The generalized continuous analog of Newton's method for the numerical study of some nonlinear quantum-field models*

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Fiz. Élem. Chastits At. Yadra **30**, 210–265 (January–February 1999)

A numerical method for studying nonlinear problems arising in mathematical models of physics is systematically described in this review. The unified basis for the development of numerical schemes is a generalization of the continuous analog of Newton's method, which represents a qualitatively new development of the Newtonian evolution process on the basis of the integration of concepts from perturbation theory and the theory of evolution in parameters. The results are presented of numerical studies of quantum-field models of the polaron, the solvated electron, the binucleon, and also QCD potential models for some commonly used potentials.
 [S1063-7796(99)00501-X]

1. INTRODUCTION

Twenty-five years have passed since the publication of the first review in the Soviet Journal of Particles and Nuclei on the use of the continuous analog of Newton's method (CANM) for the numerical solution of nonlinear equations in mathematical models of physics.[1] During this time, owing largely to the efforts of the group at the JINR, this method has been transformed into a powerful tool for constructing effective numerical schemes to solve a wide variety of nonlinear problems arising in physics. Moreover, it can now be stated with certainty that an approach which is qualitatively new compared to the CANM has been developed for designing algorithms for the numerical analysis of complex, multiparameter, nonlinear physics models.

The development of this approach has largely been the product of experience in solving a wide variety of practical problems. The method thus incorporates, along with the CANM concepts, the most attractive features of several well known methods which are widely used to solve physics problems.

These are perturbation theory,[2] the method of continuation in a parameter,[3] and the method of differentiation with respect to a parameter,[4] which in nuclear physics is also known as the method of coupling-constant evolution.[5]

In the developed iteration schemes, the problem of choosing the initial approximations is in some sense solved, and the solution of the linear problem for the iteration corrections is simplified. Moreover, it is possible to construct an iteration process without inversion of the linear operator in this problem.

As a result, the numerical schemes possess the features of such well known methods as the splitting method,[6] multigrid methods,[7] and several regularization methods.[8]

Our approach therefore follows the modern trends in the development of computer architecture and the programming techniques for numerical processes.[9]

In spectral problems of quantum mechanics, our generalization of the CANM can serve as a unified theoretical basis for describing a series of well known methods, such as the method of inverse iterations, and the method of inverse iterations with a shift and with a Rayleigh partial.[10] The realization of the numerical schemes used in these problems is discussed in reviews.[11,12]

Our work on the development of the generalized CANM has initiated research on optimization of the convergence of Newtonian iteration schemes,[13,14] and also schemes with parameter continuation.[15] In this review we present the results of a numerical study of nonlinear models used in the theory of polarons and QCD potential models. These represent completely different areas of theoretical physics, but the numerical methods used in them are based on the generalized CANM.

The collaboration responsible for this review is made up of specialists in the numerical analysis of nonlinear physics models and theoretical physicists who actively use the method. We hope that the material presented here will help the interested reader, acquainted with the basic ideas behind the generalized CANM and the technique of numerical analysis of some nonlinear models in physics, to extend the range of its applicability.

2. MODIFIED CANM-BASED ITERATION SCHEMES

A number of mathematical models of quantum field theory lead to new formulations of boundary-value problems for nonlinear differential, integro-differential, and integral equations. The formulations are original in that they combine the nonlinear boundary-value and spectral problems, which leads to systems of the corresponding equations. The general features of such systems are that they are singular and involve many parameters, i.e., the model parameters and the spectral parameters. The problems can be reduced to a unified formulation as the equation

$$\varphi(\mathbf{a},\boldsymbol{\lambda},y)=0, \tag{1}$$

where y is an element from some region of the B space Y, and $\boldsymbol{\lambda}\in R_m$ and $\mathbf{a}\in R_l$ are vectors from the Euclidean spaces of the corresponding dimensions. For a given vector $\mathbf{a}$, the nonlinear function φ takes the elements $z=\{\boldsymbol{\lambda},y\}$ from the space $R_m\times Y$ to the space $R_l\times U$, where U is a B space and $U\supseteq Y$. It is assumed that for each given vector $\mathbf{a}$, Eq. (1) has a countable set of solutions $\{y_n^*\}$, $n=0,1,2,\ldots$, and an eigenvalue vector $\boldsymbol{\lambda}_n^*$ corresponds to each solution y_n^*. A solution $z_n^*=\{\boldsymbol{\lambda}_n^*,y_n^*\}$ of Eq. (1) is a function of the parameter vector $\mathbf{a}$.

These problems have the following features.

1. As a rule, there is definite information about the existence and qualitative behavior of the desired solutions. This information can be obtained from the physical properties of the studied processes or from the study of simplified models, particularly in asymptotic regions of the parameter variation.

2. In problems which are an approximation to more complicated multidimensional ones, and also in going from infinite ranges of variation of independent variables to finite ranges, problems arise with estimating the accuracy of the approximations used. In many cases such estimates can be obtained only numerically, by performing calculations at several values of the parameters of the approximation.

Therefore, in the formulation (1) the vector of "external" parameters $\mathbf{a}$ is extended to include not only the "physical" parameters of the model, but also the parameters of the approximation to the problem, including those of the numerical scheme. The numerical study of the model usually reduces to performing a large number of calculations in a wide range of variation of these parameters, allowing the simultaneous study of both the properties of the models, i.e., the behavior of the solutions as functions of the "physical" parameters, and the accuracy of the results as a function of the parameters of the approximation to the original problem.

In what follows, we shall not write out the dependence of the function φ on the parameters $\mathbf{a}$ and $\boldsymbol{\lambda}$ wherever this cannot lead to confusion.

2.1. Newtonian iteration schemes

The author of Ref. 16, where the CANM method was first proposed, studied a group of single-step iteration methods of solving a nonlinear equation in B space:

$$\varphi(z)=0,$$

in which at each step k of the iteration process the correction Δz_k to a known approximation z_k of the desired solution is calculated from the expression

$$\Delta z_k=\psi(z_k),$$

$$z_{k+1}=z_k+\Delta z_k,\quad k=0,1,2,\ldots,$$

z_0 is a given element.

The method of constructing the function $\psi(z)$ is selected according to the iteration method used. In particular, for Newton's method,

$$\psi(z)=-\varphi'(z)^{-1}\varphi(z),$$

where $\varphi'(z)$ is a linear operator, the Fréchet derivative of the function $\varphi(z)$. For each iteration process of a given type it is possible to construct its continuous analog by introducing, instead of the discrete variable k ($k=0,1,2,\ldots$), a continuous parameter t ($0\leqslant t<\infty$). Assuming that the dependence $z=z(t)$ is continuous and introducing the derivative $(d/dt)z(t)$ in place of the increment Δz_k, we obtain the differential equation

$$\frac{d}{dt}z(t)=\psi(z(t)),\quad z(0)=z_0. \tag{2}$$

As a result, the solution of (1) is found by solving the Cauchy problem (2) on the semiaxis $0\leqslant t<\infty$. The study cited earlier[16] proves a number of statements about the convergence of continuous analogs of iteration methods for $t\to\infty$ to an isolated solution z^* of (1).

For the CANM this proof is based on transformation of (2) to the form

$$\frac{d}{dt}\varphi(z(t))=-\varphi(z(t)),\quad z(0)=z_0, \tag{3}$$

from which there follows the existence of the integral

$$\varphi(z(t))=e^{-t}\varphi(z_0).$$

When the function $\varphi(z)$ is smooth and a bounded operator $\varphi'(z)^{-1}$ exists in the neighborhood of the initial approximation z_0, it can be proved that a root z^* of Eq. (1) exists in this neighborhood and that the trajectory $z(t)$ converges to this root for $t\to\infty$.

In Ref. 16 it was proposed that the Cauchy problem (2) be solved approximately by using suitable numerical methods, which are expected to be stable for asymptotic stability of $z=z(t)$.

The earlier review[1] describes a very simple method for the approximate integration of (2): the Euler method for the CANM. On a discrete grid $\{t_k,\ k=0,1,2,\ldots;\ t_{k+1}-t_k=\tau_k\}$ this method leads to a sequence of linear problems

$$\varphi'(z_k)v_k=-\varphi(z_k),$$

$$z_{k+1}=z_k+\tau_k v_k,\quad k=0,1,2,\ldots, \tag{4}$$

where z_0 is a given element. For $\tau_k\equiv 1$ the sequence of Newton's method is obtained.

The convergence of the Euler method was proved[1] on the finite interval $0\leqslant t\leqslant T$ for $\tau_k\to 0$. However, in practice the treatment of the parameter τ_k as an integration step is not interesting. In fact, in order that $z=z(T)$ differ little from the desired solution z^*, it is necessary to take $t=T$ to be rather large. At the same time, to calculate the value of $z=z(T)$ more accurately by the Euler method it is necessary to take τ_k to be sufficiently small. These requirements are contradictory, because we are not interested in all the approximate values $z_k\approx z(t_k)$, but in only the required element $z(T)$.

In order to find a representation of the parameter τ_k satisfying the requirement of minimal computational time to reach the required accuracy of the solution z^*, we recall that Newton's method, which converges quadratically in the near neighborhood of the solution, ensures that the discrepancy is minimal for the linear part of $\varphi(z)$ (Ref. 17).

To generalize this feature, we shall treat τ_k as an iteration parameter in the iterations (4), the optimal choice of which gives the minimum transition function $\psi_{k+1}(\tau)$ in the estimate[18]

$$\|\varphi(z_{k+1})\| \leq \psi_{k+1}(\tau_k)\|\varphi(z_k)\|.$$

If we assume that in the neighborhood of the desired solution

$$\|\varphi'(z)^{-1}\| \leq B, \quad \|\varphi''(z)\| \leq M, \tag{5}$$

the transition function is defined as

$$\psi_{k+1}(\tau) = 1 - \tau + \frac{\tau^2}{2} MB^2 \|\varphi(z_k)\|, \quad 0 < \tau \leq 1.$$

It has been shown[18] that the algorithm for determining the iteration parameter

$$\tau_k = \|\varphi'(z_k)\|^{-1} \|\varphi(z_{k-1})\| \tau_{k-1}, \quad 0 < \tau_0 \leq \tau_k \leq 1, \tag{6}$$

ensures, for a suitable choice of τ_0, nearly optimal calculation of the sequence $\{\tau_k\}$, and, in the case of convergence, passage to the iterations (4) of Newton's method. It should be noted that the algorithm (6) was first proposed in Ref. 19, and it has been used successfully to solve many nonlinear problems.[20]

The local convergence of the iterations (4) with the iteration parameter (6) has been studied in Ref. 18.

Theorem 1 *(Ref. 18). Let the conditions (5) and*

$$q_0 = \frac{\tau_0}{2} MB^2 \|\varphi(z_0)\| < 1$$

be satisfied in the sphere

$$\bar{D}_1 = \left\{ \|z - z_0\| < \frac{B}{1 - q_1} \|\varphi(z_0)\| \right\}.$$

Let there exist a positive integer K such that

1) $1 > \tau_k = \dfrac{\|\varphi(z_{k-1})\|}{\|\varphi(z_k)\|} \tau_{k-1}, \quad k = 1,2,\ldots,K-1;$

2) $\tau_{k+j} = 1, \quad j = 0,1,\ldots;$

3) $\tau_0 > q_1^K, \quad q_1 = \psi_1(\tau_0).$

Then Eq. (1) has a solution $z^* \in \bar{D}_1$ *to which the iterations (4) beginning with* z_0 *converge. The rate of convergence is determined by the inequality*

$$\|z^* - z_k\| < Bq_1^{2^{k-K-1}+K} \|\varphi(z_0)\|, \quad k > K.$$

In Ref. 18 it was also shown that the region of convergence of the CANM-based iterations for this choice of τ_k is larger than in the classical Newton method.

Since the CANM ensures convergence to a solution of (1) only in the neighborhood of a local solution,[1] the problem of constructing the initial approximations is very important. In general, this problem is not algorithmizable and is solved in different ways, depending on the features of the problem in question.

In particular, for the numerical analysis of most models in theoretical physics, there is often *a priori* information about the nature of the solutions, which can be used in choosing the initial approximations.

In the software package SLIPH4,[21] which realizes the solution of the Sturm–Liouville problem, the initial approximations are efficiently constructed by the method proposed in Ref. 22. It is based on an algorithm for calculating the roots of a polynomial by Newton's method with elimination of a calculated root.[23] In that study, and also in Ref. 24, an additional orthogonalization of the calculated approximate solution is performed at each iteration in order to eliminate convergence to the solution already found.

A numerical study of several parameter-dependent problems was performed in Ref. 25 for various physical models using a combination of Newtonian iterations and the continuation method.[3] Here the computation was organized in such a way that the solution known for some set of parameters is used as the initial approximation to solve the problem with new parameter values. The small change of the parameters and the continuous dependence of the solution on them guarantee the convergence of the Newtonian iteration scheme.

It should be noted that difficulties in the practical application of the CANM can arise when $\|\varphi'(z)\|$ is close to zero. They are related to the fact that the system (4) in this case becomes incorrect. Several versions of regularization of the iteration process (4) are studied in Ref. 13.

An iteration procedure based on a combination of Newtonian iterations and the buildup method[27] was suggested in Ref. 26. Its advantage over the scheme (4) is its wider applicability in cases close to degenerate ones ($\|\varphi'(z)\| \to 0$).

2.1.1. Estimates of the accuracy of Newtonian iteration schemes

Let us discuss the accuracy of numerical schemes based on the CANM. As already noted above, in practical realizations of Newtonian iteration schemes Eq. (1) is replaced by an approximating equation in the grid space:

$$\varphi_h(z_h) = 0. \tag{7}$$

Let z_h^* be an exact solution of (7). Then in the grid norm we have the estimate

$$\|z^* - z_h^k\| \leq \|z^* - z_h^*\| + \|z_h^* - z_h^k\|, \tag{8}$$

where z_h^k is the approximation to the solution obtained after the kth iteration when the condition

$$\|\varphi_h(z_h^k)\| \leq \varepsilon \tag{9}$$

is satisfied, where $0 < \varepsilon \ll 1$.

Since

$$\|z^* - z_h^*\| \leq O(h^p) \quad \text{(Ref. 28)},$$

$$\|z_h^* - z_h^k\| \leq B\|\varphi_h(z_h^k)\| \quad \text{(Ref. 16)},$$

then for $B\|\varphi_h(z_h^k)\| \ll O(h^p)$, which is satisfied for sufficiently small ε in (9), the accuracy of the approximate solution is close to the theoretical estimate of the difference method of approximating Eq. (1):

$$\|z^* - z_h^k\| \sim O(h^p). \tag{10}$$

The accuracy can be studied in detail for a sequence of successively finer grids. It is possible to improve the difference solution using Padé or Richardson extrapolation (see, for example, Ref. 7).

When the original problem is singular, the estimate of the accuracy acquires an additional term characterizing the error in approximating the singular problem by the corresponding regular problem.[29] This error can be estimated by performing successive calculations on wider and wider intervals. A relation between the parameters of the numerical scheme is eventually reached, such that the main contribution corresponds to the error of the difference solution, i.e., such that Eq. (10) is satisfied.

According to Ref. 30, classical spectral problems for linear operators can be treated as nonlinear functional equations. For this, the eigenvalue problem in the form

$$\mathcal{D}y-\lambda y=0$$

is supplemented by the normalization condition for an eigenelement,

$$\Gamma(y)=0,$$

where Γ is a normalizing functional, for example,

$$(y,y)-1=0.$$

In this formulation, the eigenvalue problem is a nonlinear functional equation (1) for the unknown $z=\{\lambda,y\}$. Therefore, the CANM can also be used to solve eigenvalue problems.[20]

2.1.2. Generalization of the CANM

At present, various modifications of the CANM which raise its efficiency for particular classes of problems and extend its range of applicability have been developed and are widely used.

One such modification used in a number of studies is a generalization of the CANM in which the parametrization of (1) by the additional parameter t is effected by having φ depend explicitly on t. The continuous parameter t is introduced into (1) in such a way that for $t=0$ we obtain the simple equation

$$\varphi(0,z(0))\equiv\varphi_0(z_0)=0,$$

which can easily be solved, and

$$\lim_{t\to\infty}\varphi(t,z(t))=\varphi(z).$$

Thus, for the nonlinear functional equation (1) an evolution equation in the continuous parameter t is constructed which is similar to Eq. (3):

$$\frac{d}{dt}\varphi(t,z(t))=-\varphi(t,z(t)),\quad 0\leqslant t<\infty, \tag{11}$$

with the initial condition $z(0)=z_0$.

Writing $A(t)=\varphi_z'(t,z(t))$, from (11) we obtain

$$\frac{dz}{dt}=-A(t)^{-1}[\varphi(t,z(t))+\varphi_t'(t,z(t))]. \tag{12}$$

Since the integral of (11) is $\varphi(t,z(t))=e^{-t}\varphi(0,z_0)$, $\|\varphi(t,z(t))\|\to 0$ for $t\to\infty$, and asymptotically stable convergence of $z(t)$ to the desired solution z^* can be expected.

In the approximation of (12) using the Euler scheme, the continuous parameter t is discretized: $(t_0,t_1,\ldots,t_k)$; $t_0=0$, $t_{k+1}-t_k=\tau_k$, which gives the iteration sequence

$$z_{k+1}=z_k+\tau_k V_k, \tag{13}$$

where

$$V_k=-B_k[\varphi(t_k,z_k)+\varphi_t'(t_k,z_k)],\quad B_k=A(t_k)^{-1}. \tag{14}$$

Calculating the iteration correction V_k and the step τ_k for each value of t_k, we obtain a new approximation z_{k+1} to the solution z^*. The iteration process (13) and (14) must be continued until the inequality

$$\delta_k=\|\varphi(t_k,z_k)\|<\varepsilon \tag{15}$$

is satisfied.

One variant of the parametrization based on the generalized CANM is realized by using the scalar function $g(t)$ (Ref. 31), referred to as the function which switches on the perturbation. Here $g(0)=g(\infty)-1=g'(\infty)=0$, and the function $\varphi(t,z(t))$ is represented as the sum

$$\varphi(t,z(t))=\varphi_0(z(t))+g(t)[\varphi(t,z(t))-\varphi_0(z(t))]. \tag{16}$$

It is easy to find the solution of the equation $\varphi_0=0$, or else it is assumed to be known. This variant can be viewed as a combination of the CANM and the parameter-variation method.[4] In Ref. 32 the function $g(t)$ is calculated in the iteration process through the iteration correction, and in Refs. 33–38 the functional dependence $g(t)$ is specified explicitly.

The conditions for convergence of the Newtonian evolution process (11) and (16) for $g(t)=1-\exp(-t)$ are studied in Ref. 31.

Theorem 2 *(Ref. 31). On the sphere*

$$D:\|z-z_0\|\leqslant\frac{B}{1-q}\|\varphi(z_0)\|,\quad 0<q<1,$$

let the functional equation (1) be represented as

$$\varphi(z)=\varphi_0(z)+\varphi_1(z)=0,$$

and the parametric dependence have the form

$$\varphi(t,z(t))=\varphi_0(t,z(t))+g(t)\varphi_1(t,z(t)).$$

Let there exist Fréchet derivatives $\varphi_0'(z)$, $\varphi_1'(z)$ and linear derivatives $\varphi_0''(z)$, $\varphi_1''(z)$, where the linear operator $\varphi_0'(z)$ is invertible, and let the inequalities

$$\|\varphi_0'(z)^{-1}\|\leqslant B,\quad \|\varphi_1'(z)^{-1}\|\leqslant C,\quad q=2BC<1,$$

be satisfied. Let also the operators φ_0'' and φ_1'' be bounded in the neighborhood of each point from the sphere D. Then the following are true:

(1) Equation (11) has a solution $z=z(t)$ for all t from $[0,\infty)$, with its values lying in D.

(2) The limit $\lim_{t\to\infty}z(t)=z^*$ exists, and serves as the root of Eq. (1).

Theorem 3 *(Ref. 31). Let Eq. (1) have a unique solution z^* in some open region D of the space X, and let all the*

conditions of Theorem 2 be satisfied in this region. Then there exists a sphere $S:\|z-z_0\|\leq\epsilon$ *belonging to the region D such that for any* $z_0\in S$ *the differential equation (11) has a unique solution* $z(t)$ *for all* $t\in[0,\infty)$ *and* $\lim_{t\to\infty}z(t)=z^*$.

One advantage of this approach is the constructive solution of the problem of choosing the initial approximation, which can be taken to be the known solution of the equation

$$\varphi_0(z)=0.$$

Another possible application of this approach is to construct modified iteration schemes where, instead of inverting the operator $\varphi'(z)$ at each iteration, the derivative of a specially selected operator φ_0 having a simple structure is inverted. The convergence of such schemes is also discussed in Ref. 31.

In Refs. 34–38 a parametrization of this type was used to develop efficient numerical schemes of higher accuracy.

Numerical schemes based on generalization of the CANM for solving integro-differential equations are given in Ref. 33. The integral part of the equation is treated as a perturbation and is introduced via the function switching on the perturbation.

The presence of an integral operator in problems of this type makes it necessary to invert the high-order, dense matrices approximating it at each iteration. The approach mentioned above allows this step, which takes a large amount of computer time, to be avoided and significantly simplifies the solution of the problem.

As was shown in Ref. 31, realization of the Newtonian evolution process (12)–(14) leads to regularization processes of the Newtonian type studied in Refs. 8 and 39.

2.2. The Newtonian iteration scheme with simultaneous calculation of the operator inverse to the derivative operator of a nonlinear function

The use of vectorized and parallelized numerical schemes makes it essential to develop special algorithms and programs which take efficient advantage of their possibilities. In this section we present a modified algorithm based on the generalized CANM which does exactly this. An iteration process has been developed[40] in which inversion of the derivative operator of a nonlinear function is replaced in each iteration by two multiplications of linear operators.

The idea behind this approach for finding inverse matrices as applied to the parameter-variation method was described in Refs. 41 and 42. Its advantage is the absence of the division operation throughout the calculations. Division by a small number, which can occur in the inversion of poorly conditioned matrices, is thereby eliminated. This results in greater stability and accuracy of the calculations.

Test calculations performed for a number of problems have confirmed the efficiency of this algorithm for the vector and parallel system used at the JINR.

2.2.1. Description of the modified algorithm

Instead of Eq. (1), we shall study the following system of functional-operator equations:

$$\begin{cases}\varphi(z)=0,\\ BA-I=0,\end{cases}\tag{17}$$

where $A=\varphi'_z$, $B=A^{-1}$, and I is the unit operator.

Introducing the continuous parameter t $(0\leq t<\infty)$ and passing, according to the generalized CANM, to the system of evolution equations, we obtain

$$\begin{cases}\dfrac{d}{dt}\varphi(t,z(t))=-\varphi(t,z(t)),\\ \dfrac{d}{dt}[B(t)A(t)-I]=I-B(t)A(t).\end{cases}\tag{18}$$

After simple transformations we obtain

$$\begin{cases}\dfrac{d}{dt}z(t)=-B(t)[\varphi(t,z(t))+\varphi'_t(t,z(t))],\\ \dfrac{d}{dt}B(t)=[I-B(t)(A(t)+A'(t))]B(t).\end{cases}\tag{19}$$

Discretizing the continuous parameter, using the Euler scheme we obtain expressions for calculating $z_{k+1}=z(t_{k+1})$ and $B_{k+1}=B(t_{k+1})$, assuming that z_k and B_k are known at each step k:

$$\begin{cases}z_{k+1}=z_k+\tau_k V_k,\\ B_{k+1}=B_k+\tau_k W_k,\end{cases}\tag{20}$$

where

$$V_k=-B_k[\varphi(t_k,z_k)+\varphi'_t(t_k,z_k)],\tag{21}$$

$$W_k=[I-B_k(A_k+(A_k)'_t)]B_k.\tag{22}$$

Therefore, if we have the initial approximation z_0 and B_0, we can successively find all the approximations z_k and B_k.

The iteration process is continued until the inequality (15) is satisfied.

A special feature of this algorithm is the parallel calculation of the inverse operator B_k in the iteration process, which opens up additional possibilities for parallelizing the computational process.

On the other hand, the inversion of the derivative of a nonlinear functional operator in this modification is replaced by multiplications of auxiliary operators, so that in the program realizing this scheme it becomes necessary to perform the corresponding operations using the matrices approximating these operators. Since, in the scalar version, a single matrix inversion takes a time close to that for multiplying two matrices,[43] the computational time using the modified scheme should be about twice that for the unmodified scheme.

However, from the viewpoint of vectorizing the operations,[44] matrix multiplication is preferable to matrix inversion, and the modified algorithm gives a gain in time when used as part of a vector computational scheme. Naturally, this gain will be obtained at the expense of additional requirements on the machine memory needed to store the auxiliary matrices.

The convergence of this iteration scheme is discussed in Ref. 45.

2.2.2. An iteration scheme for solving the eigenvalue problem for a linear integral equation

As an illustration, let us consider an iteration scheme for solving the equation

$$\Phi(z)\equiv\begin{pmatrix}\varphi(z)\\ \Gamma(z)\end{pmatrix}=0, \tag{23}$$

where

$$\Phi(z)\equiv y(x)(Q(x)-\lambda)+\alpha\int_0^R K(x,x')y(x')dx'=0, \tag{24}$$

$K(x,x')$ is known, $z=(y(x),\lambda)$, and the normalization condition is

$$\Gamma(z)\equiv\int_0^R y^2(x)dx-N=0. \tag{25}$$

We introduce the parameter t $(0\leqslant t<\infty)$ and the function switching on the perturbation $g(t)=1-e^{-t}$, and then write $\Phi(t,z)$ as

$$\Phi(t,z)=\Phi_0(z)+g(t)(\Phi(z)-\Phi_0(z)), \tag{26}$$

where $\Phi_0(z)=0$ is a simple functional equation with known solution z_0 used as the initial approximation.

Using the fact that $z(t)=(y(x,t),\lambda(t))$ and passing to the evolution equation, for (26) we obtain

$$\begin{aligned}&[(\Phi_0(z(t)))'_y+g(t)[(\Phi(z(t)))'_y-(\Phi_0(z(t)))'_y]]y'_t\\&\quad=-[\Phi_0(z(t))+(g(t)+g'_t(t))(\Phi(z(t))\\&\quad-\Phi_0(z(t)))]-[(\Phi_0(z(t)))'_\lambda+g(t)((\Phi(z(t)))'_\lambda\\&\quad-(\Phi_0(z(t)))'_\lambda)]\lambda'_t(t).\end{aligned} \tag{27}$$

Applying the approach described above, denoting $y_k(x)=y(x,t_k)$, $g_k=g(t_k)$, $g'_k=g'(t_k)$, $v_k=y'_t(x,t_k)$, $\mu_k=\lambda'_t(t_k)$, $A_k=\Phi'_y$, $B_k=A_k^{-1}$, for each t_k using (21) and (22) we find

$$v_k=-B_k[G_k+\mu_k F_k], \tag{28}$$

$$W_k=[I-B_k(A_k+A'_{k_t})]B_k, \tag{29}$$

where

$$\begin{aligned}A_k(v_k(x))=\Phi'_{0y}(z_k)v_k(x)+g_k\Big[&(Q(x)-\lambda_k)v_k(x)\\&+\alpha\int_0^R K(x,x')v_k(x')dx'\\&-\Phi'_{0y}(z_k)v_k(x)\Big],\end{aligned} \tag{30}$$

$$\begin{aligned}A'_{k_t}(v_k(x))=(\Phi'_{0y}(z_k))'_t v_k(x)+g'_k\Big[&(Q(x)-\lambda_k)v_k(x)\\&+\alpha\int_0^R K(x,x')v_k(x')dx'\\&-\Phi'_{0y}(z_k)v_k(x)\Big]-g_k v_k(x)[\mu_k\\&+(\Phi'_{0y}(z_k))'_t],\end{aligned} \tag{31}$$

$$G_k=\Phi_0(z_k)+(g_k+g'_k)\Big[(Q(x)-\lambda_k)y_k(x)+\alpha\int_0^R K(x,x')y_k(x')dx'-\Phi_0(z_k)\Big], \tag{32}$$

$$F_k=\Phi'_{0_\lambda}(z_k)-g_k(1+\Phi'_{0_\lambda}(z_k)). \tag{33}$$

The iteration correction v_k is calculated as

$$v_k=v_k^{(1)}+\mu_k v_k^{(2)}, \tag{34}$$

where

$$v_k^{(1)}=-B_kG_k,\quad v_k^{(2)}=-B_kF_k. \tag{35}$$

The expression for calculating μ_k is derived from the normalization condition (25) and has the form

$$\mu_k=\frac{N-\int_0^R y_k(x)(y_k(x)-2v_k^{(1)}(x))dx}{\int_0^R 2y_k(x)v_k^{(2)}(x)dx}. \tag{36}$$

After calculating the iteration corrections μ_k, v_k, and W_k, we can find the new approximation by using the Euler scheme:

$$\begin{aligned}y_{k+1}&=y_k+\tau_k v_k,\\ \lambda_{k+1}&=\lambda_k+\tau_k\mu_k,\\ B_{k+1}&=B_k+\tau_k W_k.\end{aligned} \tag{37}$$

The numerical approximation of (24) on a discrete grid in x $(0=x_0<x_1<\ldots<x_n=R)$ leads to a system of n equations:

$$\Phi_i=y_i(Q_i-\lambda)+\alpha\sum_{j=1}^n K_{ij}y_j\xi_j, \tag{38}$$

where $y_i=y(x_i)$, $Q_i=Q(x_i)$, $K_{ij}=K(x_i,x_j)$, and ξ_j are the coefficients of the quadratic formula for the numerical integration. The operators A, A'_t, F, and G in Eqs. (28)–(33) are respectively approximated by the matrices $\{a_{ij}\}$, $\{\tilde{a}_{ij}\}$ and the vectors (F_i), (G_i). In particular, the values of the matrix elements a_{ij} and $\tilde{a}_{ij}$ at the kth step are defined as

$$a_{ij}=a_{ij}^{(0)}+g_k[(Q_i-\lambda_k)\delta_{ij}+\alpha K_{ij}\xi_j-a_{ij}^{(0)}], \tag{39}$$

$$\begin{aligned}\tilde{a}_{ij}=\tilde{a}_{ij}^{(0)}&+g'_k[(Q_i-\lambda_k)\delta_{ij}+\alpha[K_{ij}\xi_j-\tilde{a}_{ij}^{(0)}]\\&-g_k[\mu_k+\tilde{a}_{ij}^{(0)}],\end{aligned} \tag{40}$$

where δ_{ij} is the Kronecker delta, and $a_{ij}^{(0)}$ and $\tilde{a}_{ij}^{(0)}$ are the elements of the matrices approximating the operators $\Phi'_{0y}(z_k)$ and $[\Phi'_{0y}(z_k)]'_t$, respectively, on the discrete x grid.

2.3. The Newtonian iteration scheme with parametric dependence on the asymptote of the solutions

The modeling of nonlinear effects in field-theory models leads to singular, nonlinear boundary-value problems depending on the "external" physical parameters of the model. By including their additional constraints it is often possible to decrease the number of parameters in the problem. But here additional conditions arise which, as a rule, relate the

integral characteristics of the desired solutions to their asymptotic behavior. Since the group of dependent parameters can be replaced by asymptotic relations for some of the desired solutions, it is possible to formulate an original boundary-value problem in which the equations depend not only on the desired solutions, but also explicitly on the boundary conditions for these solutions.

The iteration scheme developed in Ref. 46 for solving this new type of problem uses a combination of the CANM and the method of continuation in a parameter.[3] It makes it possible to study the dependence of the behavior of the solution on the parameters of the problem, including the external parameters of the physical model and the internal parameters of the numerical scheme.

Let us consider a system of N equations written in vector form:

$$\mathbf{R}(\bar{y})\equiv\bar{y}''+\mathbf{F}(\bar{y};\bar{y}';x;\bar{c})=0,$$
$$0\leqslant x<\infty, \tag{41}$$

where the prime denotes differentiation with respect to x, $\bar{c}$ are the parameters of the problem (an M-component vector), and $\mathbf{F}$ is a continuous vector function of its arguments $\bar{y}$, $\bar{y}'$, and $\bar{c}$, and as a function of x can have a singularity $1/x^p$, $p\leqslant 2$, for $x\to 0$.

We shall seek a solution of the system (41) (the existence of which is assumed) satisfying the asymptotic conditions

$$\mathbf{R}_L(\bar{y})\equiv\mathbf{G}_L(\bar{y}(x_L);\bar{y}'(x_L);x_L;\bar{c})=0,\quad x_L\to 0,$$
$$\mathbf{R}_R(\bar{y})\equiv\mathbf{G}_R(\bar{y}(x_R);\bar{y}'(x_R);x_R;\bar{c})=0,\quad x_R\to\infty, \tag{42}$$

and also the auxiliary functional condition

$$\mathbf{R}_A(\bar{y})\equiv\mathbf{S}(\bar{y};\bar{y}';x,\bar{c})=0, \tag{43}$$

where $\mathbf{G}_L$ and $\mathbf{G}_R$ are N-component vector functions and $\mathbf{S}$ is a p-component vector function, with $p\leqslant M$. We note that for $p=M$, by solving (43) for $\bar{c}$ (if possible) and substituting the result into (41), we can completely eliminate the parameters of the problem. If $p<M$, some free parameters always remain. In what follows we shall assume that $p=M$ with no loss of generality.

Therefore, in solving the boundary-value problem (41), (42), taking into account the auxiliary condition (43), we need to find the unknowns $\{\bar{y}(x),\bar{c}\}$. In the numerical solution of the singular boundary-value problem (41)–(43) on the semiaxis ($0\leqslant x<\infty$) we need to define the corresponding boundary conditions on the finite interval ($0\leqslant x\leqslant x_R$). Here there is an additional problem related to transferring the asymptotic conditions for the desired solutions to finite points ($x=x_L$, $x=x_R$) and estimating the accuracy of this approximation. In general, such estimates can be made only numerically, using the calculations for a sequence of values of the parameters x_L, x_R. We shall assume that the boundary conditions (42) for finite values $x_L=0$ and $x_R<\infty$ include the asymptotic properties of the desired solutions sufficiently accurately. We use the continuous analog of Newton's method to solve the problem (41)–(43) on the finite interval ($0\leqslant x\leqslant x_R$). The Newtonian iterations for this problem amount to solving at each step k the linear problem

$$\bar{v}_k''+\mathbf{F}'_{\bar{y}},\bar{v}_k'+\mathbf{F}'_{\bar{y}}\bar{v}_k=-\mathbf{R}(\bar{y})-\bar{\mu}_k^T\mathbf{F}'_{\bar{c}} \tag{44}$$

with the boundary conditions

$$\mathbf{G}'_{L\bar{y}},\bar{v}_k'(0)+\mathbf{G}'_{L\bar{y}}\bar{v}_k(0)=-\mathbf{R}_L(\bar{y})-\bar{\mu}_k^T\mathbf{G}'_{L\bar{c}},$$
$$\mathbf{G}'_{R\bar{y}},\bar{v}_k'(x_R)+\mathbf{G}'_{R\bar{y}}\bar{v}_k(x_R)=-\mathbf{R}_R(\bar{y})-\bar{\mu}_k^T\mathbf{G}'_{R\bar{c}} \tag{45}$$

and the auxiliary condition

$$\mathbf{S}'_{\bar{y}},\bar{v}_k'+\mathbf{S}'_{\bar{y}}\bar{v}_k=-\mathbf{R}_D(\bar{y})-\bar{\mu}_k^T\mathbf{S}'_{\bar{c}} \tag{46}$$

for the iteration correction $\bar{v}_k=\Delta\bar{y}_k$, $\bar{\mu}_k=\Delta\bar{c}_k$ to the known approximation $\{\bar{y}(x)_k,\bar{c}_k\}$ of the desired solution. We shall seek a solution of the system (44) in the form

$$\bar{v}_k=\bar{v}_k^{(1)}+\bar{\mu}_k^T\bar{v}_k^{(2)}. \tag{47}$$

Substituting (47) into (44) and (45), we find

$$(\bar{v}_k^{(1)})''+\mathbf{F}'_{\bar{y}},(\bar{v}_k^{(1)})'+\mathbf{F}'_{\bar{y}}\bar{v}_k^{(1)}=-\mathbf{R}(\bar{y}) \tag{48}$$
$$\mathbf{G}'_{L\bar{y}},(\bar{v}_k^{(1)}(0))'+\mathbf{G}'_{L\bar{y}}\bar{v}_k^{(1)}(0)=-\mathbf{R}_L(\bar{y}),$$
$$\mathbf{G}'_{R\bar{y}},(\bar{v}_k^{(1)}(x_R))'+\mathbf{G}'_{R\bar{y}}\bar{v}_k^{(1)}(x_R)=-\mathbf{R}_R(\bar{y}) \tag{49}$$

and

$$(\bar{v}_k^{(2)})''+\mathbf{F}'_{\bar{y}},(\bar{v}_k^{(2)})'+\mathbf{F}'_{\bar{y}}\bar{v}_k^{(2)}=-\mathbf{F}'_{\bar{c}}, \tag{50}$$
$$\mathbf{G}'_{L\bar{y}},(\bar{v}_k^{(2)}(0))'+\mathbf{G}'_{L\bar{y}}\bar{v}_k^{(2)}(0)=-\mathbf{G}'_{L\bar{c}},$$
$$\mathbf{G}'_{R\bar{y}},(\bar{v}_k^{(2)}(x_R))'+\mathbf{G}'_{R\bar{y}}\bar{v}_k^{(2)}(x_R)=-\mathbf{G}'_{R\bar{c}}. \tag{51}$$

To find the functions $\bar{v}_k^{(1)}$ and $\bar{v}_k^{(2)}$ we solve the boundary-value problems (48), (49) and (50), (51). By substituting (47) into (46) we obtain a system of equations for the $\bar{\mu}_k$. Therefore, at each iteration it is necessary to solve the boundary-value problems (48), (49) and (50), (51) and the system of algebraic equations (46) to find $\bar{\mu}_k$. The passage to the next approximation is effected by the formulas

$$\bar{y}_{k+1}=\bar{y}_k+\tau_k\bar{v}_k$$
$$\bar{c}_{k+1}=\bar{c}_k+\tau_k\bar{\mu}_k, \tag{52}$$

where τ_k is the iteration parameter, which can be chosen so as to ensure the optimal conditions for convergence of the iterations.[13] The iterations stop when the condition

$$\delta_k<\epsilon$$

is satisfied, where the discrepancy δ_k can be defined as

$$\delta_k=\max_j\max_i\max_{x\in[x_L,x_R]}|\mathbf{R}_i(y_{ik}(x),c_{jk})|,\quad i=1,2,\cdots,N,$$
$$j=1,2,\cdots,M,$$

with $\epsilon>0$ a given small number.

3. NUMERICAL STUDY OF SEVERAL NONLINEAR, SELF-CONSISTENT QUANTUM FIELD MODELS USING THE GENERALIZED CANM

Various physical processes occurring in condensed media can in many cases be modeled in terms of self-localized states. The study of such processes is therefore very important, and for the last few years great efforts have focused on

the single-particle self-consistent description of multiparticle systems (see, for example, Ref. 47 and references therein).

One example which can be cited is that of the polaron,[48] which is, on the one hand, a very simple model of quantum field theory and, on the other, an object with numerous applications in the physics of condensed matter. The problem of a polaron as a nonrelativistic particle interacting with a quantum field was initially formulated as the problem of a self-localized electron in an ionic crystal.

At present there are many physical examples in which the electron forms a self-localized state. Among these are magnetically ordered crystals, in which magnetic polarons can be formed, polar liquids, in which solvated electrons form self-localized states, and numerous others (see references in Ref. 47). The single-particle spectrum for a charged test particle interacting with an electron gas has been studied in an approximation where the particle is associated with plasions and forms a self-localized state.[49]

From the mathematical point of view, the appearance of self-localized states is associated with the appearance of particle-like solutions at some value of the coupling constant describing the interaction of a test particle with a quantum field.[50]

The modeling of nonlinear effects in condensed media and quantum field models leads to nonlinear eigenvalue problems for differential equations depending on the external physical parameters of the model. Therefore, the essence of the problem is largely concerned with studying the solutions of the equations which arise for strong interaction between the particle and the field, when the formation of self-localized states becomes possible.

In this section we shall formulate problems within some self-consistent models which have been studied numerically using Newtonian iteration schemes. We shall discuss the generalized polaron equation in the Luttinger–Lu model,[51] the self-consistent model of a solvated electron,[52] and the quantum field model of a binucleon in the strong-coupling limit.[53]

3.1. The polaron equation in the Luttinger–Lu model

3.1.1. General statement of the problem

In the strong-coupling limit, the calculation of the characteristics (energy levels and wave functions) of the polaron reduces to solving a nonlinear system of differential equations for the eigenvalues:

$$\Delta_r\Psi(\mathbf{r})+\phi(\mathbf{r})\Psi(\mathbf{r})+E\Psi(\mathbf{r})=0,$$
$$\Delta_r\phi(\mathbf{r})+C\Psi^2(\mathbf{r})=0, \tag{53}$$

in which the function $\Psi(\mathbf{r})$ satisfies the condition $\int\Psi^2(\mathbf{r})d\mathbf{r}=1$ (here E is the eigenvalue and C is a parameter). The system (53) was obtained by Pekar from the phenomenological theory.[54] In the fundamental study by Bogolyubov,[55] the equations in (53) were obtained constructively from the consistent microscopic theory of the motion of a nonrelativistic particle interacting with a quantum field.

The spherically symmetric solutions of (53) are now well studied. Approximate solutions of (53) of this form were first obtained in Ref. 54 for the ground state by the direct variational method with trial functions chosen in the form of polynomials and exponentials. The variational calculations of the polaron ground state were improved in Ref. 56 by numerical integration of (53). The CANM was used to calculate the ground state in Ref. 57. The solutions of (53) corresponding to four different self-consistent excited states of a particle in a quantum field were first obtained in Ref. 58. Since physico-chemical reactions in condensed media occur via excited states, the quantitative study of the physical characteristics of such states is very important. Accordingly, interest has grown in solving the polaron problem not only in the strong-coupling limit, but also in the entire range of particle–field coupling constant. The physical aspects of the problem are discussed in many articles and reviews (see, for example, Ref. 47 and references therein).

As is well known, at present the best approximation for the polaron at intermediate values of the electron–phonon coupling is the Feynman path-integral approach.[59] Unfortunately, this approach is directly applicable only to calculating the polaron ground state. This method is essentially analogous to the direct variational method for the Schrödinger equation. An important development of the Feynman approach was made by Luttinger and Lu (Ref. 51; see also subsequent publications[60]). Their studies allow the Feynman approach to be reformulated in the language of differential equations. At the present time this is the only method by which differential equations can be used to describe the passage from the limit of weak particle–field coupling to strong coupling. It is crucial that in the strong-coupling limit the resulting equations are asymptotically exact, i.e., they become the Bogolyubov–Tyablikov equations corresponding to the strong–coupling limit.

Thus, the simplest self-consistent model of the polaron for arbitrary coupling is obtained from the general problem formulated in Ref. 61. In that study the polaron energy levels and wave functions $\{\epsilon_n, u(\bar{r})\}$ in the Luttinger–Lu model are determined by the eigenvalue problem for an integro-differential equation in three-dimensional coordinate space:

$$\left[-\frac{1}{2\mu}\nabla^2-\frac{\alpha\sqrt{2}}{\mu}\int d\bar{r}'\frac{|u(\bar{r}')|^2}{|\bar{r}-\bar{r}'|}(1-e^{-C|\bar{r}-\bar{r}'|})\right]u(\bar{r})$$
$$=\epsilon u(\bar{r}), \tag{54}$$

where ∇^2 is the three-dimensional Laplacian, $\mu=m/(1+m)$ is the reduced mass of the electron, α is the coupling constant, and $C=\mu\sqrt{2}/\sqrt{1-\mu}$. The normalization condition takes the form

$$\int d\bar{r}|u(\bar{r})|^2=1.$$

The problem (54) can be formulated in dimensionless quantities as a nonlinear eigenvalue problem for the system of equations

$$\Delta\psi(\mathbf{r})-\lambda\psi(\mathbf{r})+A(V_1(\mathbf{r})-V_2(\mathbf{r}))\psi(\mathbf{r})=0,$$
$$\Delta V_1(\mathbf{r})+|\psi(\mathbf{r})|^2=0, \tag{55}$$
$$\Delta V_2(\mathbf{r})-C^2V_2(\mathbf{r})+|\psi(\mathbf{r})|^2=0$$

with the normalization condition

$$\int_0^\infty |\psi(\mathbf{r})|^2 d\mathbf{r} = 1, \tag{56}$$

where Δ is the three-dimensional Laplacian, A and C are the physical parameters of the problem, and λ are the eigenvalues determining the energies of the polaron states.

3.1.2. The spherically symmetric case

Writing the spherically symmetric solutions of (54) as

$$u(\bar{r}) = x^{-1}\psi(x), \quad x = |\bar{r}|,$$

we obtain the following eigenvalue problem, the solutions of which determine the polaron energy levels and wave functions in the case of spherical symmetry:[61]

$$\psi''(x) - \lambda\psi(x) + A\psi(x)V(x,\psi,(x)) = 0, \tag{57}$$

where

$$V(x,\psi(x)) = \frac{1}{x}\int_0^\infty D(x,x')\frac{\psi^2(x')}{x'}dx',$$

the boundary conditions have the form

$$\psi(0) = \psi(\infty) = 0,$$

the normalization condition is

$$\int_0^\infty \psi^2(x)dx = \frac{1}{4\pi}, \tag{58}$$

$$D(x,x') = \begin{cases} x' - \dfrac{1}{C}\exp(-Cx)\sinh Cx', & x' < x, \\ x - \dfrac{1}{C}\exp(-Cx')\sinh Cx, & x < x', \end{cases}$$

$A = 8\sqrt{2}\pi\alpha$, and $\lambda = 2\mu\epsilon$, $\epsilon > 0$, are the energy levels. In the limiting case of strong coupling for $\mu = 1$, corresponding to the statement of the problem in the Pekar model,[54] the function $D(x,x')$ takes the form

$$D(x,x') = \begin{cases} x', & x' < x, \\ x, & x < x'. \end{cases}$$

This problem was solved in Ref. 62 using a program based on a modification of the CANM.[63]

Another statement of the eigenvalue problem (57) is[65]

$$\begin{cases} \psi''(x) - \lambda\psi(x) + A\psi(x)\dfrac{V_2 - V_1}{x} = 0, \\ V_1'' + \dfrac{\psi^2}{x} = 0, \\ V_2'' - CV_2 + \dfrac{\psi^2}{x} = 0 \end{cases} \tag{59}$$

with the normalization condition (58). The desired solutions of the system (59) must satisfy the following asymptotic conditions:

$$\psi(0) = \psi(\infty) = 0, \quad V_1(0) = V_1'(\infty) = 0,$$

$$V_2(0) = V_2(\infty) = 0.$$

The solutions of (57) are the solutions of (59) and vice versa. The system (59) was solved numerically in Ref. 64 using a modified CANM-based algorithm, which is described below for the more general nonspherically symmetric case.

After some algebra, the spectral problem (57)–(59) can be reduced[61] to a parametrically dependent system of nonlinear equations of the form

$$\begin{cases} \phi'' - \phi + \dfrac{1}{x}\phi(W_1 - W_2) = 0, \\ W_1'' + \dfrac{1}{x}\phi^2 = 0, \\ W_2'' - a^2 W_2 + \dfrac{1}{x}\phi^2 = 0 \end{cases} \tag{60}$$

with the boundary conditions

$$\phi(0) = \phi(\infty) = 0, \quad W_1(0) = W_1'(\infty) = 0,$$

$$W_2(0) = W_2(\infty) = 0.$$

The solutions $z = \{\phi, W_1, W_2\}$ are calculated for various values of the parameter a. A feature of this formulation is the fact that the energy levels and other physical parameters of the problem can be determined only after finding the solution of the system for some value of the parameter a. A Newtonian iteration scheme for the numerical study of the problem (60) is given in Ref. 61. The first five spherically symmetric states of the polaron were first found in that study. The results of solving the eigenvalue problem in the formulations (57) and (59) obtained in Refs. 62 and 64, respectively, agree with the results of Ref. 61.

3.1.3. The nonspherically symmetric case

If we write the solution of (55) as an expansion in spherical harmonics $Y_{lm}(\theta,\phi)$,

$$\begin{cases} \psi(\mathbf{r}) = \displaystyle\sum_{l=0}^{\infty}\sum_{m=-l}^{l}\frac{\psi_{lm}(r)}{r}Y_{lm}(\theta,\phi), \\ V_i(\mathbf{r}) = \displaystyle\sum_{l=0}^{\infty}\sum_{m=-l}^{l}\frac{V_{ilm}(r)}{r}Y_{lm}(\theta,\phi), \end{cases} \quad i = 1,2, \tag{61}$$

substitute this expansion into (55), multiply on the left by $Y^*(\theta,\phi)$, and integrate over $d\Omega = \sin\theta d\theta d\phi$, we obtain the following system of equations for the expansion coefficients $\psi_{lm}(r)$ and $V_{ilm}(r)$:

$$\begin{aligned} &\psi_{lm}''(r) - \lambda\psi_{lm}(r) - \frac{l(l+1)}{r^2}\psi_{lm}(r) \\ &\quad + \frac{A}{r}\sum_{l_1=0}^{\infty}\sum_{m_1=-l_1}^{l_1} Q_{lml_1m_1}(r)\psi_{l_1m_1}(r) = 0, \\ &V_{1lm}''(r) - \frac{l(l+1)}{r^2}V_{1lm}(r) + S_{lm}(r) = 0, \\ &V_{2lm}''(r) - \frac{l(l+1)}{r^2}V_{2lm}(r) - C^2V_{2lm}(r) + S_{lm}(r) = 0, \\ &l = 0,1,2,\ldots, \quad m = -l,\ldots,l, \end{aligned} \tag{62}$$

with the normalization condition

$$\sum_{l=0}^{\infty}\sum_{m=-l}^{l}\int_0^{\infty}\psi_{lm}^2(r)dr=1, \tag{63}$$

where

$$Q_{lml_1m_1}=\sum_{l_2=0}^{\infty}\sum_{m_2=-l_2}^{l_2}W_{lml_1m_1l_2m_2}(V_{1l_2m_2}(r)-V_{2l_2m_2}(r)),$$

$$S_{lm}=\frac{1}{r}\sum_{l_1=0}^{\infty}\sum_{m_1=-l_1}^{l_1}\sum_{l_2=0}^{\infty}\sum_{m_2=-l_2}^{l_2}\bar{W}_{lml_1m_1l_2m_2}\times\psi_{l_1m_1}(r)\psi_{l_2m_2}(r), \tag{64}$$

$$W_{lml_1m_1l_2m_2}=\int d\Omega Y_{lm}^*Y_{l_1m_1}Y_{l_2m_2}^*,$$

$$\bar{W}_{lml_1m_1l_2m_2}=\int d\Omega Y_{lm}^*Y_{l_1m_1}Y_{l_2m_2}^*.$$

The desired solutions of (62) satisfy the following asymptotic conditions:

$$\psi_{lm}(r)_{r\to0}\to A_{1lm}r^{l+1},\quad \psi_{lm}(r)_{r\to\infty}\to A_{2lm}e^{-\sqrt{\lambda}r},$$
$$V_{1lm}(r)_{r\to0}\to B_{1lm}r^{l+1},\quad V_{1lm}(r)_{r\to\infty}\to B_{2lm}r^{-l},$$
$$V_{2lm}(r)_{r\to0}\to C_{1lm}r^{l+1},\quad V_{2lm}(r)_{r\to\infty}\to C_{2lm}r^{-Cr}, \tag{65}$$

where A_{1lm}, A_{2lm}, B_{1lm}, B_{2lm}, C_{1lm}, and C_{2lm} are constants.

The numerical solution of the problem (62)–(64) with the boundary conditions (65) is obtained on the finite interval $0\leqslant r\leqslant R_m$, $R_m\gg1$, with the number of terms in the expansions (61) restricted to L_m for $\psi(\mathbf{r})$ and $L_v=2L_m$ for $V_i(r)$, $i=1,2$.

As already mentioned, the best-studied case is that of the spherically symmetric solutions $\psi(r,\theta,\phi)\to\psi(r)$, corresponding to the value $L_m=0$, when the problem (62)–(65) can be reduced to the statements given in the preceding section.

Let us discuss the more general case $\psi(r,\theta,\phi)\to\psi(r,\theta)$. Then the function $Y_{lm}(\theta,\phi)$ in the expansion (61) must be replaced by

$$Y_{l0}=\sqrt{\frac{2l+1}{4\pi}}P_l(\cos\theta),$$

where P_l is the Legendre polynomial and $l=0,1,\ldots,L_m$.

Introducing the more convenient notation $\psi_{l0}=\psi_l$, $V_{1l0}=V_{1l}$, $V_{2l0}=V_{2l}$, $S_{l0}=S_l$, $Q_{l0l_10}=Q_{ll_1}$, $W_{l0l_10l_20}=W_{ll_1l_2}$, and taking into account the above restrictions, the system (62)–(65) can be rewritten as

$$\psi_l''(r)-\lambda\psi_l(r)-\frac{l(l+1)}{r^2}\psi_l(r)+\frac{A}{r}\sum_{l_1=0}^{L_m}Q_{ll_1}(r)\psi_{l_1}(r)=0,$$

$l=0,1,\ldots,L_m$, (66)

$$V_{1l}''(r)-\frac{l(l+1)}{r^2}V_{1l}(r)+S_l(r)=0, \tag{67}$$

$$V_{2l}''(r)-\frac{l(l+1)}{r^2}V_{2l}(r)-C^2V_{2l}(r)+S_l(r)=0, \tag{68}$$

where $l=0,1,\ldots,L_v$, and the normalization condition has the form

$$\sum_{l=0}^{L_m}\int_0^{R_m}\psi_l^2(r)dr=1. \tag{69}$$

Here

$$Q_{ll_1}(r)=\sum_{l_2=0}^{L_v}W_{ll_1l_2}(V_{1l_2}(r)-V_{2l_2}(r)), \tag{70}$$

$$S_l(r)=\sum_{l_1=0}^{L_m}\sum_{l_2=0}^{L_m}W_{ll_1l_2}\psi_{l_1}(r)\psi_{l_2}(r), \tag{71}$$

$$W_{ll_1l_2}(r)=2\pi\sqrt{\frac{2l+1}{4\pi}}\sqrt{\frac{2l_1+1}{4\pi}}\sqrt{\frac{2l_2+1}{4\pi}}\times\int_{-1}^{+1}P_l(x)P_{l_1}(x)P_{l_2}(x)dx. \tag{72}$$

Using the asymptotic properties of the solutions (65), we can write down the boundary conditions on the finite interval $0\leqslant r\leqslant R_m$:

$$\psi_{1A}(0)\psi_l'(0)-\psi_{1A}'(0)\psi_l(0)=0, \tag{73}$$

$$\psi_{2A}(R_m)\psi_l'(R_m)-\psi_{2A}'(R_m)\psi_l(R_m)=0, \tag{74}$$

$$V_{i1A}(0)V_{il}'(0)-V_{i1A}'(0)V_{il}(0)=0, \tag{75}$$

$$V_{i2A}(R_m)V_{il}'(R_m)-V_{i2A}'(R_m)V_{il}(R_m)=0, \tag{76}$$

where

$$\psi_{1A}=A_{1l}r^{l+1},\quad \psi_{2A}=A_{2l}e^{-\sqrt{\lambda}r},\quad V_{11A}=B_{1l}r^{l+1},$$
$$V_{12A}=B_{2l}r^{-l},\quad V_{21A}=C_{1l}r^{l+1},\quad V_{22A}=C_{2l}e^{-Cr},$$

A_{il}, B_{il}, and C_{il} are constants, and $i=1,2$.

The practical application of the CANM to this problem requires the solution of fairly complex systems of (L_m+2L_v+3) nonlinear differential equations at each iteration. A different approach for solving this system was proposed in Ref. 66. By analogy with the splitting method,[67] instead of a system of (L_m+2L_v+3) nonlinear differential equations, it is possible to successively solve simpler problems: the eigenvalue problem for a system of (L_m+1) linear differential equations (66) and $2(L_v+1)$ boundary-value problems for the linear differential equations (67) and (68).

The iteration procedure for solving the problem (66)–(76) has the following sequence of steps.[66]

Having specified some set $\{\lambda^{(0)},\psi_l^{(0)}(r),l=0,1,\ldots,L_m\}$ (the initial approximation), Eq. (71) is used to calculate the coefficients $S_l(r)$ for (67) and (68). Solving (67) and (68) with the boundary conditions (75) and (76), we find $V_{1l}^{(0)}(r)$ and $V_{2l}^{(0)}(r)$. Then, using (70)–(72) we calculate the effective potentials $Q_{ll_1}^{(0)}(r)$. Solving the eigenvalue problem for the system (66) with the boundary conditions (73) and (74), the normalization condition (69), and the obtained potential $Q_{ll_1}^{(0)}(r)$, we obtain new functions

$\{\lambda^{(1)}, \psi_l^{(1)}(r),\ l=0,1,\ldots,L_m\}$, which in turn are used to calculate the solutions $V_{1l}^{(1)}(r)$ and $V_{2l}^{(1)}(r)$ and to construct the effective potential $Q_{ll_1}^{(1)}(r)$ for the next iteration.

This process continues until the eigenvalues and wave functions $\{\lambda^{(k)}, \psi_l^{(k)}(r),\ l=0,1,\ldots,L_m\}$, and also the functions $V_{il}^{(k)}(r)$, $i=1,2$, $l=0,1,\ldots,L_v$ obtained after two successive iterations coincide with each other to within a specified accuracy ϵ, i.e., until the condition

$$\delta \leqslant \epsilon$$

is satisfied, where

$$\delta = \max\{|\lambda^{(k+1)} - \lambda^{(k)}|,$$

$$\max_{r_j \in [0,R_m]} \{ \max_{l \in [0,\ldots,L_v], i=1,2} |V_{il}^{(k+1)}(r_j) - V_{il}^{(k)}(r_j)|,$$

$$\max_{l \in [0,\ldots,L_m]} |\psi_l^{(k+1)}(r_j) - \psi_l^{(k)}(r_j)|\}\}.$$

A similar algorithm was also used in Ref. 64 to find the spherically symmetric solutions.

The iteration method described here can be viewed as a variant of a combination of the buildup method and Newtonian iterations, the theoretical justification of the convergence of which is given in Ref. 26.

This algorithm has also been used successfully to solve a number of other nonlinear problems.

The results of a numerical study of this problem agree with the theoretical results of Ref. 68. The more general case $m \neq 0$ was studied in Ref. 69. In that study we presented the CANM-based algorithm and the results of a numerical study of this system in the strong-coupling limit.

3.2. Self-localized electron states in a liquid

Self-localized electron states in a liquid, the so-called solvated electron, are described[70] by a system of three nonlinear equations:

$$\begin{cases} \xi''(x) - \xi(x) + \xi(x)\dfrac{\eta_1(x) - \eta_2(x)}{x} = 0, \\ \eta_1''(x) + \dfrac{1}{x}\xi^2(x) = 0, \\ \eta_2''(x) - \dfrac{\alpha^2}{d} x \sinh\left(\dfrac{d\eta_2(x)}{x}\right) + \dfrac{b}{x}\xi^2(x) = 0, \end{cases} \tag{77}$$

with boundary conditions

$$\xi(0) = \xi(\infty) = \eta_1(0) = \eta_1'(\infty) = \eta_2(0) = \eta_2(\infty) = 0, \tag{78}$$

where α, b, and d are the parameters of the physical model.

The same system with a linearized final equation $[\sinh(d\eta_2(x)/x) \sim (d\eta_2(x)/x)]$ and the same boundary conditions (78) coincides with the system (60) and was solved in Ref. 58.

Additional constraints between these parameters are proposed in some physical models. In the boundary-value problem (77), (78) the conditions

$$m = \frac{dT_1^2}{5.2629 \cdot 10^2},$$

$$n = m\frac{d\alpha^2}{b \cdot 6.2125 \cdot 10^2} \tag{79}$$

are satisfied, while in the problem (65), (78) the condition

$$b\left(\frac{T_1^2}{\alpha}\right)^2 = 0.84713\frac{m^2}{n} \tag{80}$$

is satisfied, where

$$T_1 = \int_0^\infty \xi^2(x)dx = \eta_1(\infty), \tag{81}$$

$$A_1 = dT_1^2, \quad A_2 = d\alpha^2,$$

m is the effective electron mass, and n is the ion concentration. These parameters m and n are convenient because they are determined from the experimental data.

Thus, with the conditions (79) and (80) the original boundary-value problems depending on three independent parameters can be reduced to boundary-value problems with a single parameter and the auxiliary condition (81) relating the integral condition on one desired function to the asymptotic behavior of the other function.

A similar approach can be used to formulate the boundary-value problem with auxiliary conditions, described in the preceding section.

In the problem of the solvated electron, using the notation $\xi = y_1$, $\eta_1 = y_2$, and $\eta_2 = y_3$, we have the system (77) with the boundary conditions

$$\begin{aligned} &G_{L1} \equiv y_1(0) = 0, \\ &G_{L2} \equiv y_2(0) = 0, \\ &G_{L3} \equiv y^3(0) = 0, \\ &G_{R1} \equiv y_1'(x_R) + y_1(x_R) = 0, \\ &G_{R2} \equiv y_2'(x_R) - C = 0, \\ &G_{R3} \equiv y_3'(x_R) + \sqrt{\frac{A_2}{A_1}} C y_3(x_R) = 0, \end{aligned} \tag{82}$$

approximating the asymptotic conditions (78), and the auxiliary condition

$$Q_1 \equiv \int_0^{x_R} y_1^2(x)dx - C = 0, \tag{83}$$

which in the iteration process leads to the system of linear equations

$$\begin{cases} v_{1k}'' - v_{1k} + \dfrac{y_{2k} - y_{3k}}{x} v_{1k} + \dfrac{v_{2k} - v_{3k}}{x} y_{1k} = -R_1, \\ v_{2k}'' + \dfrac{2}{x} y_{1k} v_{1k} = -R_2, \\ v_{3k}'' - \dfrac{A_2}{A_1} C^2 \cosh\left(\dfrac{A_1 y_{3k}}{C^2 x}\right) v_{3k} + \dfrac{2b}{x} y_{1k} v_{1k} \\ \quad = -R_3 + \mu\left(\dfrac{A_2}{A_1^2} 4C^3 x \sinh\left(\dfrac{A_1 y_{3k}}{C^2 x}\right)\right. \\ \quad \left. - \dfrac{A_2}{A_1} 2C y_3 \cosh\left(\dfrac{A_1 y_{3k}}{C^2 x}\right)\right), \end{cases} \tag{84}$$

with boundary conditions

$$\begin{cases} v_{1k}(0) = -G_{L1}, \\ v_{2k}(0) = -G_{L2}, \\ v_{3k}(0) = -G_{L3}, \\ v'_{1k}(x_R) + v_{1k}(x_R) = -G_{R1}, \\ v_{2k}(x_R) - \mu = -G_{R2}, \\ v'_{3k}(x_R) + \sqrt{\dfrac{A_2}{A_1}} C v_{3k}(x_R) = -G_{R3} - \mu \sqrt{\dfrac{A_2}{A_1}} y_{3k}(x_R) \end{cases} \tag{85}$$

and auxiliary condition

$$2\int_0^{x_R} y_{1k}(x) v_{1k}(x) dx - \mu_k = -Q_1. \tag{86}$$

A detailed description of the algorithm for solving this problem is given in Ref. 46, along with the numerical results.

3.3. The quantum field model of the binucleon in the strong-coupling limit

There have been many studies devoted to the description of the binucleon (a bound state of a neutron and a proton); references to them can be found in the books and reviews dealing with this topic.[71,72] However, this problem remains important, because its solution gives direct information about the nuclear forces.

The basic characteristics of the binucleon were calculated in Ref. 73 using the quantum field model proposed in Ref. 53. According to this approach, the description of the interaction of the nucleons with the meson field in the strong-coupling limit reduces to a system of nonlinear differential equations in three-dimensional space.

According to Ref. 53, the total-energy functional in the quantum field model of the binucleon for the case of a point interaction of the nucleons with scalar and pseudoscalar meson fields has the form

$$\begin{aligned} F = {} & \frac{\hbar^2}{m}\int |\nabla\psi|^2 dV - \frac{g^2}{\pi} \\ & \times \int \frac{e^{-k_s|r-r'|/2}}{|r-r'|} |\psi(r)|^2 |\psi(r')|^2 dV dV' - \tilde{f}^2 \\ & \times \int (\sigma\nabla_r)(\sigma\nabla_{r'}) \frac{e^{-k_{ps}|r-r'|/2}}{|r-r'|} |\psi(r)|^2 \\ & \times |\psi(r')|^2 dV dV', \end{aligned} \tag{87}$$

where k_s is the mass of the scalar meson, k_{ps} is the mass of the pseudoscalar meson, m is the nucleon mass, g and $\tilde{f}$ are the constants describing the interaction with the scalar and pseudoscalar meson fields, σ is the spin operator (a unit vector directed along the z axis), and $\hbar$ is Planck's constant.

From the condition for the functional (87) to be a minimum on the class of functions $\psi(\mathbf{r})$ satisfying the normalization condition

$$\int d\mathbf{r} |\psi(\mathbf{r})|^2 = 1, \tag{88}$$

we obtain the system of equations

$$\begin{cases} \dfrac{\hbar^2}{m}\Delta\psi - \varepsilon\psi + \dfrac{2g^2}{\pi} V_1\psi + 2\tilde{f}^2[(\sigma\nabla_r)V_2]\psi = 0, \\ \Delta V_1 - \left(\dfrac{k_s}{2}\right)^2 V_1 = -4\pi|\psi|^2, \\ \Delta V_2 - \left(\dfrac{k_{ps}}{2}\right)^2 V_2 = -4\pi(\sigma\nabla_r)|\psi|^2. \end{cases} \tag{89}$$

Then, writing

$$V_3 = (\sigma\nabla_r)V_2$$

and setting $\hbar^2 = 1$, we rewrite the system (89) as

$$\begin{cases} \dfrac{1}{m}\Delta\psi - \varepsilon\psi + \dfrac{2g^2}{\pi} V_1\psi + 2\tilde{f}^2 V_3\psi = 0, \\ \Delta V_1 - \left(\dfrac{k_s}{2}\right)^2 V_1 = -4\pi|\psi|^2, \\ \Delta V_3 - \left(\dfrac{k_{ps}}{2}\right)^2 V_3 = -4\pi(\sigma\nabla_r)^2|\psi|^2. \end{cases} \tag{90}$$

Solving this system (90) on the class of functions $\psi(\mathbf{r})$ bounded for $0 < \mathbf{r} < \infty$, and satisfying the normalization condition (88) and the asymptotic conditions

$$\begin{cases} \lim\limits_{r\to 0} \psi(\mathbf{r}) = \text{const}, & \lim\limits_{r\to 0} V_1(\mathbf{r}) = \text{const}, & \lim\limits_{r\to 0} V_3(\mathbf{r}) = \text{const}, \\ \lim\limits_{r\to \infty} \psi(\mathbf{r}) = \text{const}, & \lim\limits_{r\to \infty} V_1(\mathbf{r}) = \text{const}, & \lim\limits_{r\to \infty} V_3(\mathbf{r}) = \text{const}, \end{cases} \tag{91}$$

we can determine the binucleon energy levels ε and wave functions ψ. (Here $r = \sqrt{x^2+y^2+z^2}$.) Then the binucleon radius R and its quadrupole moment Q are calculated from the expressions

$$R = \int d\mathbf{r} r|\psi|^2, \quad Q = \int d\mathbf{r}(3z^2 - r^2)|\psi|^2. \tag{92}$$

Making transformations of the form

$$\mathbf{r} = r_0\bar{\mathbf{r}}, \quad \psi = \gamma\varphi, \tag{93}$$

the system (90) can be rewritten in dimensionless quantities (henceforth the bar over the vector $\bar{\mathbf{r}}$ will be dropped):

$$\begin{cases} \Delta\varphi - \lambda\varphi + (V_1 + BV_3)\varphi = 0, \\ \Delta V_1 - k_1^2 V_1 = -|\varphi|^2, \\ \Delta V_3 - k_2^2 V_3 = -(\sigma\nabla_r)^2|\varphi|^2, \end{cases} \tag{94}$$

where

$$\lambda = \varepsilon m r_0^2, \quad k_1^2 = \left(\frac{k_s}{2}\right)^2 r_0^2, \quad k_2^2 = \left(\frac{k_{ps}}{2}\right)^2 r_0^2,$$

$$B = \frac{\tilde{f}^2}{g^2}\frac{\pi}{r_0^2}, \quad 8g^2 m r_0^4 \gamma^2 = 1. \tag{95}$$

Using the change of variables (93), we rewrite (88), (92), and (87) as

$$\hat{N} = \int d\mathbf{r}|\varphi|^2 = \frac{1}{r_0^3\gamma^2}, \quad R = r_0^4\gamma^2\hat{R}, \quad \hat{R} = \int d\mathbf{r} r|\varphi|^2, \tag{96}$$

$$Q = r_0^5\gamma^2\hat{Q}, \quad \hat{Q} = \int d\mathbf{r}(3z^2 - r^2)|\varphi|^2,$$

$$F=(\varepsilon/\lambda)[(\hat{T}-W_{13}/2)/\hat{N}], \tag{97}$$

where

$$T=r_0\gamma^2\hat{T}, \quad \hat{T}=\int d\mathbf{r}|\nabla\varphi|^2,$$

$$W_{13}=\int d\mathbf{r}(V_1+BV_3)|\varphi|^2. \tag{98}$$

These quantities are related to each other as

$$R=r_0(\hat{R}/\hat{N}), \quad Q=r_0^2(\hat{Q}/\hat{N}). \tag{99}$$

Here the expressions in parentheses are dimensionless.

The system of differential equations for the binucleon (94) represents a nonlinear three-parameter eigenvalue problem. The numerical integration of (94) in the limit $k_{ps}\to\infty$ was performed in Ref. 53. The problem (94) for finite k_{ps} was studied numerically in Ref. 73.

As an example, let us present a formulation of the boundary-value problem for the system (94) in the special case where the solutions are symmetric about an axis, i.e., $\Phi(\rho,z,\phi)\to\Phi(\rho,z)$ (cylindrical coordinates). In addition, we go from a semi-infinite integration range to a finite range ($-z_M\leq z\leq z_M$, $0\leq\rho\leq\rho_M$). Then the description of the binucleon reduces to solving the two-dimensional spectral problem for a system of nonlinear differential equations.

Let us formulate the problem in such a way that it is reduced to a one-dimensional system of equations.

We shall seek a solution of (94) in cylindrical coordinates in the form

$$\begin{cases} \varphi(\rho,z)=\sum_{n=1}^{\infty} y_n(z)\Phi_n(\rho), \\ V_1(\rho,z)=\sum_{n=1}^{\infty} V_{1n}(z)\Phi_{1n}(\rho), \\ V_3(\rho,z)=\sum_{n=1}^{\infty} V_{3n}(z)\Phi_{3n}(\rho), \end{cases} \tag{100}$$

where the eigenvalues and eigenfunctions $\{\mu_n,\Phi_n\}$ are defined as the solutions of the following spectral problem:

$$\begin{cases} \Phi_n''+\frac{1}{\rho}\Phi_n'+\mu_n\Phi_n=0, \quad 0\leq\rho\leq\rho_M, \\ \Phi_n'(0)=0, \quad \Phi_n'(\rho_M)-A_{\rho_M}\Phi_n(\rho_M)=0, \\ \int d\rho\rho\Phi_n^2=1. \end{cases} \tag{101}$$

Here A_{ρ_M} is determined from the expressions

$$A_{\rho_M}=\left.\frac{\frac{d}{d\rho}[\Phi_A(\rho)]}{\Phi_A(\rho)}\right|_{\rho=\rho_M},$$

$$\Phi_A(\rho)=\int_{-z_M}^{z_M} dz y_0(z)\varphi_A(z,\rho).$$

In finding the sets $\{\mu_{1n},\Phi_{1n}\}$ and $\{\mu_{3n},\Phi_{3n}\}$ the function φ_A is replaced by V_{1A} and V_{3A}, respectively, and the function $y_0(z)$ by V_{10} and V_{30}, respectively, where $y_0(z)$, V_{10}, and V_{30} are some initial approximations. In a special case we can use only one set of functions $\{\Phi_n\}$.

Substituting the expansion (100) into the system (94), we find

$$\begin{cases} y_n''-(\lambda+\mu_n)y_n+\sum_{m=1}^{\infty} W_{nm}y_n=0, \quad n=1,2,..., \\ V_{1j}''-(k_1^2+\mu_{1j})V_{1j}=-J_{1j}, \quad j=1,2,..., \\ V_{3j}''-(k_2^2+\mu_{3j})V_{3j}=-J_{3j}, \end{cases} \tag{102}$$

where

$$W_{nm}=\sum_{j=1}^{\infty}[Q_{1njm}V_{1j}+BQ_{3njm}V_{3j}], \tag{103}$$

$$J_{1j}=\sum_{n,m=1}^{\infty} Q_{1njm}y_ny_m, \quad J_{3j}=\sum_{n,m=1}^{\infty} Q_{3njm}\frac{d^2}{dz^2}(y_ny_m), \tag{104}$$

$$Q_{injm}=\int_0^{\rho_M} d\rho\rho\Phi_n(\rho)\Phi_{ij}(\rho)\Phi_{im}(\rho), \quad i=1,3. \tag{105}$$

The functions y_n, V_{1j}, and V_{3j} satisfy the following boundary conditions:

$$\begin{cases} y_n'(z_M)-A(z_M)y_n(z_M)=0, \\ y_n'(-z_M)-A(-z_M)y_n(-z_M)=0, \\ V_{1j}'(z_M)-A_1(z_M)V_{1j}(z_M)=0, \\ V_{1j}'(z_M)-A_1(-z_M)V_{1j}(-z_M)=0, \\ V_{3j}'(z_M)-A_3(z_M)V_{3j}(z_M)=0, \\ V_{3j}'(-z_M)-A_3(-z_M)V_{3j}(-z_M)=0, \end{cases} \tag{106}$$

where

$$A(z_M)=\left.\frac{\frac{d}{dz}[y_A(z)]}{y_A(z)}\right|_{z=z_M},$$

$$y_A(z)=\int_0^{\rho_M} d\rho\rho\Phi_0(\rho)\varphi_A(z,\rho),$$

$$A_1(z_M)=\left.\frac{\frac{d}{dz}[V_{1A}(z)]}{V_{1A}(z)}\right|_{z=z_M},$$

$$V_{1A}(z)=\int_0^{\rho_M} d\rho\rho\Phi_{10}(\rho)V_{1A}(z,\rho),$$

$$A_3(z_M)=\left.\frac{\frac{d}{dz}[V_{3A}(z)]}{V_{3A}(z)}\right|_{z=z_M},$$

$$V_{3A}(z)=\int_0^{\rho_M} d\rho\rho\Phi_{30}(\rho)V_{3A}(z,\rho).$$

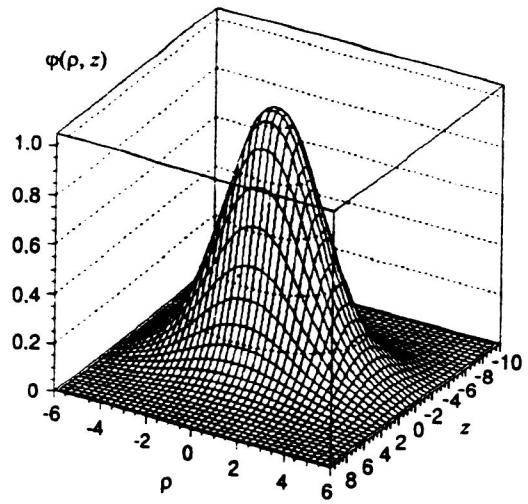

FIG. 1. The binucleon wave function $\varphi(\rho,z)$.

The coefficients $A(-z_M)$, $A_1(-z_M)$, and $A_3(-z_M)$ are defined analogously. The normalization condition for the system (102) takes the form

$$\sum_n \int_{-z_M}^{z_M} dz y_n^2(z) = \frac{1}{2\pi r_0^3 \gamma^2} = \hat{N}_c .$$

Using the expansion (100), Eqs. (96) and (97) for calculating the required physical quantities have the form

$$\hat{R} = 2\pi \int_{-z_M}^{+z_M} dz \int_0^{\rho_M} d\rho\rho \sqrt{(z^2+\rho^2)}\varphi^2(z,\rho), \qquad (107)$$

$$\hat{Q} = 2\pi \int_{-z_M}^{+z_M} dz \int_0^{\rho_M} d\rho\rho (2z^2-\rho^2)\varphi^2(z,\rho), \qquad (108)$$

$$F = (\varepsilon/\lambda)[\hat{T}_c - \hat{W}_c/2]/(2\pi N_c), \qquad (109)$$

where

$$\hat{T}_c = 2\pi \int_{-z_M}^{+z_M} dz \int_0^{\rho_M} d\rho\rho \left[\left| \frac{\partial\varphi^2}{\partial\rho} \right| + \left| \frac{\partial\varphi^2}{\partial z} \right| \right],$$

$$\hat{W}_c = 2\pi \sum_{jnm} \int_{-z_M}^{+z_M} dz [V_{1j}(z) + BV_{3j}(z)] y_n(z) y_m(z).$$

The symmetry of the problem can be used to solve the system (102) on the interval $0 \leq z \leq z_M$. Here it is necessary to change the boundary conditions and the normalization condition accordingly.

This problem was studied numerically in Ref. 73 using a modified CANM-based algorithm similar to the one described in Sec. 3.1.3. As an illustration, in Fig. 1 we show the binucleon wave function $\varphi(\rho,z)$. The calculations showed that the numerical solutions of the two-nucleon system in the limit of strong coupling to the scalar and pseudoscalar fields lead to values of the deuteron binding energy, effective radius, and quadrupole moment consistent with experiment.

We conclude by noting that a system of the form (53) arises in widely different cases of particle–field interactions, for example, the self-localized states of electrons in electrolytes[70,74] and electron states in biological macromolecules,[75,76] in particular, electron transport over large distances in biological systems. Certain nuclear-physics models (the Hartree–Fock and Hartree–Fock–Slater models[77]) also lead to nonlinear self-consistent systems.

A common feature of all these cases and many other problems is the need to solve the nonlinear self-consistent spectral problem. The development of methods for studying self-localized states numerically therefore acquires special importance.

The algorithms and CANM-based programs developed for the above problems are widely applicable and can be used to solve a broad range of nonlinear self-consistent problems.

4. NUMERICAL STUDY OF SEVERAL QUARKONIUM POTENTIAL MODELS USING THE GENERALIZED CANM

The physics programs of experiments at meson factories present the theories of elementary particles with the problem of constructing a model for the unique description of the spectrum and form factors of the interactions of light and heavy mesons. This problem has been solved in several studies[78–83] using a quantum field generalization of the nonrelativistic potential model of one-gluon exchange. The main feature of such an approach is the description of the spontaneous breakdown of chiral symmetry using the Schwinger–Dyson equation. Then the description of the meson spectrum reduces to solving boundary-value problems for the Schwinger–Dyson (SD) and Bethe–Salpeter (BS) equations in three-dimensional form. The SD equation describes the quarks "inside" the meson and allows the use of the same phenomenological potential as in the spectroscopy of heavy quarkonia for calculating the "dynamical" quark mass, which is a measure of the spontaneous breakdown of chiral symmetry for light quarks. The solutions of the BS equation (the eigenvalues and eigenfunctions) are compared with the masses and wave functions of free mesons. Then, by comparing the resulting solutions with the experimental data for the masses and decay constants, one can study the problem of constructing an effective QCD potential independent of the quark flavor. In the limit of heavy quarks the equations of the model become the Schrödinger equation.

In Refs. 79–83 the quark potential model with various phenomenological potentials (like the harmonic oscillator, a linearly growing plus Coulomb potential, and the Richardson potential) was used to describe a broad range of meson masses, wave functions, and leptonic decay constants (F_π and so on). The authors of those studies consider their main result to be the qualitative description of the mass spectra of all mesons represented as a quark–antiquark bound state. In particular, in Ref. 84 a large difference between the ρ- and π-meson masses was obtained in the oscillator-potential approximation as a consequence of the spontaneous breakdown of chiral symmetry, neglecting the quark–antiquark spin–spin interaction, which is usually added to the interaction potential. In addition, in the studies cited above, values of the meson leptonic decay constants (for example, F_π) considerably smaller than the experimental data were obtained.

One difficulty in the numerical study of relativistic potential models (see, for example, Ref. 84) is related to the fact that, as in the nonrelativistic case,[85] the effective potential in those models is usually taken to be a combination of the Coulomb and linear potentials, which leads to divergences in the kernels of the integral equations. In the literature this problem is often solved by the method of "renormalization of the quark wave function inside the meson." Essentially, here the singularities are removed, owing to counterterms introduced into the Hamiltonian. Up to now there has been no self-consistent method of regularizing singularities when the quark is off-shell and is a constituent of the hadron.

Another method of solving the singularity problem is to modify the original potential at the level of the coordinate representation by approximating it by several functions with "good" properties. In particular, several functions approximating the Coulomb and linear potentials are studied in Ref. 86. The properties of these approximations are studied for the example of the nonrelativistic Schrödinger equation and compared with calculations[87] in which the divergence problem is solved in a different way.

From the mathematical point of view, the SD problem is a system of two nonlinear integral equations in three-dimensional momentum space. Its solutions are the quark wave function and energy function, which are used in the BS equation. The statement of the problem includes asymptotic conditions which are imposed by physical arguments on the dynamical quark mass and energy.

The system of BS equations in this model is an eigenvalue problem for a system of linear integral equations in three-dimensional momentum space. The eigenvalues and eigenfunctions of the BS system are physically interpreted as the meson energy levels and wave functions.

Thus, theoretical studies of the quark characteristics using this model lead to the numerical solution of singular boundary-value problems for systems of nonlinear differential, integro-differential, and integral equations. These problems are characterized by a countable set of solutions, which can be used to describe the quark spectra, which, in turn, depend on the physical parameters of the model: the quark mass and charge, and the characteristics of the model potential.

The study of these problems is a complicated numerical task. In general, each of these problems can be viewed as a nonlinear functional equation in B space.[88] The unified approach to the numerical analysis of these problems based on the generalized continuous analog of Newton's method allows the design of efficient numerical methods which maximally take into account the specific features of the particular problem. The algorithms and programs which have been developed have permitted the successful solution of the problem of computing the mass spectra and leptonic decay constants for a number of effective interaction potentials.

For example, the SD and BS equations with the oscillator potential were studied numerically in Ref. 89, and solutions were obtained for the π, π', K, and K' meson spectra. The spectra of pseudoscalar, scalar, vector, and axial-vector mesons were calculated for the same potential in Ref. 90. Numerical solutions of the SD and BS equations were obtained in Ref. 91 for a potential containing oscillator and Coulomb terms. The first successful description of the experimental value of the leptonic decay constant of the pseudoscalar pion was obtained in Ref. 92 using the approximation of the Gaussian potential. A numerical analysis of the modified SD and BS equations using the CANM was performed in Refs. 97–99 for the Yukawa potential, a combination of the oscillator and Gaussian potentials, and also the linear and Coulomb potentials.

The explicit form of these equations depends on the choice of effective potential. Below, we present a general statement of the SD and BS problems within this approach. We shall give the forms of potentials popular in meson spectroscopy, and also discuss methods for the numerical study of these problems on the basis of the generalized CANM.

4.1. The Schwinger–Dyson equation

The system of SD equations for a given potential $V(|\mathbf{p}-\mathbf{q}|)$ has the form[83]

$$\begin{cases} E(p)\cos(2v(p))=m_0 \\ \quad +\dfrac{1}{2}\displaystyle\int d\mathbf{q}V(|\mathbf{p}-\mathbf{q}|)\cos(2v(q))/(2\pi)^3, \\ E(p)\sin(2v(p))=p \\ \quad +\dfrac{1}{2}\displaystyle\int d\mathbf{q}V(|\mathbf{p}-\mathbf{q}|)\xi\sin(2v(q))/(2\pi)^3, \end{cases} \tag{110}$$

where the integration runs over the three-dimensional space of coordinates of the vector $\mathbf{q}$, $\xi=(\mathbf{p}/p,\mathbf{q}/q)$ is the scalar product of three-dimensional unit vectors, m_0 is a given constant (the quark current mass), and $E(p)$ and $v(p)$ are respectively the quark energy and wave function, which must be found.

After the integration over angles $\Omega\mathbf{q}$, the system (110) takes the form

$$\begin{cases} E(p)\cos(2v(p))=m_0+I_1(p), \\ E(p)\sin(2v(p))=p+I_2(p), \end{cases} \tag{111}$$

where

$$I_1(p)=\int_0^\infty dqV_1(p,q)\cos(2v(q)),$$

$$I_2(p)=\int_0^\infty dqV_2(p,q)\sin(2v(q)), \tag{112}$$

$$V_1(p,q)=\frac{1}{2}\frac{1}{(2\pi)^3}q^2\int d\Omega V(|\mathbf{p}-\mathbf{q}|),$$

$$V_2(p,q)=\frac{1}{2}\frac{1}{(2\pi)^3}q^2\int d\Omega\xi V(|\mathbf{p}-\mathbf{q}|). \tag{113}$$

The solutions of the system of equations (111)–(113) depend both on the form of the potential, and on the asymptotic behavior of the functions $V_1(p,q)$ and $V_2(p,q)$ for

$$p\to 0, \quad q=\text{const} \ (\text{or } q\to 0, \quad p=\text{const}),$$

$$p\to\infty, \quad q=\text{const} \ (\text{or } q\to\infty, \quad p=\text{const}),$$

$|p-q|\to 0$.

In addition, from physical considerations the functions $I_1(p)$ and $I_2(p)$ must satisfy certain asymptotic conditions for $p\to 0$ and $p\to\infty$:

$$\lim_{p\to\infty} I_1=0,\quad \lim_{p\to\infty} I_2=0,\quad \lim_{p\to 0} I_1=\text{const}<\infty,$$

$$\lim_{p\to 0} I_2=\text{const}<\infty. \tag{114}$$

This imposes constraints on the class of allowed potentials.

As already mentioned, for some of the potentials used in hadron spectroscopy the integrals $I_1(p)$ and $I_2(p)$ have divergences at asymptotically small and large momenta. To eliminate these, for a set of selected potentials some authors have proposed that the system (111) be replaced by a system of so-called renormalized equations (a trick often used in perturbation theory):

$$\begin{cases} E(p)\cos(2v(p))=m_0(1-Z_m)+I_1(p), \\ E(p)\sin(2v(p))=p(1-Z)+I_2(p), \end{cases}$$

where

$$Z_m=\text{const}<\infty,\quad Z=\text{const}<\infty.$$

By choosing Z_m and Z, for some potentials it is possible to satisfy the requirements (114) imposed on the system (111). Several authors have suggested that the constants Z_m and Z be replaced by specially selected functions $Z_m(p)$ and $Z(p)$. These questions are discussed, in particular, in Refs. 80–82.

A more general approach to modifying the system (111) is the following. While preserving the form of the SD system, we introduce into (112) the new functions $f_1(p,q)$ and $f_2(p,q)$:

$$\begin{cases} I_1(p)=\int_0^\infty dq V_1(p,q)\cos(2v(q))f_1(p,q), \\ I_2(p)=\int_0^\infty dq V_2(p,q)\sin(2v(q))f_2(p,q). \end{cases} \tag{115}$$

For different choices of the functions f_1 and f_2 we obtain different modifications of the SD equation. For example, taking

$$f_1=\frac{\cos(2v(p))-m_0/\sqrt{p^2+m_0^2}}{\cos(2v(p))},$$

$$f_2=\frac{\sin(2v(p))-1}{\sin(2v(p))},$$

we obtain the system of SD equations studied in Ref. 81. For $f_1\equiv 1$ and $f_2\equiv 0$ we have one of the modifications of the SD equation studied in Ref. 92, and so on. Another possibility is to choose the functions f_1 and f_2 to be analytic solutions of the Schrödinger equation with the corresponding potential, or to be functions of the form $p^a\exp(-bp)$ or $cp^a/(p^a+1)^b$, and so on, where $a\geq 0$, $b\geq 1$, and $c>0$. Since the solutions $E(p)$ and $v(p)$ of the system (111), (113), and (115) describe not free quarks, but quarks in a bound state ("inside" the meson), the choice of functions f_1 and f_2 can be related not only to the solutions of the SD system, but also to the solutions $U_1(p)$ and $U_2(p)$ of the BS equation, i.e., $f_1=f_1(p,U_1(p))$ and $f_2=f_2(p,U_2(p))$. In this case the SD and BS equations must be solved as a single system of equations. Here we shall not discuss the physical justification for replacing the system (111)–(113) by the system (111), (113), and (115), or the specific choice of the functions f_1 and f_2. The criteria specifying the form of these functions in this case are the correct asymptotic behavior of the solutions, the absence of divergences in the integrals I_1 and I_2, and also the qualitative and quantitative description of the characteristics of mesons as bound states of a quark and antiquark.

The system of SD equations therefore reduces to the boundary-value problem for the system of nonlinear equations (111), (113), and (115) with the boundary values

$$\lim_{p\to 0} v(p)=0,\quad \lim_{p\to\infty} v(p)=\pi/4,\quad \lim_{p\to 0} E(p)=\text{const},$$

$$\lim_{p\to\infty} E(p)=p.$$

4.2. The Bethe–Salpeter equation

Let us consider the BS equation for pseudoscalar mesons consisting of quarks of various masses:[83]

$$ML_{\binom{2}{1}}(\mathbf{p})=E_t(p)L_{\binom{1}{2}}(\mathbf{p})-\int\frac{d\mathbf{q}}{(2\pi)^3}V(|\mathbf{p}-\mathbf{q}|)\times[C_p^{(-)}C_q^{(+)}+\xi S_p^{(-)}S_q^{(+)}]L_{\binom{2}{1}}(\mathbf{q}), \tag{116}$$

where

$$C_p^{(-)}=\cos(v_1(p)\pm v_2(p)),\quad S_p^{(-)}=\sin(v_1(p)\pm v_2(p)),$$

v_1, v_2 and E_1, E_2 are the solutions of the SD equation for a quark and antiquark with current masses m_{01} and m_{02}, respectively, $E_t(p)=E_1(p)+E_2(p)$ is the total meson energy, M is the eigenvalue (the mass of the bound state), and $L_{\binom{1}{2}}$ are the wave functions. The normalization condition has the form

$$\frac{4N_C}{M}\int\frac{d\mathbf{q}}{(2\pi)^3}L_1(\mathbf{q})L_2(\mathbf{q})=1, \tag{117}$$

where $N_C=3$ is the quantum number. These solutions of the system (116) can be used to calculate the leptonic decay constants of pseudoscalar mesons:

$$F_\pi=\frac{4N_C}{M}\int\frac{d\mathbf{q}}{(2\pi)^3}L_2(\mathbf{q})\cos(v_1(q)+v_2(q)). \tag{118}$$

We shall seek solutions of (116) in the form of an expansion in spherical harmonics $Y_{lm}(\theta,\phi)$:

$$L_{\binom{2}{1}}(\mathbf{p})=\frac{1}{p}\sum_{l,m}U_{\binom{2}{1}lm}(p)Y_{lm}(\theta,\phi). \tag{119}$$

In the spherically symmetric case ($l,m=0$), writing for brevity $U_{\binom{2}{1}00}=U_{\binom{2}{1}}$ we find

$$MU_{\binom{2}{1}}(p)=E_t(p)U_{\binom{1}{2}}(p)-2\int_0^\infty dq[C_p^{(\bar{+})}C_q^{(\bar{+})}\hat{V}_1(p,q)$$

$$+S_p^{(\bar{+})}S_q^{(\bar{+})}\hat{V}_2(p,q)]U_{\binom{1}{2}}(q), \quad (120)$$

$$\frac{4N_C}{M}\frac{1}{(2\pi)^3}\int_0^\infty dqU_1(q)U_2(q)=1, \quad (121)$$

where

$$\hat{V}_1(p,q)=\frac{p}{q}V_1(p,q), \quad \hat{V}_2(p,q)=\frac{p}{q}V_2(p,q),$$

and $V_1(p,q)$ and $V_2(p,q)$ are given by (113).

The expression for the leptonic decay constant takes the form

$$F_\pi=\frac{4N_C}{M}\frac{1}{(2\pi)^3}\sqrt{4\pi}\int_0^\infty dqqU_2(q)\cos(v_1(q)$$

$$+v_2(q)). \quad (122)$$

The solutions of (120) must satisfy the asymptotic conditions

$$\lim_{p\to 0}U_{\binom{1}{2}}(p)=0, \quad \lim_{p\to\infty}U_{\binom{1}{2}}(p)=0. \quad (123)$$

We have thus obtained the eigenvalue problem for the system (120) with the normalization condition (121) and boundary conditions (123). We again note that the expressions defining the BS problem involve the solutions (v_1,E_1) and (v_2,E_2) of the SD system for two quark masses m_{01} and m_{02}.

4.3. The interaction potentials

In this section we present the most commonly used effective interaction potentials and discuss methods of numerically solving the SD and BS problems with these potentials.

4.3.1. The Gaussian and Yukawa potentials

The Gaussian potential is usually used for simplifying a model (see, for example, Refs. 92 and 93). The coordinate representation of this potential is

$$V_G=v_g\exp(-\mu^2r^2)+C, \quad (124)$$

where C is a constant and $v_g>0$ and $\mu>0$ are parameters. The momentum representation of this potential is

$$V(|\mathbf{p}-\mathbf{q}|)=\frac{v_g}{(\sqrt{\pi})^3}R^3\exp(-R^2|\mathbf{p}-\mathbf{q}|^2)$$

$$+C(2\pi)^3\delta(|\mathbf{p}-\mathbf{q}|),$$

$$R=\mu/2. \quad (125)$$

The potential corresponding to the difference of two Yukawa potentials has the coordinate and momentum forms

$$V=\frac{\alpha}{r}\{\exp(-\mu_1r)-\beta\exp(-\mu_2r)\}+C, \quad (126)$$

TABLE I. $m_{01}=m_{02}=0.01$.

h	M (Gaussian potential) $\beta=3$	M (Yukawa potential) $\mu_1=0.001$, $\mu_2=5$, $\alpha=1.8$
0.100	0.192851	0.461893
0.050	0.202286	0.463275
0.025	0.201669	0.463363
$\sigma_M=\frac{M_h-M_{h/2}}{M_{h/2}-M_{h/4}}$	15.17	15.71

$$V(\mathbf{p}-\mathbf{q})=4\pi\alpha\left\{\frac{1}{\mu_1^2+|\mathbf{p}-\mathbf{q}|^2}-\frac{\beta}{\mu_2^2+|\mathbf{p}-\mathbf{q}|^2}\right\}$$

$$+C(2\pi)^3\delta(|\mathbf{p}-\mathbf{q}|), \quad (127)$$

where α, μ_1, μ_2, and C are the potential parameters. For $\beta=0$ we have only a single Yukawa potential. Obviously, for $\beta=0$ and $\mu_1r\ll 1$ the potential becomes similar to the Coulomb potential. The difference of two Yukawa potentials ($\beta=1$) for $\mu_1\ll\mu_2$ can be viewed as a method of regularizing the Coulomb potential in the ultraviolet region ($|\mathbf{r}-\mathbf{q}|^2\gg\mu_2^2$).

The renormalized system (111), (113), and (115) with the potential (124), (125) for $f_1\equiv 1$ and $f_2\equiv 0$ was solved in Ref. 94 using a modified Newtonian algorithm.[95] By means of simple transformations, the problem was reformulated as a nonlinear integral equation determining the quark mass function:

$$m(p)=m_0+\int_0^\infty dqV(q,p)m(q)/\sqrt{m^2(q)+q^2}), \quad (128)$$

where

$$V(p,q)=\alpha_g\frac{p}{q}[\exp(-\beta_g(p^2+q^2))\sinh(2\beta_gpq)], \quad (129)$$

and α_g and β_g are parameters.

The SD problem was solved in Refs. 92 and 97 by the iteration process described in Ref. 92. The numerical results obtained by solving the SD equation in this way agree with the results for Eqs. (128) and (129) obtained by using the modified Newtonian iteration scheme described in Ref. 95.

The BS system (120) for the potentials (124), (125) and (126), (127) is an eigenvalue problem for two linear integral equations with the normalization condition (121). It was solved numerically using the program package SYSINT (SYSINTM),[96] designed to solve the eigenvalue problem for a system of linear integral equations using modified iteration schemes based on the generalized CANM. The integrals were calculated using the quadratic Simpson's rule, which gives the order of the approximation $O(h^4)$, as confirmed by numerical experiments with a sequence of successively finer grids with argument step h, $h/2$, $h/4$ (see Table I).

4.3.2. The oscillator and Gaussian potentials

The oscillator potential, with coordinate and momentum representations

$$V_O(r)=-v_0r^2,$$

$$V_O(|\mathbf{p}-\mathbf{q}|)=-(2\pi)^3v_0\Delta_{\mathbf{p}}\delta(|\mathbf{p}-\mathbf{q}|), \tag{130}$$

is often used as a linear approximation to simplify a model (Refs. 80, 89–91, and 98). As was shown in Refs. 89 and 90, the SD equation can be reduced to a nonlinear differential equation of the form

$$\psi''(p)+2\psi'(p)/p-2p\sin\psi(p)+\sin 2\psi(p)/p^2+2m_0 -2\cos\psi(p)=0 \tag{131}$$

with the boundary conditions

$$\psi(0)=\pi/2, \quad \psi(\infty)=m_0/\sqrt{p^2+m_0^2}.$$

In the studies cited above, Eq. (131) was studied numerically using Newton's iteration scheme. A modification of the problem (131) allowing a more accurate description of some experimental characteristics was studied in Ref. 98. It was also solved using the CANM.

Let us consider a more general case, namely, a combination of the oscillator and Gaussian potentials:

$$V=V_G+V_O, \quad V_G=v_g\exp(-\mu^2r^2)+C, \quad V_O=-v_0r^2. \tag{132}$$

The momentum representation of (132) has the form

$$V(|\bar p-\bar q|)=\frac{v_g}{(\sqrt{\pi})^3}R^3\exp(-R^2|\bar p-\bar q|^2)+C(2\pi)^3 \times\delta(|\bar p-\bar q|)-v_0(2\pi)^3\Delta_{\bar p}\delta(|\bar p-\bar q|),$$

$$R=1/(2\mu). \tag{133}$$

Equations (112) take the form

$$\begin{cases}\tilde I_1=\left[(\sin(\phi(\bar p)))''+\dfrac{2}{p}(\sin(\phi(\bar p)))'\right]+\tilde J_1,\\ \tilde I_2=\left[(\cos(\phi(\bar p)))''+\dfrac{2}{p}(\cos(\phi(\bar p)))'-\dfrac{2}{p^2}\cos(\phi(\bar p))\right] +\tilde J_2,\end{cases}$$

where

$$J_1=\hat\alpha\int_0^\infty dqV_1(p,q)\cos(2v(q)),$$

$$J_2=\hat\alpha\int_0^\infty dqV_2(p,q)\sin(2v(q)), \tag{134}$$

$$V_1=R\frac{q}{p}[\exp(-R^2(p^2+q^2))\sinh(2R^2pq)], \tag{135}$$

$$V_2=\frac{1}{2}\frac{1}{Rp^2}\{\exp(-R^2(p^2+q^2))[2R^2pq\cosh(2R^2pq) -\sinh(2R^2pq)]\}. \tag{136}$$

The system (115), (134)–(136) was studied numerically in Ref. 99. In this case the SD equation reduces to a nonlinear boundary-value problem for a single integro-differential equation [for $V_g=0$ and $f_1\equiv f_2\equiv 1$ we obtain the differential equation (131)]. This problem was solved numerically using the modified Newtonian algorithm studied in Ref. 63.

The statement of the problem (120) for the potential (132) has the form of an eigenvalue problem for a system of two linear integro-differential equations:

$$MU_{\binom{2}{1}}(p)+U''_{\binom{1}{2}}(p)+W_{\binom{1}{2}}(p)U_{\binom{1}{2}}(p) =-2\int_0^\infty dq[C_p^{(-)}C_q^{(+)}\hat V_1(p,q) +S_p^{(-)}S_q^{(+)}\hat V_2(p,q)]U_{\binom{1}{2}}(q), \tag{137}$$

with normalization condition (121), where

$$W_1=-\left\{E_t+\frac{1}{4}(\phi_1'+\phi_2')^2+\frac{2}{p^2}\cos^2\left(\frac{\phi_1+\phi_2}{2}\right)\right\}, \tag{138}$$

$$W_2=-\left\{E_t+\frac{1}{4}(\phi_1'-\phi_2')^2+\frac{2}{p^2}\sin^2\left(\frac{\phi_1-\phi_2}{2}\right)\right\}, \tag{139}$$

$$\phi_i=-2v_i+\pi/2, \quad i=1,2.$$

The problem (137), (138) was solved in Ref. 99 using the CANM modification proposed in Ref. 63. The program package[24] SLIPS2 was used for the case $V_g=0$, where the equations of the system become differential equations.

4.3.3. A combination of the Coulomb and linear potentials

The coordinate representation of a combination of Coulomb and linear potentials has the form

$$V(r)=-\alpha_c\frac{1}{r}+\sigma r, \tag{140}$$

where α_c and σ are parameters. In momentum space we have

$$V(|\bar p-\bar q|)=-\alpha_c\frac{4\pi}{|\bar p-\bar q|^2}-\sigma\frac{8\pi}{|\bar p-\bar q|^4}. \tag{141}$$

Using the identity

$$\frac{1}{|\bar p-\bar q|^4}=\frac{1}{6}\Delta_p\frac{1}{|\bar p-\bar q|^2}, \tag{142}$$

the system (115) can be rewritten as

$$\begin{cases}E(p)\cos(2v(p))=m_0+I_{1K}+I_{1L}\\ E(p)\sin(2v(p))=p+I_{2K}+I_{2L},\end{cases}$$

where

$$\bar\alpha=-\frac{\alpha_c}{2\pi}, \quad \bar\sigma=-\frac{\sigma}{\pi}, \quad I_{1C}=\frac{\bar\alpha\hat I_{1C}}{p},$$

$$I_{2C}=\frac{\bar\alpha\hat I_{2C}}{p}, \quad I_{1L}=\frac{\bar\sigma\hat I''_{1C}}{2p}, \quad I_{2L}=\frac{\bar\sigma}{2p}\left[\hat I''_{2C}-\frac{2\hat I_{2C}}{p^2}\right],$$

TABLE II. The interval [0,6.], $m_0=0.1$, $\bar{\alpha}=0.1$, $\bar{\sigma}=0.1$.

h	M	$U_1(0.6)$	$U_2(0.6)$
0.100	1.7691	7.8183	6.6219
0.050	1.7744	7.7721	6.6048
0.025	1.7757	7.7761	6.6005
	$\frac{M_h-M_{h/2}}{M_{h/2}-M_{h/4}}=4.16$	$\frac{(U_{1,h}-U_{1,h/2})}{U_{1,h/2}-U_{1,h/4}}=4.05$	$\frac{U_{2,h}-U_{2,h/2}}{U_{2,h/2}-U_{2,h/4}}=3.94$

$$\begin{cases} \hat{I}_{1C}(p)=\int_0^\infty dqq\ln\left|\frac{p+q}{p-q}\right|\cos(2v(q))f_1(p,q), \\ \hat{I}_{2C}(p)=\int_0^\infty dqq\left[-1+\frac{p^2+q^2}{2pq}\ln\left|\frac{p+q}{p-q}\right|\right] \\ \qquad \times\sin(2v(q))f_2(p,q). \end{cases}$$

This system was solved numerically in Ref. 100 using the algorithm described in Ref. 92.

In Ref. 100 it was also shown that the BS equation for the potential (140)–(141) can be reduced to a system of the form

$$\begin{cases} V_{13}(p)U_1''(p)+V_{12}(p)U_1'(p)+V_{11}(p)U_1(p) \\ \quad -MU_2(p)-2J_{12}(U_1,U_2,p)=0, \\ V_{23}(p)U_2''(p)+V_{22}(p)U_1'(p)+V_{21}(p)U_2 \\ \quad -MU_1(p)-2J_{22}(U_1,U_2,p)=0, \end{cases} \tag{143}$$

where the functions J_{12} and J_{22} depend nonlinearly on the eigenfunctions U_1 and U_2.

The system (143) was solved numerically in Ref. 100 by developing a modified Newtonian scheme similar to the algorithm proposed in Ref. 66, combining the CANM with the method of successive approximations. The numerical scheme was realized using a uniform grid in the argument p with step h and has second-order convergence, as confirmed by calculations on a sequence of grids smaller by a factor of two. These results are presented in Table II.

4.3.4. Analysis of the numerical results

The SD and BS equations were studied numerically in Refs. 92, 97, 99, and 100 for various forms of the effective potentials. Results were obtained for the pion as a bound state of a quark and an antiquark having nonzero current masses.

Since, as mentioned above, in some studies by various authors the calculated values of the leptonic decay constants did not agree with the existing experimental data, the goal of these calculations was to try to describe the experimental value of the leptonic decay constant F_π for the ground state of the pseudoscalar pion.

Therefore, the criterion for choosing the free parameters of the model was chosen to be the experimental value of the ratio of the pion mass and leptonic decay constant, $M_\pi/F_\pi \sim 1.04$. The parameters and the modified SD system satisfying this experimental value were found for each of the potentials listed above.

In particular, in Ref. 92 it was shown for the first time that there is a scheme for renormalizing the solutions of the SD problem which allows the value of F_π to be described within this class of models.

The parameters fixed according to this criterion were also used to calculate radially excited states of the pion. However, for this method of choosing the model parameters the energy levels of radially excited states turned out to be lower than the experimental values given in Ref. 101. The exception was the oscillator potential,[83] for which the energies of the radially excited states significantly exceed the experimental data.

4.4. Generalization of a QCD-inspired model to the case of finite temperatures

The generalization of the SD and BS equations to the case of finite temperature and baryon density proposed in Refs. 93 and 102 is interesting from the viewpoint of solving the important problem of describing hot, dense hadronic matter (the quark–gluon plasma).[103] Since up to now[104,105] this problem has mainly been studied using the Nambu–Jona-Lasinio model,[106] which is equivalent to a separable approximation[107] of the equations, comparison of the results from numerically solving the full system of SD and BS equations with the results obtained in the separable approximation is useful for analyzing the validity of the theoretical model.

Such a study was performed in Ref. 108. As in Refs. 92 and 93, the model was simplified by taking the effective potential to be a Gaussian.

In the formulation of the problem, the inclusion of the temperature dependence leads to the appearance of an additional equation for the chemical potential. As a result, as was shown in Ref. 109, the SD problem takes the form of a system of three nonlinear integral equations in three-dimensional momentum space:

$$\begin{cases} E(p)\cos(2v(p))=m_0+\frac{1}{2}\int d\mathbf{q}V(|\mathbf{p}-\mathbf{q}|) \\ \qquad \times[1-f(q)-\bar{f}(q)]\cos(2v(q))/(2\pi)^3, \\ E(p)\sin(2v(p))=p+\frac{1}{2}\int d\mathbf{q}V(|\mathbf{p}-\mathbf{q}|)\xi[1-f(q) \\ \qquad -\bar{f}(q)]\sin(2v(q))/(2\pi)^3, \end{cases} \tag{144}$$

$$\mu(p)=\mu_0+\frac{1}{2}\int d\mathbf{q}V(|\mathbf{p}-\mathbf{q}|)[f(q)-\bar{f}(q)]/(2\pi)^3, \tag{145}$$

where

$$f(p)=\frac{1}{1+\exp[\beta_T(E(p)-\mu(p))]},$$

$$\bar{f}(p)=\frac{1}{1+\exp[\beta_T(E(p)+\mu(p))]}. \tag{146}$$

As in Sec. 4.1, the integration runs over three-dimensional momentum space, $\xi=(\mathbf{p}/p,\mathbf{q}/q)$ is the scalar product of three-dimensional unit vectors, $\beta_T=1/T$, T is the temperature, and $E(p)$, $v(p)$, and $\mu(p)$ are respectively the

quark energy, wave function, and chemical potential, which must be found. The quark current mass m_0 and the initial chemical potential μ_0 are treated as given parameters of the model.

After integrating over angles $\Omega\mathbf{q}$, changing to dimensionless quantities, and performing some algebra, we obtain the system

$$\begin{cases} \cot(2v(p))=\dfrac{m_0+I_1(p)}{p+I_2(p)}, \\ E(p)=\dfrac{1}{2}C[1-f(p)-\bar{f}(p)]+[m_0+I_1(p)] \\ \qquad \times\cos(2v(p))+[p+I_2(p)]\sin(2v(p)), \\ \mu(p)=\mu_0(p)+\dfrac{1}{2}C[f(p)-\bar{f}(p)] \\ \qquad +\displaystyle\int_0^\infty dqV_1(p,q)[f(q)-\bar{f}(q)], \end{cases} \tag{147}$$

where

$$I_1=\int_0^\infty dqV_1(p,q)[1-f(q) -\bar{f}(q)]\cos(2v(q))f_1(p,q),$$

$$I_2=\int_0^\infty dqV_2(p,q)[1-f(q) -\bar{f}(q)]\sin(2v(q))f_2(p,q),$$

$$\begin{cases} V_1=R\dfrac{q}{p}\exp\left(-R^2\left(p^2+q^2\right)\right)\sinh\left(2R^2pq\right), \\ V_2=\dfrac{1}{2}\dfrac{1}{Rp^2}\exp\left(-R^2\left(p^2+q^2\right)\right)\left[2R^2pq\cosh\left(2R^2pq\right)\right. \\ \qquad \left.-\sinh\left(2R^2pq\right)\right]. \end{cases} \tag{148}$$

Let us now turn to the BS problem. As was shown in Ref. 109, in the case of unequal quark current masses for pseudoscalar mesons, the BS equation has the form of the eigenvalue problem for a system of four integral equations:

$$(E^{\binom{N}{A}}(p)-M)L^{\binom{N}{A}}_{\binom{2}{1}}(\mathbf{p})=\alpha^{\binom{N}{A}}_{\binom{+}{-}}\int\frac{d\mathbf{q}}{(2\pi)^3}V(|\mathbf{p}-\mathbf{q}|)[c_p^{\binom{-}{+}}c_q^{\binom{-}{+}} +\xi c_p^{\binom{-}{+}}c_q^{\binom{+}{-}}]L^{\binom{N}{A}}_{\binom{1}{2}}(\mathbf{q}), \tag{149}$$

where

$$c_p^{\binom{+}{-}}=\cos(v_1(p)\pm v_2(p)), \quad s_p^{\binom{+}{-}}=\sin(v_1(p)\pm v_2(p)),$$

$$\alpha^{\binom{N}{A}}_{\binom{+}{-}}=(a_+^{\binom{N}{A}}\pm a_-^{\binom{N}{A}})/2, \quad E^{\binom{N}{A}}=E_1\pm E_2,$$

$$a_+^N=1-f_1-\bar{f}_2, \quad a_-^N=1-\bar{f}_1-f_2,$$

$$a_+^A=f_2-f_1, \quad a_-^A=\bar{f}_2-\bar{f}_1,$$

$$f_i=\frac{1}{1+\exp[\beta_T(E_i-\mu_i)]}, \quad \bar{f}_i=\frac{1}{1+\exp[\beta_T(E_i+\mu_i)]},$$

$i=1,2,$

v_1, v_2, E_1, E_2, and μ_1, μ_2 are the solutions of the SD equation and the chemical potentials for the quark and antiquark with given current masses m_{01} and m_{02}, M is the eigenvalue (the mass of the bound state), and $L^{\binom{N}{A}}_{\binom{1}{2}}$ are the wave functions.

The normalization condition has the form

$$\frac{N_C}{M}\int\frac{d\mathbf{q}}{(2\pi)^3}\left(\frac{(L_1^N(\mathbf{q})+L_2^N(\mathbf{q}))^2}{a_+^N}-\frac{(L_1^N(\mathbf{q})-L_2^N(\mathbf{q}))^2}{a_-^N} -\frac{(L_1^A(\mathbf{q})+L_2^A(\mathbf{q}))^2}{a_+^A}+\frac{(L_1^A(\mathbf{q})-L_2^A(\mathbf{q}))^2}{a_-^A}\right)=1. \tag{150}$$

According to Ref. 109, the leptonic decay constants can be calculated using the obtained solutions with the expression

$$F_\pi=\frac{4N_C}{M}\int\frac{d\mathbf{q}}{(2\pi)^3}(L_2^N(\mathbf{q})\cos(v_1(q)+v_2(q)) -L_2^A(\mathbf{q})\sin(v_1(q)+v_2(q))). \tag{151}$$

For the spherically symmetric case, going to the finite integration range $[0,p_M]$, we obtain the eigenvalue problem for a system of four linear integral equations.

When the quark current masses are equal, $m_{01}=m_{02}$, the BS system simplifies somewhat and reduces to the eigenvalue problem for a system of two integral equations.

These equations were solved numerically by using the algorithms and programs described in Ref. 92 and substantially modified to take into account the particular features of this problem. The SD problem was solved by the method of simple iterations. The BS system was solved by using the SYSINT (SYSINTM) program.[96] Since the introduction of additional parameters—the temperature and chemical potential—makes the problem more complicated, it was solved successfully by the method of continuation in a parameter,[3] which allows the solutions obtained for other parameters of the problem to be used as the initial approximation.

In Table III we give some of the results of the calculations for a sequence of grids smaller by a factor of two. These results show that the numerical scheme has $O(h^4)$ convergence, corresponding to the order of the numerical approximation of the problem.

The solutions of the SD and BS problems for several parameter values are shown in Figs. 2–4. The qualitative

TABLE III. $m_{01}=m_{02}=0.1$, $T=0.1$, $\mu_0=1$.

h	M	$U_1(1.96)$	$U_2(1.96)$
0.07	0.5150346	0.6175460E-02	0.5610517E-0.2
0.035	0.5150543	0.6176788E-02	0.5611749E-02
0.0175	0.5150554	0.6176862E-02	0.5611821E-02
	$\dfrac{M_h-M_{h/2}}{M_{h/2}-M_{h/4}}=17.9$	$\dfrac{U_{1,h}-U_{1,h/2}}{U_{1,h/2}-U_{1,h/4}}=17.9$	$\dfrac{U_{2,h}-U_{2,h/2}}{U_{2,h/2}-U_{2,h/4}}=17.1$

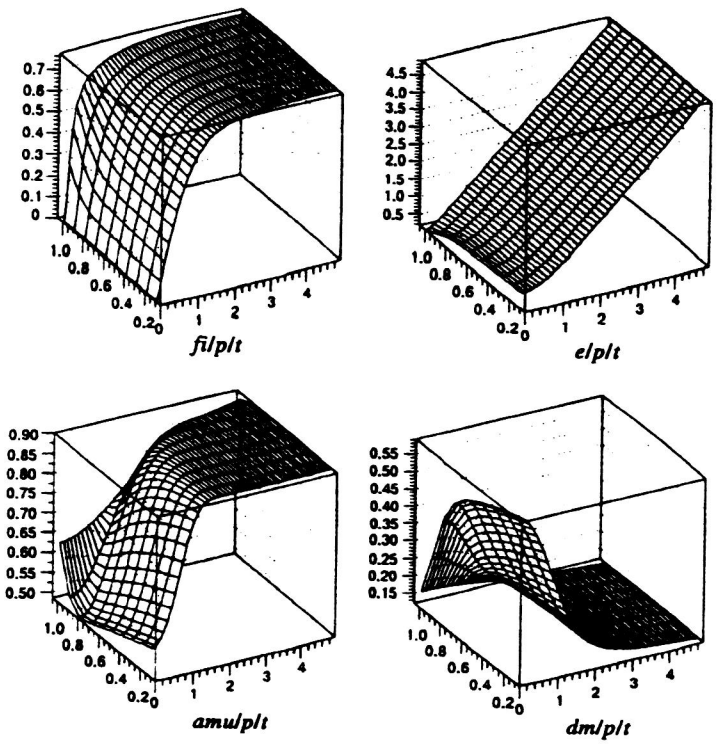

FIG. 2. Dependence of the solutions of the SD equation on the temperature T and momentum p $[v(T,p)=fi/p/t,\ E(T,p)=e/p/t,\ \mu(T,p)=amu/p/t,$ and $m(T,p)=E(T,p)\cos(2v(T,p))=dm/p/t]$ for quark current mass $m_0=0.1$ and initial chemical potential $\mu_0=0.9$ for $I_2=0$.

behavior of the solutions of these problems using the modified system ($I_2\equiv 0$) are similar to the results obtained in Ref. 109 for the Nambu–Jona-Lasinio model.

The program which has been developed can be used to find solutions for various values of the model parameters (the quark mass, the temperature, and the initial value of the chemical potential). Therefore, additional conditions are required for determining the solutions of interest in physics studies.

It should also be noted that this approach to solving these problems and its software implementation can be used for the numerical analysis of theoretical models with potentials of a different form (for example, Yukawa potentials).

Numerical investigation of the SD and BS equations with different types of potential shows that this approach can be used to obtain a quantitative description of some of the available experimental data. For example, the use of a combination of Coulomb and linear potentials allows satisfactory

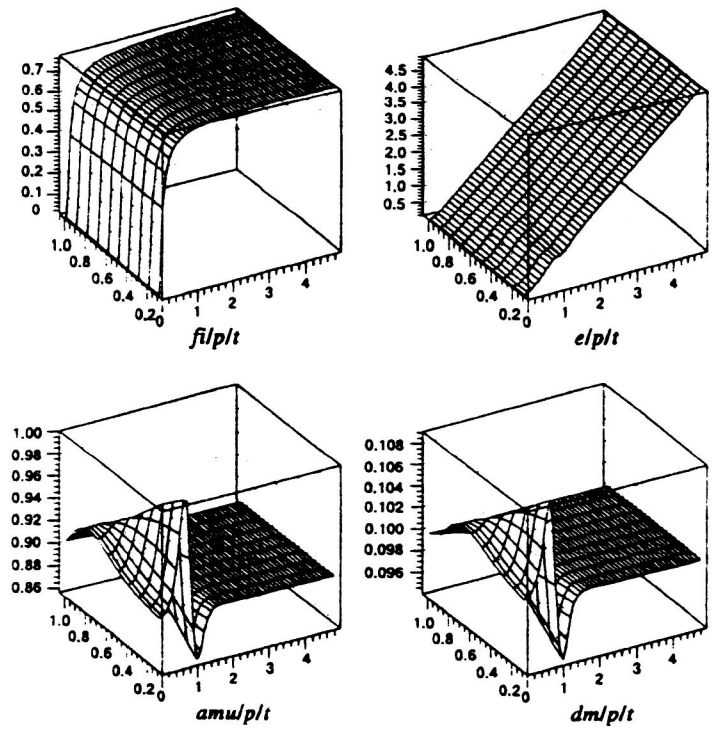

FIG. 3. Dependence of the solutions of the SD equation on the temperature T and momentum p $[v(T,p)=fi/p/t,\ E(T,p)=e/p/t,\ \mu(T,p)=amu/p/t,$ and $m(T,p)=E(T,p)\cos(2v(T,p))=dm/p/t]$ for quark current mass $m_0=0.1$ and initial chemical potential $\mu_0=0.9$ for the unmodified system ($I_2\neq 0$).

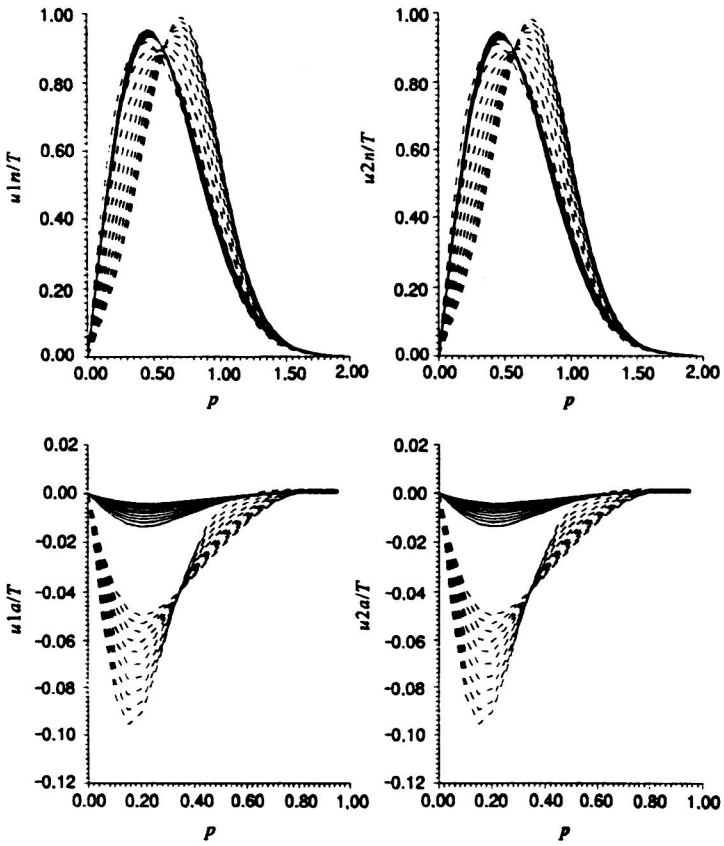

FIG. 4. Wave functions of the BS equations as a function of temperature $T=0.1(0.1)1$, for quark current masses $m_{01}=0.8$, $m_{02}=0.4$, and $\mu_0=1$ for $I_2=0$ (solid lines) and $I_2\neq 0$ (dashed lines).

description of the mass spectra and leptonic decay constants of heavy quarkonia. The oscillator potential can be used to describe the mass spectra of both heavy and light quarkonia. The possibility of correctly describing the decay constant for the pion ground state was demonstrated in Ref. 92 for the example of the Gaussian potential. Similar results have been obtained for the Yukawa potential and a combination of oscillator and Gaussian potentials.

The numerical studies which have been performed for systems of nonlinear equations, including the singular boundary-value and spectral problems, have demonstrated the effectiveness of computational schemes constructed on the basis of the generalized continuous analog of Newton's method. The broad possibilities offered by such schemes have been demonstrated for the SD and the BS problems, neglecting the temperature dependence, and also for the generalization of these equations to the case of nonzero temperature and baryon density.

The analysis of these results can serve as the foundation for the further development and experimental verification of the theoretical approaches which are used.

5. CONCLUSION

In this review we have systematically described the computational techniques used to study problems arising in several quantum field models and QCD potential models. The unified basis for the development of these techniques is a generalization of the continuous analog of Newton's method, which represents a qualitatively new development of the CANM based on combining the ideas of perturbation theory and parameter evolution. We have shown that this approach can be used to construct efficient iteration schemes with optimal step size which allow inversion of the regular part of the linear derivative operator at each iteration step, or which allow this inversion to be avoided altogether. We have justified the convergence of these iteration schemes and discussed their relation to several other existing methods.

We have presented the results of numerical studies of models of the polaron, the bipolaron, the solvated electron, and QCD potential models with various types of potential.

We have thus demonstrated the existence of an efficient numerical method for studying a large class of nonlinear models in theoretical physics.

The CANM has been developed at the JINR over more than thirty years, and it is still a viable approach. This is because it is closely related to practical problems in the mathematical modeling of physical processes, which continually impose new requirements on the method and provide new ideas which stimulate its development.

*Work performed with the financial support of the Russian Fund for Fundamental Research, Grant No. 97-01-01040.

[1] E. P. Zhidkov, G. I. Makarenko, and I. V. Puzynin, Fiz. Élem. Chastits At. Yadra **4**, 127 (1973) [Sov. J. Part. Nucl. **4**, 53 (1973)].
[2] T. Kato, *Perturbation Theory for Linear Operators*, 2nd ed. (Springer-Verlag, Berlin, 1976) [Russ. transl. of 1st ed., Mir, Moscow, 1972].
[3] J. M. Ortega and W. C. Rheinboldt, *Iterative Solution of Nonlinear Equations in Several Variables* (Academic Press, New York, 1970) [Russ. transl., Mir, Moscow, 1975].
[4] D. F. Davidenko, Ukr. Mat. Zh. **7**, No. 1, 18 (1955) [in Russian].

[5] D. A. Kirzhnits and N. G. Takibaev, Yad. Fiz. **25**, 700 (1977) [Sov. J. Nucl. Phys. **25**, 370 (1977)].
[6] G. I. Marchuk, *Splitting Methods* [in Russian] (Nauka, Moscow, 1988).
[7] G. I. Marchuk and V. V. Shaĭdurov, *Raising the Accuracy of Solutions of Difference Schemes* [in Russian] (Nauka, Moscow, 1979).
[8] L. Aleksandrov, Diff. Uravneniya **13**, 1281 (1977) [in Russian].
[9] *Parallel Processing Systems*, edited by D. J. Evans (Cambridge University Press, Cambridge, 1982) [Russ. transl., Mir, Moscow, 1985].
[10] E. K. Blum and A. F. Chang, J. Inst. Math. Appl. **22**, 29 (1978).
[11] L. Bracci and G. Fiorentini, Phys. Rep. **86**, 169 (1982).
[12] I. V. Puzynin and S. I. Vinitsky, J. Muon Catalyzed Fusion **3**, 307 (1988).
[13] V. V. Ermakov and N. N. Kalitkin, Zh. Vychisl. Mat. Mat. Fiz. **21**, 491 (1981) [USSR Comput. Math. and Math. Phys.].
[14] K. A. Lebedev, Zh. Vychisl. Mat. Mat. Fiz. **36**, No. 3, 6 (1996) [Russ. Comput. Math. and Math. Phys.].
[15] I. D. Rodionov, *Author's Abstract of Doctoral Dissertation*, JINR, Dubna (1987) [in Russian].
[16] M. K. Gavurin, Izv. Vyssh. Uchebn. Zaved. Fiz. **5**, No. 6, 18 (1958) [in Russian].
[17] L. A. Kivistik, Dokl. Akad. Nauk SSSR **136**, 22 (1961).
[18] T. Zhanlav and I. V. Puzynin, Zh. Vychisl. Mat. Mat. Fiz. **32**, 846 (1992) [USSR Comput. Math. and Math. Phys.].
[19] I. V. Puzynin, Candidate's Dissertation, JINR, Dubna (1969) [in Russian].
[20] I. V. Puzynin, Doctoral Dissertation, JINR, Dubna (1978) [in Russian].
[21] I. V. Puzynin, T. P. Puzynina, and T. A. Strizh, Report R11-87-332, JINR, Dubna (1987) [in Russian].
[22] P. G. Akishin and I. V. Puzynin, Report 5-10992, JINR, Dubna (1977) [in Russian].
[23] J. H. Wilkinson, *The Algebraic Eigenvalue Problem* (Clarendon Press, Oxford, 1965) [Russ. transl., Nauka, Moscow, 1970].
[24] T. P. Puzynina, Report R11-89-728, JINR, Dubna (1989) [in Russian].
[25] T. A. Strizh, Candidate's Dissertation, JINR, Dubna (1988) [in Russian].
[26] T. Zhanlav and I. V. Puzynin, Zh. Vychisl. Mat. Mat. Fiz. **34**, No. 2, 175 (1994) [Russ. Comput. Math. and Math. Phys.].
[27] N. S. Bakhvalov, *Numerical Methods: Analysis, Algebra, Ordinary Differential Equations* (Mir, Moscow, 1977) [Russ. original, Nauka, Moscow, 1976].
[28] A. A. Samarskiĭ, *Theory of Difference Schemes* [in Russian] (Nauka, Moscow, 1980).
[29] I. M. Glazman, *Direct Methods of Qualitative Spectral Analysis of Singular Differential Operators* [in Russian] (Fizmatgiz, Moscow, 1963).
[30] L. V. Kantorovich, Usp. Mat. Nauk **11**, No. 6, 90 (1956) [Russ. Math. Surveys].
[31] T. Zhanlav and I. V. Puzynin, Zh. Vychisl. Mat. Mat. Fiz. **31**, No. 1, 3 (1992) [USSR Comput. Math. and Math. Phys.].
[32] S. I. Vinitskiĭ, L. I. Ponomarev, I. V. Puzynin, and T. P. Puzynina, Report R4-10942, JINR, Dubna (1977) [in Russian].
[33] S. I. Vinitskiĭ, A. D. Gocheva, and I. V. Puzynin, Report R11-81-837, JINR, Dubna (1981) [in Russian]; Reports R11-82-314, R11-82-315, JINR, Dubna (1982) [in Russian].
[34] S. I. Vinitskiĭ, I. V. Puzynin, and Yu. S. Smirnov, Report R11-91-327, JINR, Dubna (1991) [in Russian].
[35] T. Zhanlav, I. V. Puzynin, and Yu. S. Smirnov, Report R11-90-501, JINR, Dubna (1990) [in Russian].
[36] S. I. Vinitskiĭ, I. V. Puzynin, and Yu. S. Smirnov, Yad. Fiz. **52**, 1176 (1990) [Sov. J. Nucl. Phys. **52**, 746 (1990)].
[37] T. Zhanlav, I. V. Puzynin, and A. V. Rakitskiĭ, Report R11-88-823, JINR, Dubna (1988) [in Russian].
[38] T. L. Boyadzhiev, T. Zhanlav, and I. V. Puzynin, Report R11-89-423, JINR, Dubna (1989) [in Russian].
[39] L. Aleksandrov, Zh. Vychisl. Mat. Mat. Fiz. **11**, No. 1, 36 (1970) [USSR Comput. Math. and Math. Phys.].
[40] I. V. Puzynin, I. V. Amirkhanov, T. P. Puzynina, and E. V. Zemlyanaya, JINR Rapid Commun. **62**, 63 (1993).
[41] D. F. Davidenko, Dokl. Akad. Nauk SSSR **131**, 500 (1960).
[42] W. Holbrow, R. Hass, R. Kalaba, and E. Zagustin, Report, Univ. of Southern California, Los Angeles (1972).
[43] N. N. Kalitkin, *Numerical Methods* [in Russian] (Nauka, Moscow, 1978).
[44] J. M. Ortega, *Introduction to Parallel and Vector Methods of Solving Linear Systems* [Russ. transl., Mir, Moscow, 1991].
[45] R. G. Airapetyan and I. V. Puzynin, Comput. Phys. Commun. **102**, 97 (1997).
[46] I. V. Amirkhanov, I. V. Puzynin, and T. A. Strizh, Report R11-91-454, JINR, Dubna (1991) [in Russian].
[47] *Perspectives of Polarons*, edited by G. N. Chuev and V. D. Lakhno (World Scientific, Singapore, 1996).
[48] Yu. A. Firsov, *Polarons* [in Russian] (Nauka, Moscow, 1975).
[49] V. D. Lakhno, in *Polarons and Applications*, edited by V. D. Lakhno (Wiley, Chichester, 1994), p. 5.
[50] I. V. Amirkhanov, I. V. Puzynin, T. A. Strizh *et al.*, in *Excited Polaron States in Condensed Media*, edited by V. D Lakhno (Manchester University Press, Manchester, 1991).
[51] J. Luttinger and Ch. Y. Lu, Phys. Rev. B **21**, 4251 (1980).
[52] A. K. Pikaev, *The Solvated Electron in Radiation Chemistry* [in Russian] (Nauka, Moscow, 1969).
[53] V. D. Lakhno, Teor. Mat. Fiz. **100**, 219 (1994) [Theor. Math. Phys. (USSR)].
[54] S. I. Pekar, Report AEC-tr-5575, U.S. Atomic Energy Commission (1963) [Russ. original, Gostekhizdat, Moscow, 1951].
[55] N. N. Bogolyubov, Usp. Mat. Nauk **2**, 3 (1950) [in Russian].
[56] S. J. Mijake, J. Phys. Soc. Jpn. **38**, 181 (1975).
[57] L. I. Komarov, E. V. Krylov, and E. D. Feranchuk, Zh. Vychisl. Mat. Mat. Fiz. **18**, 681 (1978) [USSR Comput. Math. and Math. Phys.].
[58] I. V. Amirkhanov, I. V. Puzynin, C. Rodriguez *et al.*, Report R11-85-445, JINR, Dubna (1985) [in Russian]; I. V. Amirkhanov, V. D. Lakhno, I. V. Puzynin *et al.*, in *Proceedings of the Eighth Intern. Workshop of Nonlinear Evolution Equations and Dynamical Systems, NEEDS'92*, Dubna, 1992 (World Scientific, Singapore, 1993), p. 406.
[59] R. P. Feynman, Phys. Rev. **97**, 660 (1955).
[60] Y. Lu and Ch. K. Shen, Phys. Rev. B **26**, 4707 (1982).
[61] I. V. Amirkhanov, V. D. Lakhno, I. V. Puzynin *et al.*, Preprint NTsBI, USSR Academy of Sciences, Pushchino (1988) [in Russian]; in *Excited Polaron States in Condensed Media* [in Russian] (NTsBI, USSR Academy of Sciences, Pushchino, 1990), p. 70.
[62] I. V. Amirkhanov, E. V. Zemlyanaya, and T. P. Puzynina, Report R11-91-87, JINR, Dubna (1991) [in Russian].
[63] F. A. Gareev, S. A. Goncharov, E. P. Zhidkov *et al.*, Zh. Vychisl. Mat. Mat. Fiz. **17**, 407 (1977) [USSR Comput. Math. and Math. Phys.].
[64] I. V. Amirkhanov, E. V. Zemlyanaya, and T. P. Puzynina, Report R11-91-139, JINR, Dubna (1991) [in Russian].
[65] N. L. Balabaev and V. D. Lakhno, Preprint ONTI NTsBN, USSR Academy of Sciences, Pushchino (1970) [in Russian].
[66] I. V. Amirkhanov, I. V. Puzynin, T. P. Puzynina, and E. V. Zemlyanaya, Preprint E11-92-205, JINR, Dubna (1992); in *Polarons and Applications*, edited by V. D. Lakhno (Wiley, Chichester, 1994), p. 445.
[67] G. I. Marchuk, *Methods of Numerical Mathematics*, 2nd ed. (Springer-Verlag, New York, 1985) [Russ. original, Nauka, Moscow, 1989].
[68] R. R. Gabdullin, Preprint NTsBI, USSR Academy of Sciences, Pushchino (1991) [in Russian]; Dokl. Ross. Akad. Nauk **333**, No. 1, 23 (1993) [Phys. Dokl. **38**, 452 (1993)].
[69] P. G. Akishin, I. V. Puzynin, and Yu. S. Smirnov, Zh. Vychisl. Mat. Mat. Fiz. **36**, No. 7, 109 (1996) [Russ. Comput. Math. and Math. Phys.].
[70] V. D. Lakhno and O. V. Vasil'ev, Chem. Phys. **153**, 147 (1991); Phys. Lett. A **152**, 300 (1991).
[71] T. Ericson and W. Weise, *Pions and Nuclei* (Clarendon Press, Oxford, 1988).
[72] G. E. Brown and A. D. Jackson, *The Nucleon–Nucleon Interaction* (North-Holland, Amsterdam, 1976).
[73] I. V. Amirkhanov, E. V. Zemlyanaya, V. D. Lakhno *et al.*, Mat. Modelirovanie **9**, No. 8, 52 (1997) [in Russian]; I. V. Amirkhanov, V. D. Lakhno, I. V. Puzynin *et al.*, in *Proceedings of the Third Intern. Symp. Dubna Deuteron 95*, Dubna, 1995, E2-96-100, JINR, Dubna (1996), p. 58; I. V. Amirkhanov, I. V. Puzynin, T. P. Puzynina *et al.*, in *Proceedings of the Ninth Intern. Conf. on Computational Modeling and Computing in Physics*, Dubna, 1996, D5,11-97-112, JINR, Dubna (1997), p. 48; I. V. Amirkhanov, I. V. Puzynin, T. P. Puzynina *et al.*, in *Perspectives of Polarons*, edited by G. N. Chuev and V. D. Lakhno (World Scientific, Singapore, 1996), p. 229.
[74] I. V. Amirkhanov, I. V. Puzynin, T. Strizh *et al.*, Preprint ONTI NTsBI, USSR Academy of Sciences, Pushchino (1990) [in Russian].
[75] G. N. Chuev and V. D. Lakhno, J. Theor. Biol. **163**, 51 (1993).
[76] V. D. Lakhno and G. N. Chuev, Biofizika **42**, No. 3, 313 (1997) [in Russian].
[77] D. R. Hartree, *The Calculation of Atomic Structures* (Wiley, New York, 1957) [Russ. transl., IL, Moscow, 1960].
[78] Yu. L. Kalinovskiĭ, W. Kallies, B. N. Kuranov *et al.*, Yad. Fiz. **49**, 1709 (1989) [Sov. J. Nucl. Phys. **49**, 1059 (1989)].
[79] S. Goldrey and N. Isgur, Phys. Rev. D **32**, 189 (1985); A. Le Yaouanc,

L. Oliver, P. Pene, and J. C. Raynal, Phys. Rev. D **29**, 1233 (1984); **31**, 137 (1985); S. L. Adler and A. S. Davis, Nucl. Phys. B **224**, 469 (1984); P. J. de A. Bicudo and J. E. F. T. Ribeiro, Phys. Rev. D **42**, 1611 (1990).
[80] A. Kocic, Phys. Rev. D **33**, 1785 (1986); D. W. McKay, H. J. Munczek, and B.-L. Young, Phys. Rev. D **37**, 195 (1988).
[81] A. Trzupek, Acta Phys. Pol. B **20**, No. 2, 93 (1989).
[82] R. Alkofer and P. A. Amundsen, Nucl. Phys. B **306**, 305 (1988).
[83] Yu. L. Kalinovsky, W. Kallies, L. Kaschluhn *et al.*, Fortschr. Phys. **38**, 333 (1990); Few-Body Syst. **10**, 87 (1991); R. Horvat, D. Keker, D. Klabučar, and D. Palle, Phys. Rev. D **44**, 1585 (1991).
[84] F. Gross, Phys. Rev. B **6**, 125 (1968); F. Gross and J. Milane, Phys. Rev. D **43**, 2401 (1991); **45**, 969 (1992); V. G. Kadyshevsky, Nucl. Phys. B **6**, 125 (1968); R. H. Thompson, Phys. Rev. D **1**, 110 (1970).
[85] A. A. Bykov, I. M. Dremin, and A. V. Leonidov, Usp. Fiz. Nauk **143**, 3 (1984) [Sov. Phys. Usp. **27**, 321 (1984)].
[86] I. V. Amirkhanov, E. V. Zemlyanaya, I. V. Puzynin *et al.*, Preprint R11-96-449, JINR, Dubna (1996) [in Russian]; Mat. Modelirovanie **9**, No. 10, 111 (1997) [in Russian]; I. V. Amirkhanov, I. V. Puzynin, T. P. Puzynina *et al.*, in *Proceedings of the Ninth Intern. Conf. on Computational Modeling and Computing in Physics*, Dubna, 1996, D5,11-97-112, JINR, Dubna (1997), p. 40.
[87] K. H. Maung, D. E. Kahana, and J. W. Norbury, Phys. Rev. D **47**, 1183 (1993).
[88] I. V. Amirkhanov, I. V. Puzynin, T. P. Puzynina *et al.*, in *Lecture Notes in Computer Science, Proceedings of the First Intern. Workshop on Numerical Analysis and Applications WNAA '96*, Rousse, Bulgaria, 1996, edited by L. Vulkov, J. Wasniewski, and P. Yalamov (Springer-Verlag, New York, 1997), p. 9.
[89] I. V. Amirkhanov, O. M. Zhuraev, W. Kallies *et al.*, Report R11-88-506, JINR, Dubna (1988) [in Russian]; I. V. Amirkhanov, O. M. Juraev, V. N. Pervushin *et al.*, Commun. E11-91-108, JINR, Dubna (1991).
[90] I. V. Amirkhanov, O. M. Juraev, V. N. Pervushin *et al.*, Preprint E2-90-414, JINR, Dubna (1990); I. V. Amirkhanov, O. M. Zhuraev, V. N. Pervushin *et al.*, Report R11-91-111, JINR, Dubna (1991) [in Russian].
[91] I. V. Amirkhanov, T. Z. Nasirov, and N. A. Sarikov, Report R11-93-173, JINR, Dubna (1993) [in Russian].
[92] I. V. Amirkhanov, E. V. Zemlyanaya, V. N. Pervushin *et al.*, Preprint R11-94-74, JINR, Dubna (1994); Mat. Modelirovanie **6**, No. 7, 55 (1994) [in Russian].
[93] D. Blaschke, Yu. L. Kalinovsky, V. N. Pervushin *et al.*, Z. Phys. A **346**, 85 (1993).
[94] E. V. Zemlyanaya, Candidate's Dissertation, JINR, Dubna (1994) [in Russian].
[95] I. V. Puzynin, I. V. Amirkhanov, T. P. Puzynina, and E. V. Zemlyanaya, JINR Rapid Commun. 5[62]-93, JINR, Dubna (1993), p. 63; in *Proceedings of the Intern. Conf. on Programming and Mathematical Techniques in Physics*, JINR, Dubna, 1993, edited by Yu. Yu. Lobanov and E. P. Zhidkov (World Scientific, Singapore, 1994), p. 30.
[96] E. V. Zemlyanaya, Report R11-94-120, JINR, Dubna (1994) [in Russian].
[97] I. V. Amirkhanov, Kh. F. Davlatov, E. V. Zemlyanaya *et al.*, Report R11-94-523, JINR, Dubna (1994) [in Russian].
[98] I. V. Amirkhanov, T. Z. Nasirov, V. N. Pervushin, and N. A. Sarikov, Report R11-94-406, JINR, Dubna (1994) [in Russian].
[99] I. V. Amirkhanov, V. N. Pervushin, I. V. Puzynin *et al.*, Commun. E11-94-509, JINR, Dubna (1994).
[100] I. V. Amirkhanov, E. V. Zemlyanaya, I. V. Puzynin *et al.*, Preprint R11-95-8, JINR, Dubna (1995) [in Russian]; Mat. Modelirovanie **7**, No. 7, 34 (1995) [in Russian].
[101] Particle Data Group, Phys. Rev. D **45**, 11 (1992); D. V. Amelin *et al.*, in *Proceedings of the Conf. Hadron-93*, Como, Italy, 1993.
[102] Yu. L. Kalinovsky and C. Weiss, Z. Phys. C **63**, 275 (1994).
[103] F. Karsch, in *Quark–Gluon Plasma*, edited by R. C. Hwa (World Scientific, Singapore, 1990), p. 61.
[104] M. K. Volkov, Ann. Phys. (N.Y.) **157**, 282 (1984).
[105] S. P. Klevansky, Rev. Mod. Phys. **64**, 649 (1992); Yu. L. Kalinovsky, L. Kaschluhn, and V. N. Pervushin, Phys. Lett. B **231**, 288 (1989).
[106] Y. Nambu and G. Jona-Lasinio, Phys. Rev. **122**, 345 (1961);**124**, 246 (1961); M. K. Volkov, Ann. Phys. (N.Y.) **157**, 282 (1957); D. Ebert and H. Reinhardt, Nucl. Phys. B **27**, 188 (1986); Yu. L. Kalinovsky, L. Kaschluhn, and V. N. Pervushin, Phys. Lett. B **231**, 288 (1989); Fortschr. Phys. **38**, 353 (1990).
[107] W. Kallies, V. N. Pervushin, and N. A. Sarikov, Preprint E9-94-42, JINR, Dubna (1994).
[108] I. V. Amirkhanov, E. V. Zemlyanaya, V. N. Pervushin *et al.*, Preprint R11-95-325, JINR, Dubna (1995); Mat. Modelirovanie **9**, No. 3, 73 (1997) [in Russian].
[109] S. Schmidt, D. Blaschke, and Yu. L. Kalinovsky, Phys. Rev. C **50**, 435 (1994).

Translated by Patricia A. Millard