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Numerical Methods for Solving Some Singular Boundary Value Problems of Quantum Mechanics and Quantum Field Theory. I

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This is the first of a series of papers dealing with numerical solving of certain singular boundary value problems of quantum mechanics and quantum field theory by using a common computational approach, which is briefly exposed in the Introduction. In the main body of the paper one simple problem, which arose in the theory of composite hadrons, is investigated in detail. Using this problem as a typical example we formulate a method of analytic continuation of the numerical solution defined on the real axis into the whole complex plane.

1. INTRODUCTION

Many problems of quantum mechanics and quantum field theory may be formulated in a form of the following integral equation

$$u(x) = u_0(x) + \sum_{i=1}^{n} a_i(x)\, V_i(\lambda, x), \tag{1.1a}$$

$$V_i(\lambda, x) = \int_{x_i}^{x} dy\, \mathrm{f}_i(\lambda; y, u(y)), \qquad \mathrm{f}_i \equiv b_i(x)\, \mathrm{g}_i(\lambda, x, u(x)), \tag{1.1b}$$

where $u_0(x)$, $a_i(x)$, $\mathrm{f}_i(\lambda; x, u)$ are known functions, x_i are some real numbers (usually $x_i = 0$ for $i = 1,..., m$ and $x_i = \infty$ for $i = m + 1,..., n$). The problem

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consists in finding a relation between the real or complex parameters λ for which Eq. (1.1) has solutions and in determining the corresponding functions $u(x)$ in some domain D of the complex x-plane. Note that usually $u(x)$ satisfies some normalization condition.

In this series of papers we investigate in detail several physically interesting examples of the Eq. (1.1) and of a system of similar equations. To numerically solve these problems we employ an approach (or a strategy) which is believed to be useful in a more general context. Therefore, it is in order to outline in this Introduction the main features of our approach to the general problem. In the main body of the paper we investigate a highly simplified version of Eq. (1.1) which arose in the theory of composite hadrons developed by one of the authors [1]. The exact formulation of this problem is given below.

First we introduce some other physical problems that can be expressed in the form of Eq. (1.1) and which will be treated in subsequent papers. Note that some equations of a more general type

$$u(x) = \int_0^\infty dy\, K(x, y)\, g(\lambda, y, u(y)) \tag{1.2}$$

can be approximately reduced to the form of Eq. (1.1), provided the kernel $K(x, y)$ permits the uniformly convergent approximations

$$\begin{aligned} K(x, y) &= \sum_i K^{(i)}(x, y), \\ K^{(n)}(x, y) &= \sum_{i=1}^{m} a_i(x)\, b_i(y), \qquad x > y, \\ &= \sum_{i=m+1}^{n} a_i(x)\, b_i(y), \qquad y > x. \end{aligned} \tag{1.3}$$

Keeping here a finite number of terms one arrives at Eq. (1.1). In physical problems the most singular part of the kernel $K(x, y)$ can often be approximated by finite sums (1.3) and if we solve the corresponding equation (1.1) the remaining kernel $K - K^{(n)}$ can be treated as a perturbation. Examples of using such an approach can be found in [2, 3, 5].

The equations of form (1.1) were also met with in quantum field theory, typical examples being the Bethe–Salpeter equation and Dyson–Schwinger equations (see, e.g., [5]). In the quark model introduced in [1] the zero-mass-pion Bethe–Salpeter wavefunction satisfies the equation

$$u(x) = -\epsilon \frac{\pi}{2} f \left\{ x^{1/2} N_1(x) \int_0^x dy\, \frac{y^{1/2} J_1(y)}{y^2 + \mu^2}\, u(y) + x^{1/2} J_1(x) \int_x^\infty dy\, \frac{y^{1/2} N_1(y)}{y^2 + \mu^2}\, u(y) \right\}, \tag{1.4}$$

where $\epsilon = \pm 1$, $J_1(x)$ and $N_1(x)$ are the Bessel functions of the first and second kind, respectively. In the same model the quark self-energy satisfies the nonlinear equation

$$u(x) = -\frac{\pi}{2} f \left\{ x^{1/2} N_1(x) \int_0^x dy \frac{y^{1/2} J_1(y)}{u^2(y) + y^2} u(y) + x^{1/2} J_1(x) \int_x^\infty dy \frac{y^{1/2} N_1(y)}{u^2(y) + y^2} u(y) \right\}. \tag{1.5}$$

A similar but much simpler equation for the electron self-energy was suggested by Johnson *et al.* [4] in their approach to quantum electrodynamics:

$$u(x) = \frac{3}{2\pi} \lambda \left\{ \int_0^x dy \frac{y u(y)}{u^2(y) + y^2} + x^2 \int_x^\infty dy \frac{y^{-1} u(y)}{u^2(y) + y^2} \right\}. \tag{1.6}$$

Very similar equations arise in the now most fashionable nonabelian gauge theories.

The linear problem (1.4) is treated in the present paper, the nonlinear problems (1.5) and (1.6) will be treated in the next paper. Now we outline our approach to solving these problems. The equation (1.1) is obviously equivalent to the following differential boundary value problem

$$V_i'(x) = \mathrm{f}_i \left(\lambda; x, u_0(x) + \sum_{i=1}^{n} a_i(x) V_i(x) \right); \qquad V_i(x_i) = 0. \tag{1.7}$$

If $a_i(x)$ and $\mathrm{f}_i(\lambda; x, u)$ are not very complicated functions Eq. (1.7) may be more convenient for numerical solving. However this is not the case even for Eqs. (1.4)–(1.5). Much greater simplification is possible if the functions $a_i(x)$ are n times differentiable, f_i are $(n-1)$ times differentiable with respect to the variables x and u and the Wronskian of $a_i(x)$, $W(a_1(x), a_2(x), \ldots, a_n(x))$ has no zeros in D.

Then, differentiating Eq. (1.1a) $(n-1)$ times and using the relation $V_i'(x) = \mathrm{f}_i(\lambda; x, u(x))$ for eliminating all derivatives of V_i, we arrive at a system of n linear equations for n functions V_i, which therefore can be expressed in terms of $u(x)$ and $(n-1)$ derivatives of $u(x)$. Substituting this in the nth derivative of Eq. (1.1a) obtained by the same method, we thus obtain a certain nth order differential equation for $u(x)$ with n boundary conditions $V_i(x_i) = 0$ (where V_i are expressed in terms of u and its $(n-1)$ derivatives). It can be proven that this boundary value problem is equivalent to Eq. (1.1) and to Eq. (1.7).

We illustrate this general procedure by explicitly writing the boundary value problem, corresponding to Eq. (1.1) with $n = 2$:

$$\det \begin{Vmatrix} a_1 & a_2 & (u-u_0) \\ a_1' & a_2' & [(u-u_0)' - (a_i f_i)] \\ a_1'' & a_2'' & [(u-u_0)'' - (a_i f_i)' - (a_i' f_i)] \end{Vmatrix} = 0, \tag{1.8a}$$

$$\det \begin{Vmatrix} a_2 & (u-u_0) \\ a_2' & [(u-u_0)' - (a_i f_i)] \end{Vmatrix} \xrightarrow[x \to x_1]{} 0; \qquad \det \begin{Vmatrix} a_1 & (u-u_0) \\ a_1' & [(u-u_0)' - (a_i f_i)] \end{Vmatrix} \xrightarrow[x \to x_2]{} 0. \tag{1.8b}$$

Here $(a_i f_i) = a_1 f_1(\lambda; x, u(x)) + a_2 f_2(\lambda; x, u(x))$, $(a_i' f_i) = a_1' f_1 + a_2' f_2$, and the primes denote the differentiation with respect to x, e.g., $f_1'(\lambda; x, u(x)) = (\partial f_1/\partial x) + (\partial f_1/\partial u)\, u'(x)$. The Eq. (1.8a) essentially simplifies if $a_1(x)$ and $a_2(x)$ satisfy a differential equation $a_i'' - c(x)\, a_i' - d(x)\, a_i = 0$ with some simple functions $c(x)$ and $d(x)$. It then reads

$$(u-u_0)'' - c(x)(u-u_0)' - d(x)(u-u_0) = (a_i f_i)' + (a_i' f_i) - d(x)(a_i f_i). \tag{1.9}$$

Further simplifications occur if $g_1 \equiv g_2 \equiv g(\lambda, x, u(x))$ and $(a_i b_i) \equiv a_1 b_1 + a_2 b_2 \equiv c_1(x)$, $(a_i' b_i) \equiv a_1' b_1 + a_2' b_2 \equiv c_2(x)$, where $c_1(x)$ and $c_2(x)$ are some simple functions of x. Then the right-hand side of Eq. (1.9) is $(c_1'(x) - d(x)\, c_1(x) + c_2(x))g$. Note that we call the functions "simple" if the resulting equation allows convergent power series or asymptotic expansion near its singular points and so the questions of the existence and uniqueness of the boundary value problem can be answered.

Our approach to solving the problems of the type (1.1) may be summarized as follows. Reduce Eq. (1.1) to the differential boundary value problem (1.8), find the singular points of Eq. (1.8a), obtain the asymptotic (or convergent power series) expansions near these points, prove (or disprove) the existence of the solution of the problem, and investigate the question of its uniqueness. Then, by any of available methods find a rough approximation to this solution. A simple procedure giving such an approximation consists in writing some trial functions $V_i(x)$ satisfying boundary conditions $V_i(x_i) = 0$ and depending on some parameters. These functions and the relations between parameters λ are to be determined from the requirement of the minimum error in Eq. (1.7). This procedure usually gives a reasonable first approximation and can be iterated. However, more ingenuous methods of iteration, such as continuous analog of the Newton method [6], usually provide more rapidly convergent approximations and thus they will be systematically used in our computations.

The present paper is organized as follows. In the next section the boundary value problem (2.1)–(2.3), corresponding to Eq. (1.4) is considered and solved by the JWKB method and the asymptotic expansion of $u'(x_0)/u(x_0)$ for large values of x_0 is obtained. In Section 3 the differential boundary value problem is

solved numerically by using the continuous analog of the Newton method. The approach used in this section is quite general provided we have reasonable first approximations for λ and $u(x)$ and for the behavior of $u(x)$ near singular points. JWKB method of Section 2 can be helpful for some other linear problems, when f_i are linear functions of u, however, it is useless in more general context, and the numerical methods should generally be used from the very beginning. In Section 4 the analytic continuation of the numerical solution defined on the real axis is performed. We hope that the analytic continuation method employed in this section is rather general and can be applied to other similar problems.

2. The Asymptotic Methods of Solving the Boundary Value Problem

As has been pointed out, the relativistic bound state problem for the pion composed of quarks may be written in the form of Eq. (1.4) or, equivalently,

$$\frac{d^2u(x)}{dx^2} + \left[1 + \frac{\epsilon f}{x^2 + \mu^2} - \frac{\lambda^2 - (1/4)}{x^2}\right] u(x) = 0, \tag{2.1}$$

$$u(0) = 0, \tag{2.2}$$

$$u(x) \underset{x\to\infty}{\sim} x^{1/2} N_\lambda(x), \tag{2.3}$$

where $\epsilon = \pm 1$, $N_\lambda(x)$ is the Bessel function of the second kind and for the pion problem $\lambda = 1$. The bound state function satisfies the normalization condition

$$\frac{1}{8\pi^2} \int_0^\infty \left[\frac{u(x)}{x^2 + \mu^2}\right]^2 dx = 1. \tag{2.4}$$

In this section we use the standard asymptotic methods to solve the problem (2.1)–(2.4):

I. The JWKB method is used to obtain the approximate eigenvalues $f_n(\mu)$ and eigenfunctions $u_n(x)$.

II. The asymptotic expansion in powers of x^{-1} is used to find the solutions of Eq. (2.1) for large x. On this basis the boundary condition at some finite point $x_{\max} \in [0, \infty)$ is obtained and then used for realization of the numerical method in Section 3.

Without loss of generality, we take $\lambda = 1$ and $\epsilon = -1$. The generalization to an arbitrary λ and (or) $\epsilon = +1$ is straightforward and is discussed at the end of this section. For $\mu = 0$ the exact solution of Eq. (2.1) satisfying the boundary condition (2.2) is easily found to be

$$u(x) = \text{const}\, x^{1/2} J_\nu(x), \tag{2.5}$$

where $\nu = (1 + f)^{1/2}$, and $J_\nu(x)$ is the Bessel function of the first kind. Comparing (2.5) with the asymptotic expansion of $N_1(x)$ for $x \to \infty$ and using the normalization condition (2.4) we obtain eigenvalues and normalized eigenfunctions of the problem (2.1)–(2.4) for $\mu = 0$:

$$f_{n(-)}(0) = N(N + 2), \tag{2.6}$$

$$u_{n(-)}(x) = 4\pi[2(N + 1)(N + 2)]^{1/2}\, x^{1/2} J_{N+1}(x). \tag{2.7}$$

Here $n = 0, 1, 2,\ldots$, $N = 2n + 1 = 1, 3, 5,\ldots$ and by $f_{n(\pm)}(\mu)$ and $u_{n(\pm)}(x)$ we denote the eigenvalues and the eigenfunctions of the eigenvalue problem (2.1)–(2.4) corresponding to $\epsilon = \pm 1$, respectively. The exact solution (2.5) is used later to check the accuracy of different analytic and difference approximations to the boundary value problem (2.1)–(2.4).

Consider now the problem I, i.e., the application of the JWKB method to Eq. (2.1), which resembles the nonrelativistic radial Schrödinger equation with the potential $V(x) = f(x^2 + \mu^2)^{-1}$ and $\lambda = l + \frac{1}{2}$. To perform the correct transition to a JWKB-type equation [7] it is necessary to use the generalized Langer transformation [8] or, equivalently, the simple Kramers change [9]: $\lambda^2 - \frac{1}{4} \to \lambda^2$. In so doing, we make the JWKB solutions have the correct behavior at the singular points of Eq. (2.1). Equation (2.1) on the real axis has one regular singular point $x = 0$, one irregular singular point $x = \infty$ and one turning point x_1. The JWKB solutions are of the standard form [7]:

$$u(x) = (\mathrm{B}/(|\, p(x)|)^{1/2}) \exp\left\{-\int_{x_1}^{x} |\, p(t)|\, dt\right\}, \qquad 0 \leqslant x \leqslant x_1, \tag{2.8}$$

$$u(x) = (2\mathrm{B}/(|\, p(x)|)^{1/2}) \cos\left\{\int_{x_1}^{x} p(t)\, dt - (\pi/4)\right\}, \qquad x_1 < x < \infty, \tag{2.9}$$

where B = const and

$$x_1 = [\{(1/4)(\mu^2 - f - 1)^2 + \mu^2\}^{1/2} - (1/2)(\mu^2 - f - 1)]^{1/2},$$

$$p(x) = [1 - (f/(x^2 + \mu^2)) - (1/x^2)]^{1/2}.$$

The JWKB eigenvalue condition is easily derived from the boundary condition (2.3). Noting that the behavior of the JWKB solution (2.9) for $x \to \infty$ is

$$u(x) \underset{x\to\infty}{\sim} \sin[x - C(f, \mu) + (\pi/4)], \tag{2.10}$$

where

$$C(f, \mu) \equiv \lim_{x\to\infty} \left[x - \int_{x_1}^{x} p(t)\, dt\right]$$

and comparing (2.10) with the known asymptotic behavior of $N_1(x)$ for $x \to \infty$, we obtain the JWKB eigenvalue condition

$$C(f, \mu) = (n + 1)\pi, \qquad n = 0, 1, 2, \ldots . \tag{2.11}$$

For $\mu = 0$ the JWKB eigenvalue condition gives the exact result. Noting that

$$\int_{x_1}^{x} p(t)\, dt \underset{x\to\infty}{\sim} x - (f + 1)(\pi/2),$$

we find $C(f, 0) = (f + 1)(\pi/2)$, and from Eq. (2.11) it follows that $f_{n(-)}^{\mathrm{JWKB}}(0) = N(N + 2)$, $N = 2n + 1$, which coincides with Eq. (2.6).

In the general case $0 \leqslant \mu < \infty$ $C(f, \mu)$ can be expressed in terms of the elliptic integrals:

$$\begin{aligned} C(f, \mu) = &- ((a + \alpha)/(a - c)^{1/2})\, F(\pi/2, q) + (a - c)^{1/2}\, E(\pi/2, q) \\ &+ (\mu^2/ab(a - c)^{1/2})[(b - a)\, \Pi(\pi/2, b/a, q) + aF(\pi/2, q)], \end{aligned} \tag{2.12}$$

where

$$\begin{aligned} a &= \tfrac{1}{2}(\alpha^2 + 4\mu^2)^{1/2} - \tfrac{1}{2}\alpha \equiv x_1 ; \qquad b = -\tfrac{1}{2}(\alpha^2 + 4\mu^2)^{1/2} - \tfrac{1}{2}\alpha; \\ c &= -\mu^2; \qquad \alpha = \mu^2 - f - 1; \qquad q = ((b - c)/(a - c))^{1/2}; \end{aligned}$$

and F, E, and Π are the elliptic integrals of the first, the second, and the third kind, respectively (as defined in [10, 11]).

Using Eqs. (2.11) and (2.12) we can find the asymptotic expansions of the eigenvalues for $\mu \to 0$, ∞. Omitting rather lengthy calculations we quote here only the final result

$$\mu \to 0: f_{n(-)}^{\mathrm{JWKB}}(\mu) = N(N + 2) + \frac{\mu^2}{2} \frac{N(N + 2)}{N(N + 2) + 1} + \cdots, \tag{2.13}$$

$$\mu \to \infty: f_{n(-)}^{\mathrm{JWKB}}(\mu) = 2N\mu - (N^2/2) + \cdots, \tag{2.14}$$

where $N = 2n + 1 = 1, 3, 5, \ldots$.

To check the accuracy of the JWKB method it is helpful to consider Eq. (2.1) with $\lambda = \frac{1}{2}$. In this case Eq. (2.1) can be reduced to the spheroidal differential equation which has been extensively studied [12]. The solutions of the following eigenvalue problem

$$\begin{gathered} (d^2u/dz^2) + [\mu^2 - (f/(z^2 + 1))]\, u(z) = 0, \\ u(z) \underset{z\to 0}{\sim} z; \qquad u(z) \underset{z\to\infty}{\sim} \sin(\mu z) \end{gathered} \tag{2.15}$$

are known:

$$u_n(z) = A_n(z^2 + 1)^{1/2}\, R_{1N}^{(1)}(\mu, z). \tag{2.16}$$

Here $n = 1, 2, 3,...$; $N = 2n$, A_n are the normalization constants and $R_{1N}^{(1)}(\mu, z)$ are the spheroidal functions (see [12] for definitions and useful relations). The eigenvalues $f_n(\mu)$ have the following asymptotic expansions [12]:

$$\mu \to 0: f_n(\mu) = N(N+1) + a_n\mu^2 + \cdots, \tag{2.17}$$

$$\mu \to \infty: f_n(\mu) = 2N\mu - (N^2/2) + \cdots, \tag{2.18}$$

where $a_1 = 4/7$, $a_2 = 40/77$, $a_3 = 28/55,...$. On the other hand, we can solve the eigenvalue problem (2.15) by the JWKB method, which gives the following asymptotic expansions for the eigenvalues:

$$\mu \to 0: f_n^{\text{JWKB}}(\mu) = N(N+1) + \frac{\mu^2}{2}\frac{N(N+1)}{N(N+1)+(1/4)} + \cdots, \tag{2.19}$$

$$\mu \to \infty: f_n^{\text{JWKB}}(\mu) = 2N\mu - (N^2/2) + \cdots, \tag{2.20}$$

where $N = 2n = 2, 4, 6,...$. Comparing (2.17) and (2.18) with (2.19) and (2.20) we conclude that the JWKB method provides quite a reasonable accuracy for the eigenvalue problem (2.15). The leading terms of Eqs. (2.17), (2.18) and of Eqs. (2.19), (2.20) coincide, the difference between the next to the leading terms is rather small. This comparison gives a support to using the JWKB method for treating the problems of real physical importance, such as the pion equation (2.1)–(2.3) with $\lambda = 1$.

The case $\epsilon = +1$ can be treated in the same way. The JWKB eigenvalue condition is of the same form (2.11), (2.12) as before, the only difference being in the definitions of the parameters:

$$a = \tfrac{1}{2}(\alpha^2 + 4\mu^2)^{1/2} - \tfrac{1}{2}\alpha \equiv x_1; \qquad b = -\mu^2;$$

$$c = -\tfrac{1}{2}(\alpha^2 + 4\mu^2)^{1/2} - \tfrac{1}{2}\alpha; \qquad \alpha = \mu^2 + f - 1; \qquad q = ((b-c)/(a-c))^{1/2}.$$

The asymptotic expansions of the eigenvalues of problem (2.1)–(2.3) for $\epsilon = +1$, $\lambda = 1$ and $\mu \to \infty$ are as follows:

$$\mu \to \infty: f_{n(+)}^{\text{JWKB}}(\mu) = 2N\mu + (N^2/2) + \cdots, \tag{2.21}$$

where $N = 2n + 1 = 1, 3, 5,...$. Note that in the case $\epsilon = +1$ all eigenvalue curves $f_n(\mu)$ go out of the same point $f = 1$, i.e., $f_n(0) = 1$, $n = 0, 1, 2,...$. Hence for an arbitrary fixed $f > 1$ the number of eigenvalues $\mu_n(f)$ is infinite, contrary to the case $\epsilon = -1$, for which this number is always finite.

The JWKB eigenvalue condition (2.11), (2.12) is convenient for numerical calculation of the eigenvalues $f_{n(\pm)}^{\text{JWKB}}(\mu)$ for any desired $\mu \in [0, \infty]$. The numerical results are shown in Fig. 1 and in Table I for the "ground state" $f_{O(\pm)}^{\text{JWKB}}(\mu)$, $\lambda = 1$ and in Fig. 2 for $n = 0, 1, 2$; $\lambda = 1$. The asymptotic expansions of eigenvalues

for $\mu \to \infty$ (see Eqs. (2.14) and (2.21)) are very useful as the first approximations since they are close enough to $f_{n(\pm)}^{\mathrm{JWKB}}(\mu)$ for values of μ being not too small. For instance, if $\mu \geqslant 5$ the difference between $2\mu - \frac{1}{2}$ and $f_{O(-)}^{\mathrm{JWKB}}(\mu)$ (see Fig. 1) is less than 3%.

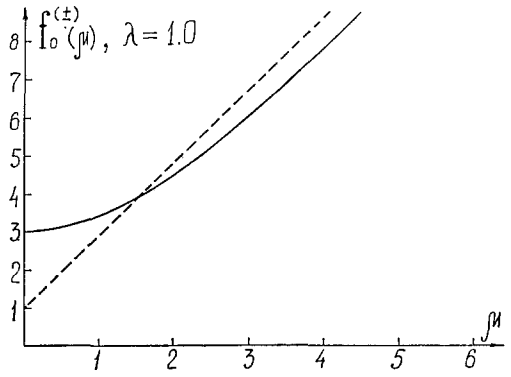

FIG. 1. Eigenvalues $f_{O(\pm)}(\mu)$ for $\lambda = 1$. The solid (dashed) lines correspond to $\epsilon = -1(+1)$.

TABLE I

Eigenvalues $f_{O(\pm)}(\mu)$ Obtained by using the Continuous Analog of the Newton Method and the JWKB Method

μ \ f, λ	$f_{O(-)}(\mu)$ $\lambda = 0.5$	$f_{O(-)}(\mu)$ $\lambda = 1.0$	$f_{O(-)}(\mu)$ $\lambda = 1.5$	$f_{O(-)}(\mu)$ $\lambda = 2.0$	$f_{O(+)}(\mu)$ $\lambda = 1.0$	$f_{O(-)}^{\mathrm{JWKB}}$ $\lambda = 1.0$	$f_{O(+)}^{\mathrm{JWKB}}(\mu)$ $\lambda = 1.0$
3.0	5.59	6.07	6.67	7.36	6.65	6.03	6.69
3.5	6.53	6.93	7.46	8.08	7.63	6.92	7.66
4.0	7.50	7.83	8.29	8.85	8.62	7.84	8.65
4.5	8.48	8.77	9.17	9.67	9.61	8.79	9.64
5.0	9.48	9.72	10.07	10.52	10.60	9.75	10.63
5.5	10.48	10.69	11.00	11.40	11.59	10.72	11.62
6.0	11.49	11.66	11.94	12.30	12.59	11.70	12.61
6.5	12.48	12.65	12.89	13.22	13.58	12.67	13.60
7.0	14.48	13.63	13.85	14.14	14.57	13.66	14.60

In conclusion of this discussion we remind the main advantages of the JWKB method: its simplicity, the wide range of applicability and reasonable accuracy at least for calculating the eigenvalues. Unfortunately, the quantitative estimation of this accuracy is rather a delicate problem [13]. The worst feature of the method is that the JWKB functions have the singularity at the turning points, while the

exact solutions are continuous. To overcome this difficulty and to improve the accuracy of the JWKB approximation the Langer comparison equation method should be used [14]. Here we do not use it as the standard JWKB method is reasonably accurate, being applied to the boundary value problem (2.1)–(2.3) (for comparison with the numerical solutions, see Section 3).

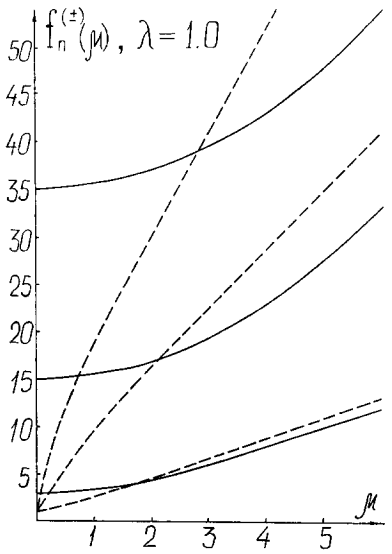

FIG. 2. Eigenvalues $f_{n(\pm)}(\mu)$ ($n = 0, 1, 2$) for $\lambda = 1$. See also the caption to Fig. 1.

Now we turn to the problem II. The formal asymptotic solution of Eq. (2.1) satisfying the boundary condition (2.3) for $x \to \infty$ are

$$u(x) \sim \sin \xi \sum_{n=0} \frac{\alpha_n}{x^{2n}} + \cos \xi \sum_{n=0} \frac{\beta_n}{x^{2n+1}}, \tag{2.22}$$

$$\frac{du(x)}{dx} \sim \cos \xi \sum_{n=0} \frac{\alpha_n'}{x^{2n}} - \sin \xi \sum_{n=0} \frac{\beta_n'}{x^{2n+1}}, \tag{2.23}$$

where $\xi \equiv x - (3\pi/4)$ and

$$\alpha_n' = \alpha_n - (2n-1)\beta_{n-1}; \qquad \beta_{-1} = 0; \qquad n = 0, 1, 2, \ldots,$$
$$\beta_n' = \beta_n + 2n\alpha_n. \tag{2.24}$$

The coefficients α_n and β_n satisfy the recurrence relations:

$$\alpha_0 = 1,$$

$$2(2n+1)\beta_n = -[2n(2n+1) - \tfrac{3}{4}]\alpha_n + f\sum_{i=0}^{n}(-\mu^2)^i \alpha_{n-i}, \tag{2.25}$$

$$2(2n+2)\alpha_{n+1} = [(2n+2)(2n+1) - \tfrac{3}{4}]\beta_n - f\sum_{i=0}^{n}(-\mu^2)^i \beta_{n-i}$$

and can be easily found for arbitrary μ and f with the help of a computer. Using the asymptotic expansions (2.22), (2.23) it is possible to find the boundary condition at some distant point $x = x_{\max}$ or, equivalently, to present the logarithmic derivative of $u(x)$ in the following form:

$$\left.\frac{u'(x)}{u(x)}\right|_{x=x_{\max}} = \frac{\operatorname{ctg}\xi_{\max}\sum_{n=0}^{n_0}(\alpha_n'/x_{\max}^{2n}) - \sum_{n=0}^{n_0}(\beta_n'/x_{\max}^{2n+1})}{\sum_{n=0}^{n_0}(\alpha_n/x_{\max}^{2n}) + \operatorname{ctg}\xi_{\max}\sum_{n=0}^{n_0}(\beta_n/x_{\max}^{2n+1})}. \tag{2.26}$$

The magnitude of n_0 is determined by the asymptotic nature of the series in (2.22), (2.23), and (2.26) [22].

The main results of this section (the JWKB eigenvalues and their asymptotic expansions for $\mu \to 0, \infty$, the boundary condition at a finite point) interesting by themselves will be used in the next section as a basis for application of the numerical methods, which allow one to improve the accuracy of solving the eigenvalue problem (2.1)–(2.4).

3. The Numerical Method of Solving the Eigenvalue Problem

If any two parameters, e.g., λ and μ, are fixed, the boundary value problem (2.1)–(2.4) may be regarded as an eigenvalue problem for the third parameter, e.g., $f = f(\lambda, \mu)$. Varying the parameters λ and μ in some ranges we can determine the function $f = f(\lambda, \mu)$. In such a formulation our problem resembles that considered by Peek [15], the only difference is that for our problem (2.1)–(2.4) the period of asymptotic oscillations does not depend on the eigenvalue f.

The numerical solution of the eigenvalue problem is obtained by using the continuous analog of the Newton method (the program SLIPI for computer is given in [16]). This method has several important advantages over the other methods. It allows one to use effectively all available information on the behavior of the solutions and to calculate simultaneously the eigenvalue f and the corresponding eigenfunction $u(x)$ of the problem as a single unknown variable $w = [f, u(x)]$ of a certain nonlinear functional equation $\varphi(w) = 0$ [6]. It should also be mentioned that the calculation procedure is stable.

Consider now some characteristic features of numerical solving of the problem (2.1)–(2.4).

To perform the calculations we replace the interval $0 \leqslant x < \infty$ by the finite interval $0 \leqslant x \leqslant x_{\max}$, where $x_{\max}$ is sufficiently large. To exclude from the consideration the unknown asymptotic constant in the condition (2.3), we formu-

for the logarithmic derivative (2.26).

The eigenvalue problem (2.1), (2.2), (2.26) on the finite interval is supplemented with the normalization condition (2.4) for the wavefunction, which follows from the physical context of the problem [1] (the Bethe–Salpeter equation). The normalization condition is significant for the realization of the continuous analog of the Newton method [6]. In the calculation procedure used here the normalization condition (2.4) is approximated by the condition

$$\frac{1}{8\pi^2}\int_0^{x_{\max}} [u(x)/(x^2+\mu^2)]^2\,dx = 1. \tag{3.1}$$

The desired accuracy has been achieved, the wavefunction must be renormalized according to the condition:

$$\frac{1}{8\pi^2}\left\{\int_0^{x_{\max}} \left[\frac{u(x)}{x^2+\mu^2}\right]^2 dx + \mathrm{D}^2 \int_{x_{\max}}^{\infty} \left[\frac{u_a(f,x)}{x^2+\mu^2}\right]^2 dx\right\} = 1. \tag{3.2}$$

Here $u_a(f, x)$ is the asymptotic expression for the wave function (2.22) and the constant D is defined as

$$u(x_{\max}) = \mathrm{D}u_a(f, x_{\max}). \tag{3.3}$$

For the differential operator it uses the three point finite-difference approximation with the accuracy of the order $O(h^2)$, h being the step of the difference scheme. According to Ref. [17], it is natural to expect that the accuracy of the result should also be of the second order in h. Substituting the approximate expressions into the finite-difference operator, we can take the maximum of the resulting error δ as a measure of the accuracy of our results for eigenvalues and eigenfunctions.

The determination of the optimum values of the parameters $x_{\max}$ and h as well as the number of the terms in Eq. (2.26), providing the required accuracy, was performed experimentally for a particular case of the problem (2.1)–(2.4), namely, for $\lambda = 1$ and $\mu = 0$, when the corresponding boundary value problem has the exact solution (2.6), (2.7). The control calculations were performed with different values of parameters $x_{\max}$ and h and with different numbers of terms in the boundary condition expansion (2.26). The results are presented in Table II. In Case I we used only the leading term in the expansion (2.22), while in Case II the three first terms were taken into account ($\sim x^{-3}$ included). This table shows that the

accuracy of our calculation depends weakly on the magnitude of $x_{\max}$. For example, the accuracy of the results for $x_{\max} = 31$ and $x_{\max} = 40$, when $h = 0.025$, is of the same order. One may also conclude that the approximation of the exact boundary condition (2.3) by the finite interval boundary condition (2.26) is sufficiently good. Moreover, the observed error of calculation depends on the step of difference scheme as $\sim h^2$. This makes it possible to conclude that the difference network with $x_{\max} = 20$ and $h = 0.0125$ gives the relative error of the results ~ 0.005. During the calculation the accuracy control was performed for some values of λ and μ by the variation of the parameters of the difference scheme. Some results are given in Tables III and IV, which show that the relative error for the eigenvalues f as well as for eigenfunctions $u(x)$ is less than 0.005. The numerical results for the "ground" state $f_{O(\pm)}(\mu)$ for different λ and μ (in the physically most interesting range of variation of parameter μ) are listed in Table I. The normalized eigenfunctions $u_{O(\pm)}(x)$ are given in Fig. 3.

TABLE II

The Dependence of the Eigenvalue $f_{O(-)}(0)$ and the Error δ on $x_{\max}$, h and the Number of Terms in Boundary Condition (2.26)

Parameters of the difference scheme	$x_{\max} = 20$ $h = 0.0125$		$x_{\max} = 31$ $h = 0.025$		$x_{\max} = 40$ $h = 0.025$		$x_{\max} = 80$ $h = 0.050$	
$f_{O(-)}(0)$; δ;	$f_{O(-)}(0)$	δ	$f_{O(-)}(0)$	δ	$f_{O(-)}(0)$	δ	$f_{O(-)}(0)$	δ
Case I	3.00035	$1.7 \cdot 10^{-7}$	3.00164	$2.2 \cdot 10^{-7}$	3.00248	$2.2 \cdot 10^{-7}$	3.02164	$2.0 \cdot 10^{-7}$
Case II	3.00031	$1.8 \cdot 10^{-7}$	3.00158	$2.5 \cdot 10^{-7}$	3.00242	$3.4 \cdot 10^{-7}$	3.02133	$2.1 \cdot 10^{-7}$

TABLE III

Convergence of $f_{O(-)}(\mu)$ with Varying $x_{\max}$ and h

$x_{\max}$	h	$f_{O(-)}(1)$	$f_{O(-)}(4)$
40	0.0250	6.264	9.487
32	0.0200	6.263	9.486
20	0.0125	6.261	9.482

For the numerical realization of the continuous analog of the Newton method it is important to take into account that the convergence of the process of successive iterations depends on the choice of the initial approximations to the eigenvalues and the eigenfunctions. Using the JWKB method, we obtained a sufficiently good

approximation to the eigenvalue f in the whole range of variation of λ and μ. The practice of calculation shows that the asymptotic JWKB expansions of eigenvalues for $\mu \to 0, \infty$ (see, for example, (2.13), (2.14), and (2.21)) can be used as very effective initial approximations for the continuous analog of the Newton method to be realized on computers. The computation time on CDC-6200 for one variant is about 70 sec.

TABLE IV

Convergence of $u_{O(-)}(x)$ with Varying $x_{\max}$ and h

x \ $u_{O(-)}(x)$, $x_{\max}$, h.	$u_{O(-)}(x)$ $x_{\max} = 32$ $h = 0.0200$	$u_{O(-)}(x)$ $x_{\max} = 20$ $h = 0.0125$
2	12.75	12.76
4	87.48	87.56
6	75.72	75.76
8	−78.19	−78.27
10	−35.97	−35.97
12	95.65	95.72
14	−28.25	−28.29
18	82.63	82.70
δ	$2.5 \cdot 10^{-6}$	$3.6 \cdot 10^{-6}$

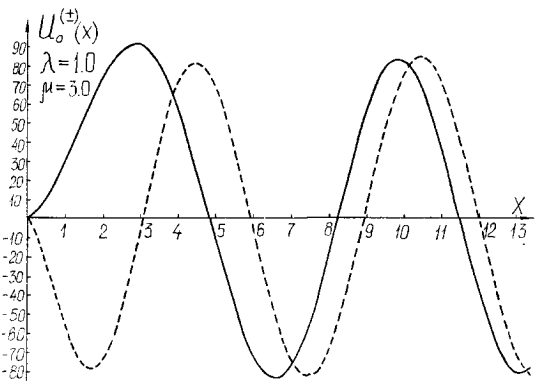

FIG. 3. Eigenfunctions $u_{O(\pm)}(x)$ for $\lambda = 1$. See also the caption to Fig. 1.

The Table I shows that the difference between the numerical value of $f_{O(\pm)}(\mu)$ obtained by the continuous analog of the Newton method and the corresponding JWKB eigenvalues (2.11) and (2.12), calculated on the computer, is about 1 % (such difference is practically indistinguishable in the scale of Figs. 1 and 2).

4. The Analytic Continuation of the Numerical Solutions. The Calculation of the Quark–Pion Coupling Constant

In the preceding sections the asymptotic (JWKB) and the numerical solutions of the boundary value problem (2.1)–(2.4) have been obtained on the interval $0 \leqslant x < \infty$. Now we turn to the problem of analytic continuation of this solutions into the whole complex plane of the independent variable x. This problem is well-posed one in the sense of Hadamard–Tikhonov [18]. In connection with this problem we will consider the following questions:

I. The application of the Frobenius method [19] to the Eq. (2.1) allowing one to construct linearly independent solutions in the form of power series converging within the circle $| x | < \mu$. By identifying the power series solution with the numerical one on the interval $0 \leqslant x \leqslant \mu$, we thus perform an approximate analytic continuation of the numerical solution into the circle $| x | < \mu$.

II. The calculation of the eigenfunctions of the boundary value problem (2.1)–(2.4) at the points $x = \pm i\mu$ by using some asymptotic method of solving the difference equation for the coefficients of the power series expansions.

III. The analytic continuation of solutions defined as power series outside the circle of convergence of these series. The determination of the asymptotic expansions of the eigenfunctions for $| x | > \mu$.

To simplify the treatment of these problems we first make, in the equation (2.1), the following change of variables

$$u(x) = x^{-1/2} v(x); \qquad z = -x^2/\mu^2. \tag{4.1}$$

Here $\mu \neq 0$; for $\mu = 0$ there exists the exact solution (2.6), (2.7). Then the function $v(z)$ satisfies the equation:

$$\frac{d^2 v(z)}{dz^2} - \frac{1}{4z}\left[\mu^2 + \frac{\epsilon f}{1 - z}\right] v(z) = 0. \tag{4.2}$$

The singular points of Eq. (2.1): $x = 0, \pm i\mu, \infty$ then transform to the singular points of Eq. (4.2): $z = 0, 1, \infty$, and our problem is to perform the analytic continuation of the numerical solutions into the domains $| z | \leqslant 1$, $| z | > 1$ and to calculate $v(1)$.

The solution of Eq. (4.2) in the form of a power series, which is absolutely and uniformly convergent in the circle $| z | < 1$ and satisfies the boundary condition (2.2), is as follows [19]:

$$v(z) = N(f, \mu) \sum_{n=1}^{\infty} C(n)\, z^n. \tag{4.3}$$

Here $N(f, \mu)$ is the normalization constant which can be determined by equating $v(z)$ to the numerical solution, obtained in Section 3, and the coefficients $C(n)$ satisfy the recurrence relations:

$$(n+2)(n+1)\,C(n+2) - [(n+1)n + (\mathrm{a} - \mathrm{b})]\,C(n+1) + \mathrm{a}C(n) = 0, \tag{4.4}$$

$$C(1) = 1; \qquad C(0) = 0; \qquad n = 0, 1, 2,..., \tag{4.5}$$

where $\mathrm{a} = \frac{1}{4}\mu^2$ and $\mathrm{b} = -\frac{1}{4}\epsilon f$. Then our problem is essentially the calculation of the normalization constant $N(f, \mu)$ for different values of μ. With this aim we divide the interval $[-1, 0]$ by k points z_i, $0 \leqslant i \leqslant k$ and in each of these points find the ratio:

$$N(\mu, z_i) = v^{\mathrm{num}}(z_i) \Big/ \sum_{n=1}^{\infty} C(n)\, z_i^n. \tag{4.6}$$

The function $v^{\mathrm{num}}(z)$ is related to the numerical solution $u(x)$ obtained in Section 3 by Eq. (4.1) and at each point z_i it is defined up to a certain error depending on the accuracy of the numerical method. The sum of the convergent power series in Eq. (4.6) can obviously be found with any desired accuracy. By calculating $N(\mu, z_i)$ for different i it is easy to determine the mean value of the normalization constant $\bar{N}(\mu)$ and the dispersion $\sigma(\mu)$:

$$\begin{aligned} \bar{N}(\mu) &= (1/k) \sum_{i=1}^{k} N(\mu, z_i), \\ \sigma(\mu) &= \left[(1/k) \sum_{i=1}^{k} \{N(\mu, z_i) - \bar{N}(\mu)\}^2\right]^{1/2}. \end{aligned} \tag{4.7}$$

As a typical example we present here in more detail the results, obtained for the eigenfunction $u_{O(-)}(x)$ (corresponding to the eigenvalue $f_{O(-)}(\mu)$) for $\lambda = 1$ and $\mu = 3$. Dividing the interval $(-1, 0)$ by the points $z_i = -i^2/36$ $(x_i = i/2)$, $i = 1, 2, 3, 4, 5$, and calculating the power series at these points with the relative error $<10^{-6}$ we obtain $\bar{N}(3) = 288.89$ and $\sigma(3) = 3 \cdot 10^{-5}$. For all values of μ, for which the calculations were made, we obtained $\sigma < 10^{-4}$, that is quite satisfactory. In such a way we can a posteriori estimate the accuracy of the numerical method used in Section 3 and obtain the function $N(\mu)$, which is important for physical applications. The normalization constant $N(\mu)$ being known, the power series expansion (4.3) provides the analytic continuation of the numerical solution of the boundary value problem (2.1)–(2.4) defined on the interval $(-1, 0)$ into the domain $|z| < 1$.

Consider now the problem II. Using the recurrence relations (4.4) and (4.5) it is easy to show that the series (4.3) converges absolutely for $|z| = 1$, performing in this way the analytic continuation of the solution on the circle $|z| = 1$. The

function $v(\cdot)$ [illegible] expansion

$$v(1) = N(\mu) \sum_{n=1}^{\infty} C(n). \tag{4.8}$$

Unfortunately, this series converges rather slowly, as $C(n) \sim_{n\to\infty} n^{-2}$. Therefore we employ here another, asymptotic method of calculation of $v(1)$, which rapidly gives quite accurate results.

The second-order linear difference equation (4.4) has two independent solutions $C_1(n)$ and $C_2(n)$ which for $n \to \infty$ can be represented in the form of the asymptotic series:

$$\begin{aligned} C_1(n) &\underset{n\to\infty}{\sim} \frac{1}{n^2}\left[1 + \frac{\alpha_1}{n} + \frac{\alpha_2}{n^2} + \cdots\right], \\ C_2(n) &\underset{n\to\infty}{\sim} \frac{1}{n!\,(n+1)!}\left[1 + \frac{\beta_1}{n} + \frac{\beta_2}{n^2} + \cdots\right]. \end{aligned} \tag{4.9}$$

The general solution of the difference equation (4.4) can be written as the linear combination of these two independent solutions [20]:

$$C(n) = A(f, \mu)\, C_1(n) + B(f, \mu)\, C_2(n), \tag{4.10}$$

and the coefficients A and B can, in principle, be determined from the boundary conditions (4.5).

To formulate the effective method for calculating the sum in (4.8) we rewrite the recurrence relations (4.4) in a more convenient form:

$$(n+2)(n+1)\, C(n+2) - (\mathrm{a} - \mathrm{b})\, C(n) + \mathrm{b} \sum_{k=1}^{n} C(k) = 0. \tag{4.11}$$

Substituting the general solution (4.10) into Eq. (4.11) and taking the limit $n \to \infty$ we immediately obtain:

$$\sum_{k=1}^{\infty} C(k) = -A(f, \mu)/\mathrm{b}. \tag{4.12}$$

This shows that the solution $C_2(n)$ does not contribute to the sum defining $v(1)$ and so the calculation of $v(1)$ is reduced to the determination of the asymptotic normalization constant $A(f, \mu)$.

In the subsequent calculations we choose a finite but large enough value of n (say, $n = 8$) and use the obvious fact that the asymptotic expansions for $C(n)$ and $C_1(n)$ are equivalent (see (4.9) and (4.10)) [4, 22]. Thus, the asymptotic normalization constant is defined by

$$A(f, \mu) = \frac{C^{\mathrm{ex}}(n)}{C^{\mathrm{as}}(n)}, \tag{4.13}$$

where C^{ex} may be easily found from the recurrence relations (4.4) by using the initial conditions (4.5), and C^{as} is defined by the asymptotic series:

$$C^{as}(n) \sim \sum_{k=0} (\alpha_k/n^{k+2}); \qquad \alpha_0 = 1. \tag{4.14}$$

Our problem is now to calculate the function $C(n)$ by using the asymptotic series (4.14) and to estimate the accuracy of these calculations. To this end, we first transform the recurrence relations (4.4) into the recurrence relations for the coefficients α_i. It is not difficult to find the expansions of $C(n \pm 1)$ in powers of n^{-1}:

$$C(n \pm 1) \sim \sum_{k=0}^{\infty} \frac{\alpha_k}{(n \pm 1)^{k+2}} = \sum_{k=0}^{\infty} \frac{\beta_k^{(\pm)}}{n^{k+2}}. \tag{4.15}$$

This may be done by expressing $\beta_k^{(\pm)}$ in terms of α_i according to the Bürmann theorem [21]. Omitting the trivial algebra, we write the result

$$\beta_k^{(\pm)} = \sum_{i=0}^{k+1} (\mp 1)^{k-i+1} C_{k+1}^i \alpha_{i-1}, \tag{4.16}$$

where $C_m{}^i \equiv m!/i!(m-i)!$ are the binomial coefficients. Substituting (4.14), (4.15), and (4.16) into the recurrence relations (4.4) and performing simple but tedious manipulations we finally obtain the recurrence relations for α_i :

$$(k+1)\,\alpha_{k+1} - \left[\mathrm{b} + \frac{(k+1)(k+2)}{2}\right] \alpha_k - \sum_{i=0}^{k-1} \alpha_i A_k{}^i = 0. \tag{4.17}$$

Here $A_k{}^i$ can be expressed simply in terms of the binomial coefficients:

$$A_k{}^i = (-1)^{k-1} C_{k+2}^i + \mathrm{a} C_{k+1}^{i+1}. \tag{4.18}$$

Using the recurrence relations (4.17) one can successively found any desired number of the coefficients α_i. By using Eq. (4.17) it is not difficult to show that $\alpha_i \sim_{i\to\infty} i!$. For this reason the term α_k/n^{k+2} as a function of k for n fixed has a minimum at $k = k_0(n)$. The maximum accuracy will be achieved [22] if we restrict the summation in the infinite asymptotic series (4.14) to the following finite sum:

$$C^{as}(n) = \sum_{k=0}^{k_0(n)} \frac{\alpha_k}{n^{k+2}}. \tag{4.19}$$

The absolute error of this calculation is proportional to the magnitude of the term corresponding to $k = k_0(n)$, i.e., $\Delta C(n) \sim \alpha_{k_0}/n^{k_0+2}$. The relative error $\varphi(n) = \Delta C(n)/C(n)$ rapidly decreases with increasing n and for any fixed n may be easily estimated. As a typical example we present here the relative error $\varphi(n)$

of the calculation of the sums (4.14), (4.19) in the case of $\lambda = 1$, $\epsilon = -1$, $\mu = 3.0$, and $f = 6.073$ for different n. The results are: $k_0(4) = 6$, $\varphi(4) = 8.18\,\%$; $k_0(5) = 9$, $\varphi(5) = 1.91\,\%$; $k_0(6) = 14$, $\varphi(6) = 0.27\,\%$.

The numerical calculations were performed by summing the slowly convergent series (4.8), (4.4), (4.5) on the computer CDC-6200 (10^4 terms of the series (4.8)) and, alternatively, by using the asymptotic method with the help of the minicomputer IME-86-S (less than 10 terms of the series (4.19)). The results are listed in Table V. In the physical problem, which has been reduced to the boundary value problem (2.1)–(2.4), the main quantities are the vertex function of the pion composed of a quark and antiquark:

$$\Gamma(x) = x^{-3/2}u(x) \tag{4.20}$$

and the coupling constant of the pion

$$g(\mu) = (\Gamma^2(x)/4\pi)|_{x^2=-\mu^2} = \frac{1}{4\pi}\,[v(1)/\mu^2]^2. \tag{4.21}$$

Thus, bearing in mind the physical applications [1], in Table V we present our numerical results in terms of the coupling constant $g(\mu)$ for $\lambda = 1$, $\epsilon = -1$, $\mu = 2.5$; 3.0; 3.5; 4.0. (i.e., for eigenfunction $u_{O(-)}(i\mu)$, see Sections 2 and 3).

TABLE V

The Pion Coupling Constant $g(\mu)$ and the Relative Error $\Delta g(\mu)/g(\mu)$ of the Asymptotic Method for Different Values of μ

μ	2.5	3.0	3.5	4.0
$g(\mu)$	13.80	32.80	78.40	122.9
$\Delta g/g$ (%)	0.12	0.55	1.30	0.46

In conclusion let us briefly discuss the problem III. The continuation of the solutions, defined by the power series, outside the circle of convergence can be performed by using a bilinear transformation [19, 23] of the independent variable

$$t = z/(z + \mathrm{p}), \tag{4.22}$$

where the parameter p is to be chosen in each case so as to optimize the convergence of the resulting series in t. The practical application of this method is the subject of [23], where the details of the method are considered and the numerical results are presented. The same problem can be solved by the method due to Ford [24]. This method has been generalized and essentially completed in [25].

5. Summary and Conclusions

We have investigated in detail the numerical method for solving the problem (1.4). We have obtained the numerical solution of this problem by using the continuous analog of the Newton method, applied to the equivalent differential boundary value problem. The transition to the differential problem was used because there was the available routine for its solving and because for differential equations it is easy to find the solutions in the form of power series as well as sufficiently accurate approximate solutions of the boundary value problems by the JWKB method. The JWKB solutions were used as the initial approximations for the realization of the continuous analog of the Newton method.

The comparison of the numerical and the JWKB solutions shows that the JWKB method gives good approximations for the eigenvalues even in such a region, where the formal conditions of its applicability are not fulfilled. To obtain the better JWKB approximations to wave function, more powerful variants of the JWKB method must be used (see, for example, papers [14] and reviews [7]).

The comparison of the numerical solutions with those represented in the form of the convergent power series makes it possible to find the analytic continuation of $u(x)$ into the whole complex plane. This can be done with the same accuracy with which the approximate solutions are known for real x. This result is very important for the physical applications

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