y)\,. \tag{6}$$

Substituting this into Eq. (4) allows us to obtain

$$f''(y) + 2Am\sinh(y)f'(y) + [\epsilon - (A^2+1)m^2 + A(2m+1)m\cosh(y)]f(y) = 0\,. \tag{7}$$

Take a new variable $z = \cosh^2(y/2)$. The above equation becomes

$$(z-1)zf''(z) + \Big[z(4Am(z-1)+1) - \frac{1}{2}\Big]f'(z) + f(z)\{Am(2m+1)(2z-1) + \epsilon_1\} = 0\,, \tag{8}$$

which can be re-arranged as

$$f''(z)+\Big[4A\,m+\frac{1}{2}\Big(\frac{1}{z}+\frac{1}{z-1}\Big)\Big]f'(z) + \frac{A\,m(1+2m)(2z-1)+\epsilon_1}{(z-1)z}y(z)=0\,, \quad (9)$$

where $\epsilon_1=\epsilon-(A^2+1)m^2$. When comparing this with the confluent Heun differential equation in the simplest uniform form[29]

$$\frac{\mathrm{d}^2H(z)}{\mathrm{d}z^2}+\Big(\alpha+\frac{1+\beta}{z}+\frac{1+\gamma}{z-1}\Big)\frac{\mathrm{d}H(z)}{\mathrm{d}z} + \Big(\frac{\mu}{z}+\frac{\nu}{z-1}\Big)H(z)=0\,, \quad (10)$$

we find the solution to (9) is given by an acceptable confluent Heun function $H_c\ (\alpha,\beta,\gamma,\delta,\eta;z)$ with

$$\alpha=4Am,\ \ \beta=-\frac{1}{2},\ \ \gamma=-\frac{1}{2},\ \ \mu=A\,m(1+2m)-\epsilon_1\,,$$
$$\nu=A\,m(1+2m)+\epsilon_1, \quad (11)$$

from which we are able to calculate the parameters δ and η involved in $H_c\ (\alpha,\ \beta,\ \gamma,\ \delta,\ \eta;\ z)$ as

$$\delta=\mu+\nu-\frac{1}{2}\alpha(\beta+\gamma+2)=4A\,m^2\,,$$
$$\eta=\frac{1}{2}\alpha(\beta+1)-\mu-\frac{1}{2}(\beta+\gamma+\beta\gamma)=\frac{3}{8}-2A\,m^2+\epsilon_1\,. \quad (12)$$

It is found that the parameter η related to energy levels is involved in the confluent Heun function. The wave functions given by this function seem to be analytical, but the key issue is how we first get the energy levels. Otherwise, the solutions become incomplete. Generally, the confluent Heun function can be expressed as a series expansion around the origin

$$H_C(\alpha,\beta,\gamma,\delta,\eta,z)=\sum_{n=0}^{\infty}v_n(\alpha,\beta,\gamma,\delta,\eta,\xi)z^n,\ \ |z|<1. \quad (13)$$

The coefficients v_n are given by a three-term recurrence relation $A_nv_n-B_nv_{n-1}-C_nv_{n-2}=0$, $v_{-1}=0$, $v_0=1$, where A_n, B_n, and C_n depend on the parameters of the Heun functions.[29] For the present case, however, we have $z\geq 1$. Thus, the series expansion method around the origin becomes invalid. Since this case is very similar to our previous discussions,[26–27] we have to study the eigenvalues numerically as done in Refs. [26–27].

3 Fundamental Properties

In this section we are going to study some basic properties of the wave functions as shown in Figs. 2–5. We first consider the positive A. Since the energy spectrum cannot be given explicitly we have to solve the second order differential equation (3) numerically. Originally, we are going to calculate the energy levels numerically by using the $MAPLE$, which includes the confluent Heun function which is unavailable in $MATHEMATICA$. However, the variable $z\geq 1$ makes the calculation difficult or impossible. We finally used the command "ParametricNDSolveValue" in $MATHEMATICA$ to solve this differential equation (3). We denote the energy levels as $\epsilon_i(i\in[1,7])$ and list them in Table 1.

Table 1 Energy levels of the Schrödinger equation with potential (1).

A	ϵ_1	ϵ_2	ϵ_3	ϵ_4	ϵ_5	ϵ_6	ϵ_7
$A=-4$	135.209	156.03	177.639	200.002	223.089	246.873	271.333
$A=-3$	87.9451	104.217	121.234	138.957	157.357	176.413	196.124
$A=-2$	50.6605	62.3303	74.6793	87.6871	101.386	115.907	131.51
$A=-1$	23.3202	30.2943	46.9152	57.3065	69.5639	83.8798	100.339
$A=-0.8$	19.0409	25.0949	32.0881	40.454	50.5962	62.7581	77.0484
$A=-0.5$	13.375	18.1533	24.2696	32.1829	42.1418	54.2419	68.5156
$A=-0.2$	8.659 31	12.4182	18.042	25.7665	35.6567	47.7300	61.9921
$A=0.2$	4.050 09	7.064 05	12.506	20.1651	30.0263	42.0844	56.3376
$A=0.5$	2.020 63	4.987 46	10.4737	18.1513	28.0230	40.0875	54.3448
$A=0.8$	1.241 69	4.587 76	10.238	17.9999	27.9157	40.0049	54.2771
$A=1.0$	1.367 13	5.185 92	11.0603	18.936	28.9071	41.0245	55.312
$A=2.0$	8.540 19	16.253	25.1475	35.1689	46.4578	59.2694	73.8672
$A=4.0$	53.045	69.6912	87.3988	106.079	125.664	146.102	167.353

We find that the energy levels ϵ_i increase with the increasing $|A|\geq 1$. However, it is seen that the ϵ_i increase with the parameter $|A|$ for the parameter interval $A\in(-1,0)$, while they decrease with $|A|$ for the parameter interval $A\in(0,1)$. As we know, the wave functions are given by $\psi(z)=\mathrm{e}^{m\,A(2z-1)}H_c(\alpha,\beta,\gamma,\delta,\eta;z)$. Generally speaking, the wave functions require $\psi(z)\to 0$ when $z\to\infty$, i.e., $x\to\infty$. Unfortunately, the present study is unlike our previous study,[26–27] in which $z\to 1$ when x goes to infinity. The energy spectra can be calculated by taking the limit $z\to 1$

after the series expansion. In addition, on the contrary to the case discussed by Konwent,[24] in which he supposed the A is taken positive, we also notice that the A can also be taken negative. In this case, the minimum value of single well will be lifted relatively. The wave functions relevant for the positive and negative A are plotted in Figs. 2 and 3.

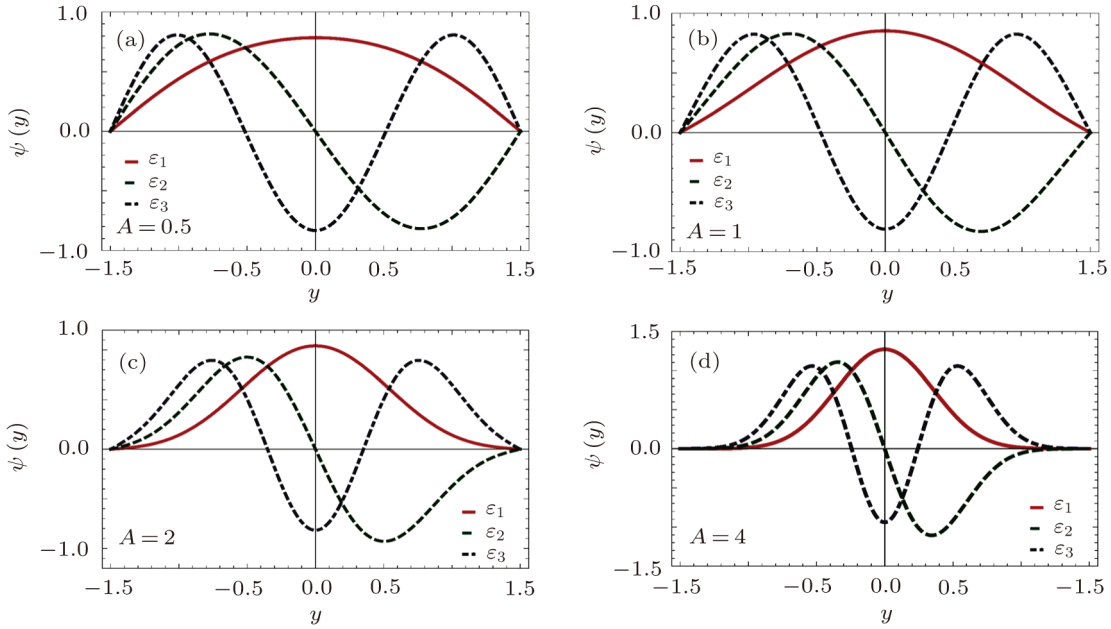

Fig. 2 (Color online) The characteristics of the wave function as a function of the position y. We take $A = 0.5, 1, 2, 4$, and $V_0 = 5$, $a = 1$.

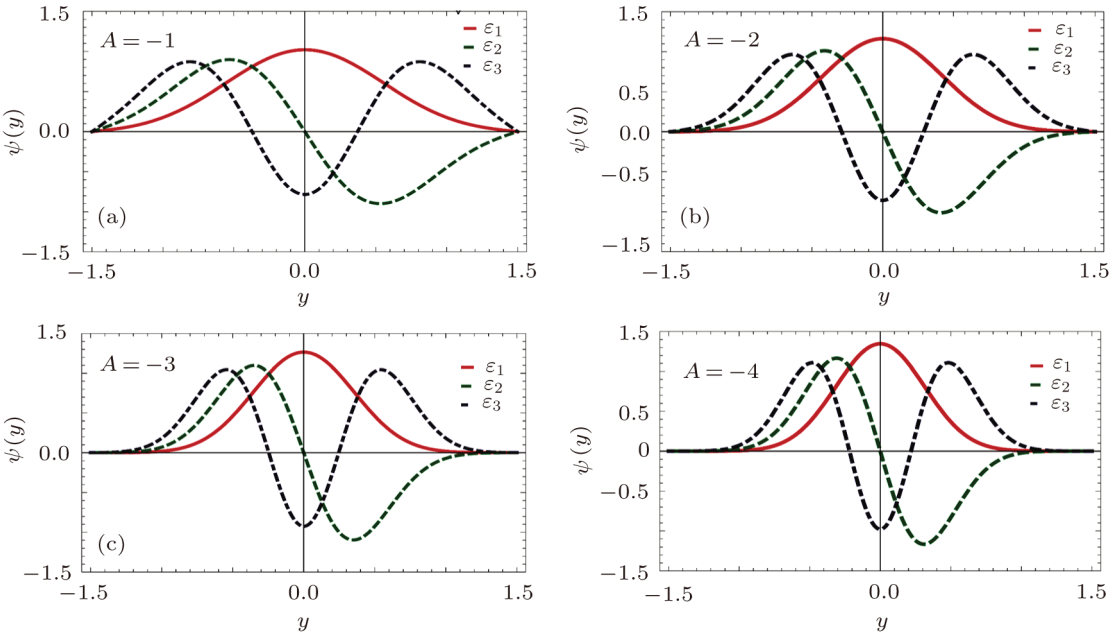

Fig. 3 (Color online) The characteristics of the wave function as a function of the position y. We take $A = -1, -2, -3, -4$, and $V_0 = 5$, $a = 1$.

We find that the wave functions are shrunk towards the origin with the increasing $|A|$. This makes the amplitude of the wave functions be increasing. For the small positive and negative A, however, the change of the wave functions is very sensitive to the parameter A, the wave functions are also shrunk towards the origin with the increasing $|A|$ as shown in Figs. 4 and 5. In particular, the amplitude of wave function of the second excited state around the origin moves towards the origin when the parameter A decreases (see Fig. 4).

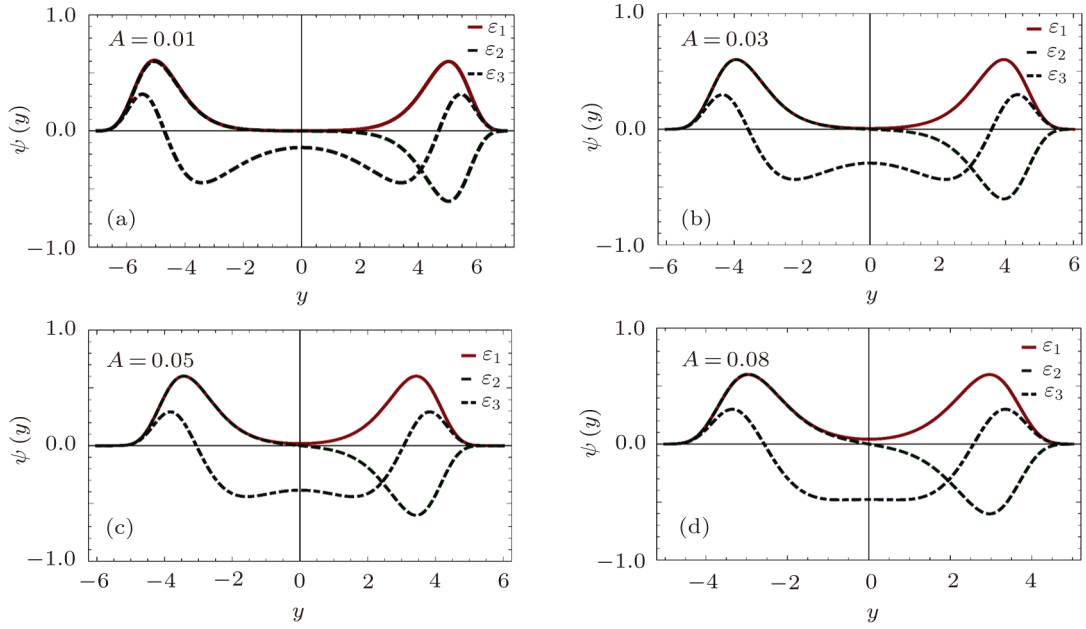

Fig. 4 (Color online) Same as above case but $A = 0.01, 0.03, 0.05, 0.08$, and $V_0 = 5$, $a = 1$.

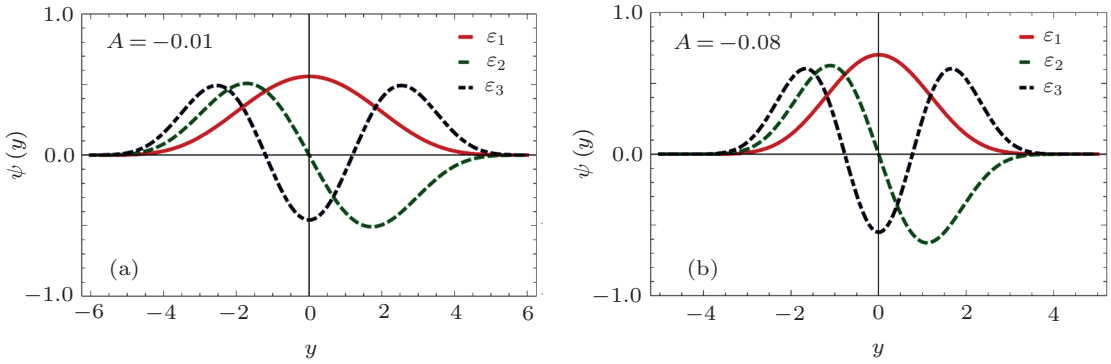

Fig. 5 (Color online) Same as above case but $A = -0.01, -0.08$, and $V_0 = 5$, $a = 1$.

4 Conclusions

In this work we have studied the quantum system with the symmetric Konwent potential and shown how its exact solutions are found by transforming the original differential equation into a confluent type Heun differential equation. It is found that the solutions can be expressed by the confluent Heun function $Hc\,(\alpha, \beta, \gamma, \delta, \eta; z)$, in which the energy levels are involved inside the parameter η. This makes us calculate the eigenvalues numerically in another way. The properties of the wave functions depending on the parameter A are illustrated graphically for given potential parameters V_0 and a. We have also noticed that the energy levels ϵ_i increase with the increasing potential parameter $|A| \geq 1$ corresponding to a single well potential. Finally, we see that the ϵ_i increase with the increasing $|A|$ for the parameter interval $0 > A > -1$, while they decrease with the increasing $|A|$ for the parameter interval $0 < A < 1$.

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