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Power Series Solution of Coupled Differential Equations in One Variable

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A precise method for solving systems of coupled ordinary differential equations of second order in one variable is presented. The method consists mostly of algebraic manipulations and is very efficient on vector computers. The method is applied to the solution of the three-body Schrödinger equation. Besides giving, in contrast to variational methods, uniformly precise expectation values of operators including the Hamiltonian, the method allows one to study the analytic structure of the wave function. Applications to the He atom, the muonic helium atom, and the μdt molecular ion are presented. No extended precision intermediate calculations are required. © 1996 Academic Press, Inc.

1. INTRODUCTION

The problem of integrating a system of coupled ordinary differential equations in one variable (ODE) arises frequently in various branches of physics. A well-known example is the reduction of the Schrödinger equation to partial waves for noncentral or spin-dependent potentials. A particular example is the few-body problem. In the three-body problem, the wave function in the center-of-mass system of coordinates is a function of six coordinates. The potential in the simplest case is a function of three variables, the distances between pairs of particles. A reparametrization of the coordinates and subsequent expansion of the wave function on an orthonormal set of functions of five ''angular'' coordinates results in an infinite set of coupled differential equations in one variable. These are truncated to a finite dimension which is then a parameter.

Numerical solvers of such systems capable of high precision are based on the Adams modification of the predictor–corrector method, or the Gear version for stiff equations [1]. These routines work with vector solutions.

In this paper we present an algebraic method of integrating systems of coupled differential equations with a regular singular point at the origin. The method represents the solution on small intervals of the independent variable, z, by matrix Taylor series; on the first interval, at $z = 0$, a modified series in z is used. The coefficients of the ODE are expanded in matrix Laurent series around $z = 0$. The solution on each interval is obtained via recurrence relations. A small number of powers of z is required.

All expansions are analytically correct which means that the accuracy of the solution depends only on the accuracy of the numerical operations, which are mostly algebraic and can therefore be well controlled. This in turn enables a separate study of the dependence of results on external parameters.

It is important, at least for the applications described in this paper, to have the solution in the form of series coefficients and not in the form of a function table. A series may be manipulated for the calculation of integrals with integrands including the solution and its derivatives with respect to external parameters, because it allows easy and numerically reliable calculation of the derivatives. The point density in numerical integration can be prescribed independently, whereas with a function table interpolation may be necessary, introducing additional errors.

It is highly desirable that the method be realizable in the usual double precision (64-bit) arithmetic. This allows the many array operations to utilize optimization (vectorization) of most machines as much as possible.

The aim of this paper is to present the numerical aspects of the solution of the ODE and to describe typical physical applications of the method.

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In Section 2, the analytical aspects of the method are presented, and in Section 3 its numerical realization is given. Section 4 describes the application of the method to precise calculations in the few-body problem. Section 5 describes the intrinsic accuracy of the solution of the ODE as a function of the parameters of the method and the accuracy of observables in the physical applications in relation to the intrinsic accuracy.

2. ALGEBRAIC METHOD

2.1. Introduction

In this paper we shall limit ourselves to equations which have one regular singular point (at the origin). Equations of this type are the Schrödinger and related equations. These equations are reducible to the Sturm–Liouville form and are self-adjoint. We shall not assume self-adjointness, however, because in some applications this property may be removed by manipulation of equations, as in our examples in Section 4. The general derivations are given in Refs. [2, 3].

2.2. Analytical Form of the Solution

We shall treat homogeneous ODE of the general form

$$\chi''(z) + P(z)\chi'(z) + Q(z)\chi(z) = 0, \tag{1}$$

where P and Q are $N \times N$ matrices. Regular singularity implies that zP and z^2Q be representable by power series in z (around $z = 0$). Equation (1) has $2N$ linearly independent vector solutions of dimension N. These solutions constitute the fundamental solution (FS) of the ODE. ODE of second order are preferred over a system of double size and first-order equations [3].

The ansatz for a solution at the origin ($z = 0$) is [2, 3],

$$X_1 = z^S z^\Lambda \sum_{n=0}^{\infty} C_{1n} z^n, \quad C_{10} = I, \tag{2}$$

where S is an upper triangular matrix and Λ is a matrix solution of the matrix indicial equation

$$\Lambda^2 + (P_{-1} - I)\Lambda + Q_{-2} = 0.$$

The recurrence relations for C_{1n} are derived in Ref. [3]. Note that ($\alpha, \beta = 1, ..., N$)

$$\lim_{z\to 0} \frac{1}{z^2} (X_1)_{\alpha\beta} = \delta_{\alpha 1}\delta_{\beta 1}.$$

The general solution is

$$\chi = X_1^{(1)} a + X_1^{(2)} b, \tag{3}$$

where $X_1^{(1)}$ and $X_1^{(2)}$ are of the form (2) and correspond to the two solutions of the indicial equation; a, b are vectors determined from boundary conditions. Usually $b = 0$ because of the regularity requirement, and

$$\lim_{z\to 0} \frac{1}{z^2} \chi_\alpha = \delta_{\alpha 1} a_1.$$

2.3. The Algebraic Method

The form (3) solves a large class of numerical problems, but not all, as follows.

The series (2) was used initially [3, 4] to solve the ground state of the He atom, using the secular equation $\det A = 0$, where A is the coefficient matrix of the unphysically increasing part of the asymptotic form of $X_1^{(1)}$ in Eq. (3). This was found not to be accurate enough [5]. The reason is twofold: (i) very large powers of z (of the order of 100) had to be used; (ii) the expansion (2) is unstable at large z against admixtures of the unphysically increasing solution.

(Recent modifications proposed in Ref. [6] may make the series (2) more tractable for numerical work by replacing the power-type expansion basis with a generalized Laguerre polynomial basis.)

Further, in applications there might be numerical difficulties associated with imposing boundary conditions, or the series (2) might not converge with sufficient numerical precision on a large enough interval.

Lack of precise boundary conditions might require as a first step, for example, the generation of the matrix FS. With a numerical integrator working with vector solutions to first-order systems, this would entail repeating N times the numerical integration of a $2N$-dimensional system.

The method described in the present paper enables the solution of these problems by the following basic idea [5]:

(i) it represents the solution on a small interval $[0, z_F)$ at the origin by the matrix series (2), but for $z > z_F$ the solution is represented by Taylor series on subintervals $[z_i, z_{i+1})$, $i = 2, 3, 4, ...$; $z_1 = 0$, $z_2 = z_F$.

(ii) the solution in the matrix form is propagated across interval boundaries. Depending on the properties of the ODE, the propagation may have to be done from z_F to a matching point, $z_M > z_F$, and from a large z, $z = z_U$, towards z_M.

The matrix Taylor series for the solution on the ith interval is

$$X_i(z) = \sum_{n=0}^{\infty} C_{in}(z - z_i)^n \tag{4}$$

and leads to the recurrence relations

$$C_{in} = -\frac{1}{n(n-1)} \left[\sum_{m=-1}^{n-2} (n-m-2)\mathcal{P}_{i,m+1} + \sum_{m=0}^{n-2} \mathcal{Q}_{im} \right] C_{i,n-m-2}, \tag{5}$$

where $\mathcal{P}$ and $\mathcal{Q}$ are defined by

$$P = \sum_{m=0}^{\infty} \mathcal{P}_{im}(z - z_i)^m,$$
$$Q = \sum_{m=0}^{\infty} \mathcal{Q}_{im}(z - z_i)^m. \tag{6}$$

If the boundary condition at $z = z_U$ is known exactly, the solution will be meaningful for all $z < z_U$. If not, z_U is to be taken large enough such that the increasing solution which is present in the initial approximation at $z = z_U$ dies out sufficiently at some $z < z_U$ which is large enough for the problem at hand.

Continuity of the solution and its derivative gives the joining equations

$$\chi_i(z_i) = C_{i0} = \chi_{i-1}(z_i),$$
$$\chi_i'(z_i) = C_{i1} = \chi_{i-1}'(z_i). \tag{7}$$

The present method can be very easily adapted to particular problems. This is discussed in Section 3.1.

The above method is appealing from the numerical standpoint: it reduces the integration of the ODE to algebraic manipulations of matrices. It can therefore be efficiently vectorized. (Presently, a very efficient vectorized code is being used.) The parallelization of the code has not yet been attempted.

3. NUMERICAL METHOD

3.1. Implementation of the Algebraic Method

We shall describe the implementation suited for equations of the Schrödinger type. Many cases would require simpler algorithms using only part of the presented material. The method of Section 2.3 eliminates large powers of z. In the Schrödinger type problems, the unphysically increasing parts of the solution are still present. (The ODE are only stable in one direction.) To solve the ODE, one has to start the propagation both from $z = 0$ and from a large $z = z_U$. Matching of the solution at some intermediate $z = z_M$ then yields a set of nonlinear equations for the optimization of an external parameter of the ODE, in this case the total energy, E.

Note that in the method it is not necessary to evaluate $X_1(0)$ at any time, thus allowing for irregular solutions.

Not only does the propagation in the reverse direction eliminate the unwanted parts of the solution, it enables one to specify approximate boundary conditions at $z = z_U$ as well. In the latter case the propagation must start at z_U which is appropriately larger than the z values of interest.

Another difficulty appears in the Schrödinger type problems. If X_i denotes the matrix solution of the form (4) on the ith interval, we have

$$\chi_i(z) = X_i(z)V_i,$$

where V_i is a constant vector. The connection equations (7) are equivalent to

$$X_i^{-1}(z_i)X_{i-1}(z_i)V_{i-1} = V_i,$$
$$(R_i(z_i) - R_{i-1}(z_i))X_{i-1}(z_i)V_{i-1} = 0,$$

where $R_i(z) = X_i'(z)\, X_i^{-1}(z)$. χ_i can change by many orders of magnitude and may become very inaccurate after a large number of intervals [5]. Therefore we replace (7) by

$$C_{i0} = I,$$
$$C_{i1} = R_{i-1}(z_i).$$

Discontinuous solutions $X_i(z)$ are propagated, and the vectors V_i are calculated only at the end. The ''R-matrices'' $R(z)$ are numerically stable.

The vectors V_i can be calculated successively if one of them can be calculated from boundary conditions. A particular way of determining the V_i will be presented in the next section.

Since in the linear system solver routines it is natural that the inverted matrix be multiplied from the left ($A^{-1}\, B$), the program works with R_i^T and C_{in}^T rather than R_i and C_{in} in order to avoid transpose operations at each interval boundary.

Interval boundaries must be specified. We recall that there are, in general, terms of the form z^{-1} and z^{-2} in P and Q. They have convergence parameters $T_z = (z_{i+1} - z_i)/z_i$ if expanded in Taylor series around z_i:

$$\frac{1}{z} = \frac{1}{z_i}\left(1 - \frac{(z - z_i)}{z_i} + \frac{(z - z_i)^2}{z_i^2} - \ldots\right).$$

These terms are dominant at small z and T_z should be constant for uniform convergence. At large z the convergence parameter $T_w = z_{i+1} - z_i$ of the solution representation (4) prevails in importance. Accordingly, the algorithm for generating the sequence $\{z_i\}$ is

$$z_1 = 0, \quad z_2 = z_F; \quad z_i = z_{i-1} + \tau \min\{T_w, z_{i-1}T_z\}, \quad i = 3, 4, \ldots, \tag{8}$$

where $\tau = 1$ if $z_i < z_M$ and -1 otherwise. Also, $z_i \neq z_M \ \forall i$. Even if $z_i > z_{i+1}$ we use the convention $[z_i, z_{i+1})$ for denoting the interval.

3.2. Derived Quantities: Integrals of the Solution

3.2.1. *Calculation of Integrals*

In integrals containing χ and its derivatives, the latter are obtainable by analytic manipulations. The integrals must frequently be calculated numerically as functions of the upper limit of integration which we denote by $z_I \leq z_U$.

3.2.2. *Extracting the Convergent Values*

Integrals may exhibit plateau-like behavior or diverge as functions of z_I, for example, when the boundary conditions at large z are approximate, causing the solution χ to be meaningless for z large enough. These plateaux can be searched for automatically in the present program package.

3.3. Estimates of the Intrinsic Parameters

Intrinsic parameters are those used to solve the ODE for a fixed N with a prescribed accuracy. They are as follows: z_F; n_F, maximum power n in the truncated series (2); T_z; T_w; n_w, maximum power n in the series (4); z_U; z_M. We shall frequently write this set as the 7-tuple $(n_F, n_w; T_z, T_w; z_F, z_M, z_U)$.

Some estimates of typical values of intrinsic parameters can be done *a priori* with little assumptions about the ODE. Some parameters form natural pairs, for example, n_w and T_w. The total CPU time spent in evaluating the recurrence relations (5) at large z (cf. Eq. (8)), is approximately given by the expression

$$t_{RR} = \text{const}\,\frac{n_w^2}{T_w}. \tag{9}$$

In many cases (at least in some part of the integration interval) a good assumption is that the coefficients in (4) are of the order (we leave out the row/column indices):

$$C_n = \mathbb{O}\left(\frac{1}{n!}\right), \quad n = 0, 1, ..., n_w.$$

Then for a prescribed accuracy ε, we must have

$$\frac{T_w e}{n_w} \approx \varepsilon^{1/n_w}.$$

Inserting in (9) and differentiating with respect to n_w we obtain that the CPU time is minimum at

$$n_w \approx m \ln 10 \approx 2.4m; \quad \varepsilon = 10^{-m}.$$

For $m = 10$, $n_w \approx 24$ and the corresponding T_w is about 4. In parts of the integration interval C_n may be more nearly $\mathbb{O}(10^{-n})$; in this case $n_w \approx 12$ and $T_w \approx 0.4$.

At smaller z, by analogy, we have the requirement

$$T_z \approx \varepsilon^{1/n_w}.$$

Together with (9) this gives $n_w \approx 1.2m$ and $T_z \approx 0.1$.

z_M should be roughly in the region in which the solution attains its largest absolute value. A useful first approximation for z_U is that it should be approximately an order of magnitude larger than z_M, or twice as large as the interval on which the solution is required to high precision. (This is similar to the Miller's method for calculating Bessel or certain other special functions from backward recurrence [7].) z_F should be an order of magnitude smaller than z_M.

4. EXAMPLE: HYPERSPHERICAL APPROACH TO THE FEW-BODY PROBLEM

4.1. The Physical Model

4.1.1. *Statement of the Problem*

For definiteness we restrict ourselves to the case of three particles with the usual Jacobi coordinates,

$$\mathbf{R} = \frac{1}{M}(m_i\mathbf{r}_i + m_j\mathbf{r}_j + m_k\mathbf{r}_k),$$

$$\mathbf{x}_k = \sqrt{\mu_k}(\mathbf{r}_i - \mathbf{r}_j),$$

$$\mathbf{y}_k = \sqrt{M_k}\left(\mathbf{r}_k - \frac{m_i\mathbf{r}_i + m_j\mathbf{r}_j}{m_i + m_j}\right).$$

Here $\mu_k = m_i m_j/(m_i + m_j)$, $M_k = m_k(m_i + m_j)/M$, $M = m_1 + m_2 + m_3$, and $\{i, j, k\}$ is a cyclic permutation of $\{1, 2, 3\}$ (spectator notation).

The angle between $\mathbf{x}_k$ and $\mathbf{y}_k$ will be called φ_k. From now on, r_k will denote the distance between the particles i and j ($r_k = |x_k|/\sqrt{\mu_k}$), and $s_k = |y_k|/\sqrt{M_k}$.

In these coordinates, the Hamiltonian operator is

$$H = -\tfrac{1}{2}\nabla^2 + V.$$

The equation to be solved is

$$(H - E)\Psi = 0.$$

The boundary conditions on Ψ are: finiteness at the origin and $\lim_{x_k, y_k \to \infty} \Psi = 0$. In this paper we restrict ourselves to systems of differential equations resulting from bound state problems.

4.1.2. *Ansatz for the Wave Function and the Derivation of the ODE*

For precision calculations, for example, in atomic physics, it is necessary to take into account the fact that the wave function has cusps on sets of points of configuration space defined by $r_k = 0$.

The central characteristic of our method is that the cusps are removed analytically before expanding in hyperspherical harmonics (HH),

$$\psi = e^{f(r_1,r_2,r_3)}\Phi$$

which gives

$$(-\tfrac{1}{2}\nabla^2 + V)\Psi = e^f(-\tfrac{1}{2}\nabla^2 + W)\Phi,$$

where Φ is the smooth part of the wave function to be expressed in HH, and the effective velocity-dependent potential is

$$W = V - \tfrac{1}{2}\nabla^2 f - \tfrac{1}{2}(\nabla f)^2 - (\nabla f)\nabla, \tag{10}$$

where $\nabla_k = (\partial/\partial \mathbf{x}_k, \partial/\partial \mathbf{y}_k)$ is the six-dimensional gradient. After the substitution

$$\Phi = \frac{1}{\rho^2}\chi$$

where $\rho^2 = \mathbf{x}_k^2 + \mathbf{y}_k^2$, we get the ODE (1) with

$$\begin{aligned} P &= \frac{1}{z} - \frac{1}{\kappa}\overline{W}^D, \\ Q &= -\frac{1}{4} - \frac{\Lambda^2}{z^2} - \frac{1}{2\kappa^2}\overline{W}^S, \end{aligned} \tag{11}$$

where $\overline{W} = \overline{W}^S + \overline{W}^D\ \partial/\partial\rho$, $\Lambda_\sigma = K_\sigma + 2$, $\sigma = 1, 2, 3, \ldots, N$, $z = 2\kappa\rho$, and $\kappa = \sqrt{-2E}$, where E is the total energy of the system.

(In scattering problems, it is natural to factorize $\rho^{-5/2}$, not ρ^{-2}. In this way one could not eliminate P, just the term z^{-2} from P. For bound states, ρ^{-2} is more natural because of the integer-power behavior at $z = 0$.)

The operator (10) makes the Hamiltonian non-self-adjoint (see Section 2.1) and the eigenvalues may have small imaginary parts, or, the spectrum may have bands. These usually become sufficiently narrow at a sufficiently large N. In addition, the energy eigenvalue E_0 does not equal the expectation value of H; the latter is the true energy.

χ is expanded in HH,

$$\chi = \sum_\alpha \chi_\alpha \mathcal{Y}_\alpha,$$

where $\mathcal{Y}_\alpha$ are the HH [5, 8]. The infinite expansion is truncated to N terms, yielding a set of ODE of dimension N for the ''hyperradial'' functions χ_α. We have $\Lambda^2\mathcal{Y}_\alpha = K_\alpha(K_\alpha + 4)\mathcal{Y}_\alpha$, where Λ is the six-dimensional quasi-angular momentum operator.

It is known [9] that to describe a three-body system one needs to include HH with $K_\alpha \approx \kappa\rho$.

4.1.3. *Reformulation of the Problem*

We are solving an eigenvalue problem with E_0 as the energy eigenvalue. This implies solving a sequence of ODE with fixed values of the energy E. The equation for E_0 fixes both E and the vectors V_i and is derived as follows.

At $z = z_M$ the continuity condition reduces to

$$(R_+(z_M) - R_-(z_M))X_+(z_M)V_+ = 0, \tag{12}$$

where the intervals left and right of z_M are denoted by $-$ and $+$, respectively. We shall write $D = D(E) = \det(R_+(z_M) - R_-(z_M))$. The spectrum of eigenvalues is the set of zeros of the function $D(E)$, i.e., the secular equation is $D(E) = 0$.

After E_0 is found, V_+ must be calculated from a homogeneous system of linear equations. From a practical point of view, $D(E_0)$ is never zero; its order of magnitude is just smaller relative to the values of $D(E)$ far away from E_0. The zero-search algorithm, in fact, decreases the magnitude of $D(E)$ until it contains no significant digits anymore.

Thus, Eq. (12) can be solved for an improved V_+ by putting $(V_+)_1 = 1$, discarding the Nth equation and using minus the first column of $(R_+ - R_-)\chi_+$ as the right-hand side. (The program implements an optional quadruple precision (usually referring to 128-bit) arithmetic code to do this part of calculation, but this has been found unnecessary in all cases; we have retained this code for possible cases where extreme precision is required.)

The solution is remarkably stable with respect to which row is ignored (see Section 5.4.1).

The V_i were not used until now at all. Now, the V_i are calculated by applying $V_i = X_i(z_i)^{-1}\chi_{i-1}(z_i)$, on all intervals proceeding in the backward directions (away from z_M).

4.1.4. *The Correlation Function*

The function f has the following general form:

$$f = \sum_{i<j} [a_k + (b_k - a_k)e^{-c_k r_k}]r_k. \tag{13}$$

Here b_k are the cusp parameters,

$$b_k = \mu_k Z_i Z_j,$$

where Z_i are charges of the particles.

The exponential term in (13) produces a smooth transition between the functions $b_k r_k$ at $r_k \to 0$ and $a_k r_k$ at $r_k \to \infty$. The

TABLE I

Eigenvalue $-E_0$ for the Infinite-Mass He Atom Ground State for Unmodified HH Expansion (HH) and for f Given by Eq. (13) with $a_k = c_k = 0\ \forall k$ (CFHH)

K_m	N	HH	CFHH
16	25	2.88754	2.90370440
20	36	2.89358	2.90374150

Note. Values are from Ref. [4].

exponential function was chosen because it is smooth enough and at the same time can be expanded in power series with a rather large ''numerical radius of convergence.'' For typical (64-bit) floating point representations, this is given by $|c_k r_k| \approx 20$.

The $c_k\ \forall k$ determine the start of the asymptotic regions and are free parameters. The a_k can be used to incorporate knowledge of asymptotic behavior (see Section 5.2).

The correlation factor $\exp(f)$ is suitable for analytic treatment but is positive definite and cannot be made similar to the wave function for excited states because it cannot reproduce its nodes. How important this is we do not know quantitatively at present, because even a positive-definite correlation factor gives very good excited states in some cases.

After the convergent values of the intrinsic parameters of the ODE (see Section 3.3) are found and convergence with external parameters like N is estimated, it may be necessary to change the parameters of f. This may in turn affect slightly the optimum values of the intrinsic parameters. From experience, this feedback is rarely necessary.

The importance of using a correlation factor is illustrated by the benchmark example of the infinite-mass He atom in Table I. A comparison of CFHHM and related methods on an exactly solvable model has been published [10].

4.2. Calculation of $\overline{W}$

We have derived algebraic formulae for the matrix elements of $\overline{W}$ [5, 8, 11] in the case the functions $r_k V$ and f are power series in r_k for all k (i.e., V can be at most Coulomb-like at $r_k \to 0$). All terms except $-\frac{1}{2}(\nabla f)^2$ are calculated algebraically. Although we have its analytic expression, this term contains a slowly converging matrix product and is calculated by numerical quadrature. The accuracy of this quadrature is easily checked separately so that it does not influence the accuracy of the solution of the ODE. Matrix elements are stored once and for all in advance and represent a minor part of the total CPU time. As a result, $\rho\overline{W}$ is represented as a matrix power series in ρ; i.e.,

$$\overline{W}_{\alpha\alpha'}(\rho) = \sum_{p=-1}^{\infty} \overline{W}^p_{\alpha\alpha'} \rho^p \tag{14}$$

which is truncated at some $p = p_W$ which is an external parameter.

Since $\mathcal{P}$, $\mathcal{Q}$ are proportional to the derivatives of P and Q at $z = z_i$ (see Eq. (6)), they have to be calculated from the series (14), which may not always converge for large z (ρ) required to obtain the solution. So far in applications it was always possible to sum enough terms for the required precision. It should be noted that at large z the sum need not be as precise as at moderate and small z; the χ at large z are approximate by construction.

4.3. Expectation Values of Observables

The calculation of expectation values of observables reduces to multidimensional integrals containing the functions χ_α, $\mathcal{Y}_\alpha$, and their derivatives, in the integrand. In the examples in Section 5 the dimension is three, the functions $\mathcal{Y}_\alpha$ depending on two ''hyperangles.''

Singular interparticle potentials result in singular behavior of some integrands in the hyperangles for any z. For Coulomb-type potentials, these singularities are integrable if the correct order of integration is chosen.

It was found that Gaussian integration is sufficiently precise, except that the grid is taken an order of magnitude denser in the vicinity of singularities. The grid has three subregions in any variable between two singularities. These subregions are subdivided further if necessary and covered with Gaussian quadrature points of order 16.

In most cases, the integrals exhibit plateaux as functions of z_I (see Section 3.2). A check of the correctness of the plateau determination is the fact that they should move uniformly toward larger z as N is increased.

5. NUMERICAL EXAMPLES

5.1. Physical Systems

To illustrate the method we present details of CFHHM calculations of the He atom, the muonic helium atom ($e^-\mu^{-4}$He), and the μdt molecular ion. These systems have very different mass ratios.

For the He atom, a linear f works, while in $e^-\mu^{-4}$He much better results are obtained with a nonlinear f. In μdt, the cusp linear f does not work at all due to the too strong positive cusp parameter of the pair $d - t$, which produces wrong asymptotic behavior.

The number of differential equations in the case of two identical particles is $N = (K_m/4 + 1)^2$; in the case of three different particles $N = (K_m/2 + 1)(K_m/2 + 2)/2$, which is almost twice as large. K_m is the maximum K_α (Section 4.1.2) included. It should be noted that due to efficient code the CPU time for $p_W = 100$ (see Eq. (14)) is only about twice as large as for $p_W = 0$ (Coulomb potential, linear f), other parameters being equal. In some cases (positronium negative ion) a nonlin-

ear f allows the use of smaller z_U, thus actually decreasing the CPU time with respect to the linear f case.

The examples presented are not necessarily the ones that led to the best results of CFHHM, but they are chosen to illustrate the numerical aspects of the method.

5.2. Determining the Parameters of f

The first choice for a_k would be expected to be $a_k = 0\ \forall k$ because this would just set the correlation factor to unity in the asymptotic regions, where $x_k \to \infty\ \forall k$. It turns out that one can incorporate some information on asymptotic behavior of the wave function in this factor and thus obtain faster convergence.

Let us discuss a three charged particle system where two of the two-particle subsystems have bound states, as is usual in atomic physics. In the leading order, and for $N = 1$, the single differential equation gives

$$\chi_1 \underset{\rho\to\infty}{\sim} e^{(f/\rho + K_{as})\rho}$$

where we chose the smaller solution,

$$K_{as} = \overline{W}_{11}^{D0} - \sqrt{(\overline{W}_{11}^{D0})^2 + 2\overline{W}_{11}^{S0} - 2E}$$

(see Eqs. (11), (14).) If particle k is separated from the bound state $\phi_k(\mathbf{x}_k)$ of particles ij (clustering k), we have

$$\chi \underset{y_k\to\infty}{\sim} e^{-\sqrt{2M_k\varepsilon_k}r_i}\phi_k(\mathbf{x}_k),$$

where $\varepsilon_k > 0$ is the particle k separation energy. Then the asymptotic conditions on a_k are

$$\begin{aligned} a_2 + a_3 + K\sqrt{M_1} &= -\sqrt{2M_1\varepsilon_1}, \\ a_3 + a_1 + K\sqrt{M_2} &= -\sqrt{2M_2\varepsilon_2}, \\ a_1 + a_2 + K\sqrt{M_3} &< 0. \end{aligned} \tag{15}$$

These equations fix f only in the clustering regions of the hypersphere and leave one of the a_k as a (partially) free parameter. If $K = 0$, asymptotics are imposed on $\exp(f)$; if $K = K_{as}$, asymptotics are imposed on Ψ. We have $K_{as} = K_{as}(a_1, a_2, a_3, E)$; using an approximate E, the Eqs. (15) represent a set of nonlinear equations for K. This system does not have to be solved by iteration but by mere tabulation since the results do not depend strongly on K and the equations are approximate. The third inequality (15) could be replaced by an equation, except that the asymptotics in the ''repulsive'' clustering is not known. It turned out in the μdt case, however, that the shape of Ψ at $r_3 = r_{dt} = 0$ depends very weakly on a_k and that good f approximate it well. (The wave function is very small in this region.)

All parametrizations of $\chi = \exp(f)$ for the μdt system disagree in shape with Ψ quite strongly in the region of equilibrium distances, where Ψ has a maximum. Particularly, χ for a linear f decays in all directions and, also, cannot describe the nodes of Ψ for excited states. Although the HH expansion is able to correct the discrepancy between Ψ and χ for any parametrization, ψ for a nonlinear f looks more similar to Ψ, its maximum, for example, being closer to the maximum of Ψ. However, in view of the small number of parameters, the shape similarity between χ and Ψ nevertheless is not a direct indicator of the suitability of a given χ.

We denote the points (a_1, a_2, a_3) corresponding to the various solutions of (15) as follows: *An*—linear f; *Bn*—nonlinear f with $K = 0$; *Cn*—nonlinear f with $K = K_{as}$; *Dn*—nonlinear f with arbitrary $a_k\ \forall k$, where n refers to the values of the free parameter.

$K = 0$ turned out to be the best choice in the μdt case using nonlinear f, as well as in the case of the positronium negative ion [12]. If these systems were calculated with linear f (using $a_k = b_k$), proper asymptotic behavior of the solution would be violated. This would force one to modify the like-charged pair a_k parameter to assume a negative value instead of the positive cusp value. This requirement is roughly equivalent to applying the constraints on Ψ at $N = 1$. Nonlinear f eliminates this necessity [12, 17].

To estimate a_1, a_2 if m_1 and m_2 are equal or of the same order of magnitude and much different from m_3 (e.g., positronium negative ion or μdt), we take approximately $a_1 = a_2$. Equations (15) constrain (a_1, a_3) to a curve in the (a_1, a_3) plane. The a_k should be kept negative and small in absolute values (close to the origin), different points on the curve should be tried, and quantities of interest (e.g., E) investigated as functions of (a_1, a_3). Even with more general mass ratios, the choice $a_3 = 0$ provided a good starting point; this seems to be even more important than satisfying Eqs. (15).

The dependence on a_k in a broad range of values turns out to be less important than dependence on N in applications. This in fact makes the CFHH method tractable.

5.3. Determining the Intrinsic Parameters

Estimates from Section 3.3 can be used as initial values of intrinsic parameters. One must then find the values at which the solution or a function of the solution converges to the required accuracy. (If the CPU time is not the issue, most cases are covered by simply taking very conservative variants of the estimates.)

The models of Section 3.3 are corroborated in applications described below, where $n_w = 16$, $T_w = 5$ are often found to be optimum (He atom). In some cases ($e\mu^4$He at intermediate z) C_n is more nearly $\mathbb{O}(10^{-n})$. All systems studied lead to a general conclusion that CPU-time-optimum values of n_w and T_w tend to be rather small, irrespective of the precise form the sequence $\{C_n\}$ assumes.

T_z of Section 3.3 also turns out to be a very good estimate for all systems calculated.

z_M in physical applications is estimated as the z at the approximate average interparticle distances. Here, too, z_U should be approximately an order of magnitude larger than z_M, and z_F should be an order of magnitude smaller than z_M.

The algorithm (8) might have to be further modified in some cases. A possible example is a very unsymmetric system like $e\mu^4$He in which the muon spends most of the time close to ^{4}He. These small distances and the distances on the electron scale are not adequately covered at the same time by the sequence $\{z_i\}$, or else too many points must be taken, making CPU time excessively large.

In physical applications presented here one does not prescribe the accuracy of the solution itself, but of derived quantities (observables). In addition, convergence is usually estimated from the dependence of observables on N. In this case one has to find the minimum necessary accuracy of the solution to give the prescribed accuracy of observables. This is extremely important if the computer time has to be saved. (For an example, see Section 5.4.3).

The following way of testing the intrinsic (and possibly other) parameters is useful in physical applications in which a parameter of the ODE (in this case the energy, E) is to be optimized. This implies that for each new set of values of intrinsic parameters the ODE would have to be solved several times until E is optimized, in order to obtain the change in E.

Consider one parameter, P, at a time. Then $D = D(E, P)$, and the relevant equation is the equation of the curve $D = 0$,

$$0 = dD = \frac{\partial D}{\partial E}\,dE + \frac{\partial D}{\partial P}\,dP \approx \frac{\partial D}{\partial E}\,\Delta E + (\Delta D)_E. \qquad (16)$$

One first performs a full optimization of $E \to E_0$ with a value $P = P_0$ which is expected to be good. (Other parameters must also be estimated conservatively.) From the sequence of optimization values of E one obtains an estimate of $\partial D/\partial E$. Then one calculates $D(E_1, P_1)$ for some P_1, where E_1 is close but not necessarily equal to E_0. This gives the estimate $(\Delta D)_E$.

The resulting value of ΔE is usually a very good estimate which replaces a full optimization of E at $P = P_1$ and decreases the CPU time proportionally to the number of optimization steps needed. An optimization (zero search) takes on the order of 10 steps, which means a CPU time reduction by almost an order of magnitude. (This decrease may be worsened somewhat by the initial attempts at finding sensible parameters to allow a successful initial optimization.)

From experience E_1 should be approximately $E_0(1 + 10^{-9})$ in order to avoid the loss of precision in D close to the optimization point (zero of $D(E)$) on a computer with the typical 64-bit floating point representation. The precise value should be tested in specific applications. (In $e^-\mu^{-4}$He, E_1 should be about $E_0(1 + 10^{-14})$.)

In some cases E may be much more stable to variations in P than the solution (pointwise), and full optimization tests might still be necessary. This is typical for the Schrödinger equation. In these cases fine tuning of intrinsic parameters is extremely important in order to keep the CPU time from increasing too much.

In our physical applications, to optimize the E eigenvalue, which is equivalent to searching for a zero of D, one usually needs only about seven calculations of D. This is due to a good zero-search method which gives fast convergence even if the function is slightly numerically unstable (inverse quadratic interpolation combined with linear interpolation and bisection) [13].

5.4. Precision of the Solution and Observables

Our aim is to calculate observables, not the wave function itself. It would be preferable to calculate the wave function precisely independently, so that the precision of the observables would not depend on the intrinsic parameters. However, large CPU times may force us to study this dependence also, i.e., make the wave function only as accurate as needed in a given calculation. This is purely a matter of economy, not of intrinsic precision of our method. It also implies that we are concerned with absolute and not with relative errors of the solution of the ODE (i.e., with the number of correct digits). This is because the wave function is a linear combination of solutions $\chi_i(z)$ at any z.

This section presents estimates of the precision of $X_i(z)$ and $\chi_i(z)$, and the precision of the expectation values related directly to intrinsic parameters.

Let us define $L_{\text{cond}}(A) = \log_{10} R_{\text{cond}}(A)$, where $R_{\text{cond}}(A)$ is the condition number of the matrix of a linear system of equations; then the number of significant digits in the solution is approximately $s - L_{\text{cond}}(A)$, where s is the number of significant digits in the matrix or the right-hand-side.

5.4.1. *He Atom*

Here we present results for the infinite mass nucleus only, although there are no restrictions on masses in our programs.

Table II presents the convergence of the Taylor series for the leading element $(X_i)_{11}$ of the matrix $X_i(z)$. Large values of the last term at $z \approx z_U$ are meaningless because (i) the increasing solution is present and (ii) the physical solution is very small.

During the iteration to find E_0, at $K_m = 24$, $L_{\text{cond}}(R_+(z_M) - R_-(z_M))$ increases from about 5 to about 19. This reflects the complete loss of significant digits in $D(E) = \det(R_+(z_M) - R_-(z_M))$ as its zero is approached. $D(E)$ itself decreases by 13 orders of magnitude.

The stability of the solution of the matching problem at $z = z_M$ has been checked at $K_m = 24$. The vector V_+ is determined to at least 12 significant digits (15 for its leading elements) even if one discards the last but fifth equation instead of the last one. L_{cond} of the reduced matrix $(R_+(z_M) - R_-(z_M))X_+(z_M)$ is about 4, implying that the accuracy of V_+ is four significant digits less than the accuracy of X_i.

$L_{\text{cond}}(X_-(z_M)) \approx 5$, implying about five digits less precise V_-

TABLE II

Largest High-Order Term in the Taylor Series for $(X_i)_{11}$ on Separate z Intervals

n_w	T_z	Interval	$\mathrm{Max}_z\,\lvert(C_{n_w})_{11}(\Delta z)^{n_w}\rvert$	Sum
15	0.1	(0.5, 5)	0.4(−16)	1.2
		(120, 80)	0.4(−2)	0.9
		(80, 5)	0.2(−12)	0.8
12	0.1	(0.5, 5)	0.1(−13)	1.2
		(120, 80)	0.1(−0)	0.9
		(80, 24)	0.4(−1)	0.8
		(24, 5)	0.3(−10)	0.8
15	0.05	(0.5, 5)	0.2(−20)	1.1
		(120, 74)	0.4(−2)	0.9
		(74, 5)	0.7(−17)	0.9

Note. Δz is the length of the interval. Parameters are (20, n_w; T_z, 5; 0.5, 5, 120). $K_m = 20$ ($N = 36$). Sum is the approximate value of the sum of the Taylor series (always of the order of 1). Inside intervals, values change monotonically. Ordering of interval boundaries indicates direction of propagation.

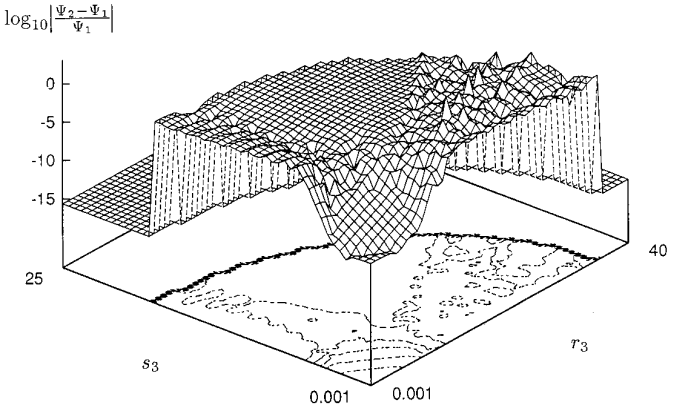

FIG. 1. Pointwise relative differences in logarithmic scale of normalized wave functions Ψ_1, Ψ_2 for the He atom ground state, for $K_m = 20$ ($N = 36$). The linear correlation function f is used ($a_k = b_k$ in Eq. (13); parametrization A1, see Section 5.2). The intrinsic parameters are (20, n_w; 0.1, 5; .5, 5, 120), Ψ_1, Ψ_2 correspond to $n_w = 15$ and 12, respectively. The angle φ_3 (Section 4.1) is 1°. z-axis: logarithm to the base 10 of the absolute value of the relative differences, bounded by machine accuracy, at grid points. The solution χ is calculated in the elliptic region corresponding to $z = z_U = 120$.

as compared with V_+. All these estimates combined would give about a nine-digit smaller accuracy of the $\chi_\alpha(z_M)$ as compared with the intrinsic accuracy of the solutions $X_i(z)$.

Accuracy of χ (see Table II) was checked by comparing χ_α for the first two, and the first and third table entries. The former case yields the χ_α accuracy at $(n_w, T_z) = (12, 0.1)$ to be only five (zero) significant digits already at $z = 25$ (50), while accurate to about 10 digits at small z. The latter case yields the χ_α accuracy at $(n_w, T_z) = (15, 0.1)$ to be 14 (8) significant digits up to $z = 60$ (100). These numbers are almost independent of α.

This result, as well as Table III and Figs. 1 and 2 show that Ψ and observables actually converge to more digits than predicted on the basis of the condition numbers. (Here we have no means of obtaining absolute estimates.) Also, if the linear systems for V_+ and V_i are solved in extended precision, the expectation values remain the same to at least the 11 significant digits examined, and $\langle H\rangle$ agrees to 16 significant digits.

Figure 1 shows pointwise relative differences in Ψ corresponding to the first entry of Table III. The Ψ precision for $(n_w, T_z) = (12, 0.1)$ is about eight significant digits (SD) but only for interparticle distances of a few a.u. This reflects on poor precision of $\langle r_k^2\rangle$. The $(X_i)_{11}$ are more precise but on a too short interval (see the last row of the second entry of Table II).

For $(n_w, T_z) = (15, 0.1)$, the accuracy of the $X_i(z)$ can be made to approach machine accuracy (affected only by the summation of the Taylor series and by the errors in calculating the matrix recurrence relations for C_n). Ψ on a large interval and the derived quantities (expectation values) are converged to about 14 significant digits. This can be seen in Fig. 2 which corresponds to the second entry of Table III and shows that the wave function is precise up to $z \approx \frac{1}{2}z_U$ which corresponds to maximum r_k from 10 to 20 a.u. (Note that the average $r_3 = 1.4$ a.u., and average $r_1 = 1$ a.u. Figure 2 is for $\varphi_3 = 1°$ but the results are insignificantly dependent on φ_3 due to cusp removal.) In summary,

TABLE III

Sensitivity of Eigenvalue E_0 and Observables on the Parameter Set (n_w, T_w)

Set 1		Set 2				
n_w	T_z	n_w	T_z	$\delta E_0/\lvert E_0\rvert$	$\delta\langle H\rangle/\langle H\rangle\rvert$	$\delta\langle\mathbb{O}\rangle$
12	0.2	15	0.1	0.2(−9)	−0.7(−9)	6–9 SD
15	0.1	15	0.05	<0.3(−16)	0.1(−13)	>13 SD

Note. Other parameters are as in Table II.

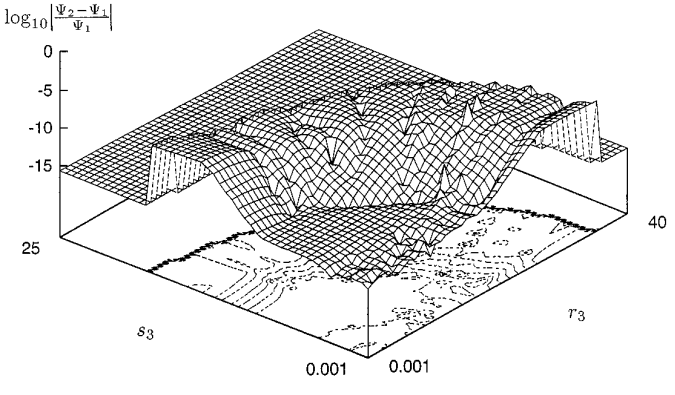

FIG. 2. As in Fig. 1, but for parameters (20, 15; T_z, 5; .5, 5, 120), where Ψ_1, Ψ_2 correspond to $T_z = 0.05$ and 0.1, respectively.

TABLE IV

As in Table II

Interval	$\mathrm{Max}_z\,\lvert(C_{n_w})_{11}(\Delta z)^{n_w}\rvert$	Sum
(0.5, 10)	0.7(−15)	1.2
(0.5, 60)	0.6(−5)	1.6
(950, 60)	0.2(−14)	1.

Note. Parameters are (20, 16; 0.1, 5; 0.5, 60, 1000). $K_m = 40$ ($N = 231$).

(i) $n_z = 12$ is sufficient for calculations with N small enough that the dependence of the derived quantities on N is stronger than on intrinsic parameters, although in the tail region the wave function is still quite unreliable;

(ii) one need not make the accuracy of Taylor series for $(X_i)_{11}$ much larger (on an appropriate interval) than the required accuracy of the observables, despite the above condition number estimates. In particular, taking $(n_w, T_z) = (15, 0.05)$ would cost twice as much CPU time as (15, 0.1) but would have a negligible effect on observables. Note also that it is difficult to estimate the value of z such that for smaller z, $X_i(z)$ must be sufficiently accurate to give precise observables; therefore Table II does not enable us to choose between its first and second entries as the latter seems reasonable but is not.

5.4.2. *Muonic He Atom* ($e^-\mu^-{}^4$He)

To illustrate the capabilities of CFHHM for large sets of ODEs, we present a test calculation with a linear f that converges slowly.

In this system the muon due to its large binding energy relative to the electron binding energy changes the z scale appreciably but does not affect much the typical distance scale of the electron. Therefore the value of z_U as compared to the He atom case is simply estimated from the formula $z = 2\sqrt{2E\rho}$ using the same ρ in both cases, and the corresponding total E: the z_U should be roughly $\sqrt{402.6/2.9} = 12$ times larger than for He. Indeed, it is about 1000, and the typical parameters are (20, 16; 0.1, 5; 0.5, 60, 1000). Also, we can only get the eigenvalue E_0 for $K_m \geq 32$ which is about $z_M/2$, as expected.

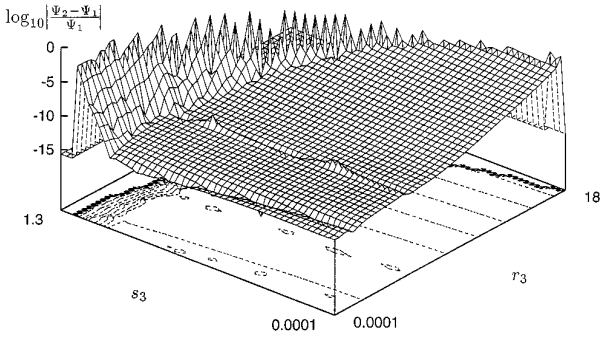

FIG. 3. As in Fig. 1, but for the $e^-\mu^-{}^4$He atom ground state, $K_m = 32$ ($N = 153$). The linear correlation function $f\,(a_k = b_k)$ is used (parametrization A1). The intrinsic parameters are (20, n_w; 0.1, 5; .5, 60, 1000); $\varphi_3 = 0.001°$. Ψ_1, Ψ_2 correspond to $n_w = 16$ and 12, respectively.

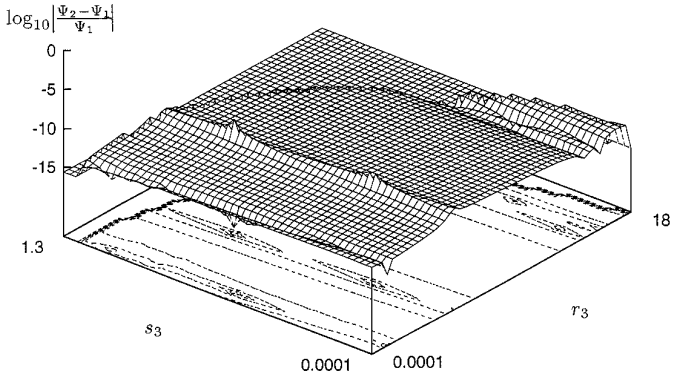

FIG. 4. As in Fig. 3, but with intrinsic parameters (20, 16; T_z, 5; .5, 60, 1000), and Ψ_1, Ψ_2 correspond to $T_z = 0.05$ and 0.1, respectively.

Figures 3 and 4 show the relative differences of the wave function Ψ corresponding to the two entries of Table V, respectively; $n_w = 16$ makes Ψ uniformly convergent to 15 digits.

At $K_m = 48$ ($N = 325$) the solutions χ_α for $T_w = 2$ and $T_w = 5$ agree to at least 10 significant digits for all α, all z; on the average, they agree to 12 digits.

The stability of the solution of the matching problem at $z = z_M$ has been checked at K_m up to 64 (N up to 561). L_{cond} of the reduced matrix $(R_+(z_M) - R_-(z_M))X_+(z_M)$ is about 4–6, even for such large systems; $L_{\mathrm{cond}}(X_-(z_M)) \approx 6$–7.

Again, the accuracy of the observables is much larger than implied by the above (see Tables V, VI), despite rather bad precision of $X_i(z)$ as $z \to 60$ from below. Also, the values of L_{cond} are almost the same if the linear system solutions for V_+ and V_i are done in extended precision. For $K_m = 48$, the expectation values in the two cases do not differ earlier than 14th digit (some are limited to less digits, due to plateaux). The solution components χ_α agree to at least 14 significant digits (except some to 13 significant digits at large z) uniformly for all α and z; this shows directly the accuracy of our solution of the ODE.

TABLE V

As in Table III

Set 1		Set 2				
n_w	T_z	n_w	T_z	$\delta E_0/\lvert E_0\rvert$	$\delta\langle H\rangle/\langle H\rangle\rvert$	$\delta\langle\mathbb{O}\rangle$
12	0.1	16	0.1	−0.5(−15)	0.2(−14)	>9 SD
16	0.1	16	0.05	<0.3(−18)	−0.2(−14)	>9 SD

Note. Other parameters are as in Table IV, except $K_m = 32$ ($N = 153$).

TABLE VI

As in Table V, except $K_m = 40$ ($N = 231$)

Set 1		Set 2				
n_w	T_z	n_w	T_z	$\delta E_0/\lvert E_0\rvert$	$\delta\langle H\rangle/\langle H\rangle$	$\delta\langle\mathbb{O}\rangle$
12	0.1	16	0.1	$-0.5(-15)$	$-1.0(-15)$	>9 SD
16	0.1	16	0.05	$0.5(-15)$	$-0.2(-14)$	>9 SD

The intrinsic precision of $\langle H\rangle$ at $K_m = 32$ is thus about 12 SD (402.637269429) but the dependence on K_m is much stronger: $-\langle H\rangle = 402.6406$ (402.6392, 402.6389, 402.6394) for $K_m = 40$ (48, 56, 64). The above examples show that it is possible to increase K_m (or N) to much larger values without reaching the intrinsic accuracy (Section 5.5).

(Nonlinear f gives much better results already at smaller K_m: $-\langle H\rangle = 402.64014341$ (402.64100308, 402.64101529, 402.64101494, 402.64101497) for $K_m = 12$ (24, 32, 40, 48). This is lower than in Refs. [14, 15].)

5.4.3. *Muonic Molecule μdt*

Figure 5 shows the relative differences of the wave functions of the ground state of μdt for $K_m = 48$ and parameters (20, 16; T_z, 1; 0.5, 15, 120), where T_z is 0.1 and 0.05. Equilibrium geometry corresponds roughly to a circle of radius 50 (units are d.a.u.). Comparing with Fig. 2 (He atom) one can see that the degree of convergence at equilibrium distances is worse by only about 3 orders of magnitude, although Fig. 5 is obtained with $N = 325$ equations and Fig. 2 with $N = 36$. In addition, T_w in Fig. 5 is 1, as opposed to 5 in Fig. 2, indicating stability with respect to both large N and a large number of intervals.

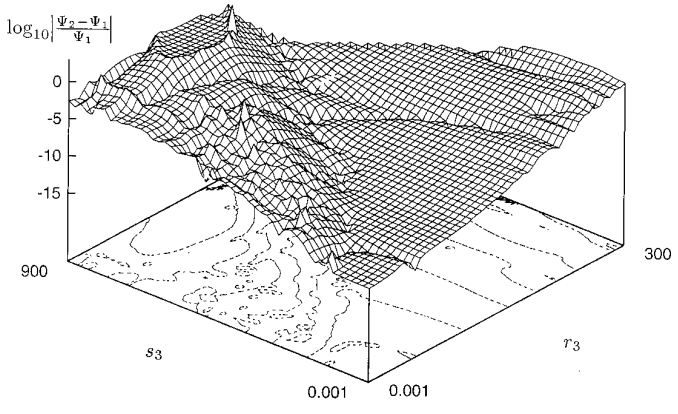

FIG. 5. As in Fig. 1, but for the μdt molecular ion ground state, $K_m = 48$ ($N = 325$). The nonlinear correlation function f (Eq. (13)) is parametrized as $a = \{b_1, b_2, -0.29\}$, $c = \{0, 0, 1/(49 \times 0.7)\}$ (parametrization C1). The intrinsic parameters are (20, 16; T_z, 1; 1.25, 15, 120); $\varphi_3 = 90°$. $\overline{W}$ is summed to $p_W = 100$ terms. Ψ_1, Ψ_2 correspond to $T_z = 0.05$ and 0.1, respectively. The value of the normalization integral is extracted from a plateau (see Section 3.2).

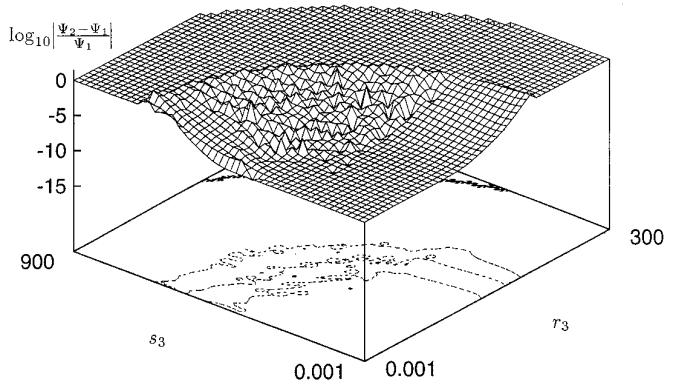

FIG. 6. As in Fig. 5, but Ψ_1, Ψ_2 corresponding to the intrinsic parameter sets (20, 16; 0.1, 1; 1.25, 15, 120) and (20, 12; 0.1, 3; 1.25, 15, 80), respectively. Also, f is parametrized as $a = \{0, 0, 0\}$, $c = \{1/(36 \times 5), 1/(38 \times 5), 1/(49 \times 0.7)\}$ (parametrization D4).

Also, μdt is a much more difficult system from the physical viewpoint (Ψ has more structure).

$z_m/2$ is about 8 and indeed the eigenvalue problem converges only for $K_m \geq 12$, which is of the same order.

In this particular example the precision of the averages at $K_m = 48$ is limited by the plateau smoothness, by the dependence on K_m, and by the dependence on the parametrization of f, which are all of the same order of magnitude and allow about 3–4 significant digits. Therefore CPU time can be reduced appreciably if one can change the parameters to their critical values giving just enough intrinsic accuracy. The most important are n_w, T_w, and z_U. Changing their respective values from (16, 1, 120) to (12, 3, 80) reduces the CPU time more than threefold, while conserving 3–6 SD in averages. The critical values were found with the prescription (16). The eigenvalue $E_0 = 0.0303442$ ... changes by -0.14×10^{-10} and $-\langle H\rangle$ by -0.60×10^{-8}. ($K_m = 48$, parametrization $D4$.) Figure 6 shows the corresponding relative differences in the normalized wave functions. As the normalization integral must be extracted from a plateau, the figure is consistent with the accuracy of the averages. Indeed, Fig. 7 shows the same, but using unnormalized wave functions, where one of them is multiplied by a constant such that their ratio is 1 at a point where the wave function is large. Figure 7 eliminates the effect of the normalization integral plateau and shows much better agreement in the region spanning a few equilibrium distances. (Ratio of normalization integrals in both cases is 0.96.)

The results of the calculations of μdt are published in [16, 17].

5.5. Numerical Stability

Due to the large number of matrix manipulations at each interval boundary, increasing the number of intervals will eventually lead to imprecisions. This was tested in the He atom case at $K_m = 20$ ($N = 36$) by calculating $D(E)$ with $T_z = 10^{-1}$, 10^{-2}, ..., 10^{-5}. E was taken equal to E_0. In this case the leading

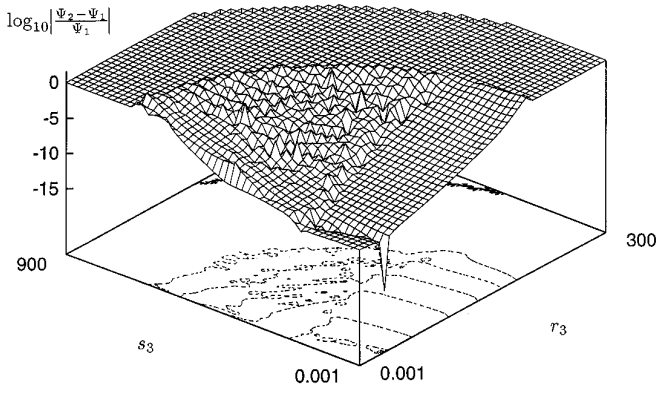

FIG. 7. As in Fig. 6, but using unnormalized Ψ_1, Ψ_2, except that one of them is multiplied by a constant such that $\Psi_1 = \Psi_2$ at $r_3 = 30$, $s_3 = 0$.

digit of D is meaningless. Until $T_z = 10^{-4}$, D only increased by an order of magnitude, causing a predicted shift of E_0, according to (16), of 0.2×10^{-13}. At $T_z = 10^{-5}$, the predicted shift increased to 0.3×10^{-11}. The smallest T_z used in applications is of the order of 0.05, thus being very far from instability.

A second measure of stability is the condition number, R_{cond}, of the matrix $R_+^{\text{T}} - R_-^{\text{T}}$, where $D = \det(R_+^{\text{T}} - R_-^{\text{T}})$. For the He atom at $K_m = 20$ ($E_0 = 2.903741$ ...), $1/R_{\text{cond}} = 0.2 \times 10^{-5}$ at $E = 2.90$, implying 10–11 digit accuracy in the calculation of D. For $e^-\mu^{-4}$He at $K_m = 40$ (56), where $E_0 = 402.662$ ... (402.667 ...) and $N = 231$ (435), $1/R_{\text{cond}} = 0.5 \times 10^{-8}$ (0.2×10^{-8}) at $E = 402.5$. For μdt at $K_m = 40$ (48), where $E_0 = 0.0303551$ ... (0.0303482 ...) and $N = 231$ (325), $1/R_{\text{cond}} = 0.6 \times 10^{-7}$ (0.2×10^{-8}) at $E = 0.0303$. This indicates only a small deterioration of accuracy with increasing K_m or N even at N of the order of 400. As $E \to E_0$, $1/R_{\text{cond}}$ becomes of the order of the machine accuracy as it should because of the loss of precision of D at its zero.

The largest calculation up to date was done on $e^-\mu^{-4}$He. It can be shown that $\langle H \rangle$ must be monotonically decreasing for large enough K_m. For the above system and linear f this is only true for $K_m \geq 64$ (see Section 5.4.2); it was also necessary to set $T_z = 0.05$. Numerical stability was complete even with this size numerical parameters ($N = 561$; 290 z intervals).

6. CONCLUSION

We have presented an algebraic method of solution of coupled systems of ODE. The method reduces the process of solution to a sequence of mostly matrix operations. As a consequence, the code has been efficiently vectorized. In general, the method allows flexibility in adaptation to different computer architectures.

The CPU time to solve the ODE on a 120 MFLOPs vector computer (He atom, $T_z = 0.1$, $z_U = 120$, $n_w = 15$) is 24 s for $N = 49$ and 800 s for $N = 169$. The total CPU time to find the eigenvalue and the wave function Ψ is an order of magnitude larger, but one must bear in mind that a uniformly precise Ψ is obtained.

An important feature of our method is the separation of analytical and numerical input. The former is exact, enabling independent testing of the numerics. The latter is easily controllable via a set of parameters, resembling the step size and the predictor/corrector extrapolation/interpolation order parameters in numerical integrators.

Since χ is given algebraically, it is straightforward to calculate derived quantities, for example, integrals containing χ in the integrand.

The stability of the method seems very large, having seen no indication to the contrary for up to 561 equations. We had no indication that extended precision should be necessary.

We have shown that the accuracy of the solution components χ_α is typically 12 significant digits, even for as many as 561 coupled ODE. This is more than expected on the basis of the condition numbers of the linear systems of equations being solved to make χ_α, χ'_α continuous.

The preferable intrinsic parameters to adjust are T_z and T_w, if n_F and n_w are sufficiently large (about 20 and 16, respectively).

If one is only interested in derived quantities (for example, integrals involving χ_α), one may save CPU time by adjusting the intrinsic parameters to their critical value for the results and not to their values required to find χ_α pointwise to the same precision.

We applied the method to physical problems. These introduce some additional parameters which may be less easily controllable, but which have no direct connection with the intrinsic precision of the solution χ. For example, the HH expansion must contain a minimum number of terms in more complicated systems in order for the eigenvalue problem to be solvable numerically. Nonhermiticity in the effective Hamiltonian also may require a large HH basis before the observables can be extracted from the solution of the ODE. One of the consequences is the fact that excited states are sometimes more difficult to calculate than ground states; in the He atom case, both can be calculated comparably well [18].

The method also permitted a very accurate calculation of the positronium negative ion annihilation rate [12], which was verified in a few months by the subsequent extremely precise computation by Ho [19]. In a recent work [20] we obtained better values than discrepancies in the literature for the fusion rate and the sticking probability of the muon to ^{4}He, for the muon catalyzed fusion reaction of μdt.

There are many instances of variational calculations giving better energy values than CFHHM, e.g., [19, 21]. This is not the case for other observables because by their nature variational wave functions are not necessarily locally correct. Also, since the intrinsic accuracy of our calculations is only a few digits less than the machine precision, we can increase the accuracy of our final physical results by increasing the size of the ODE. The preliminary numerical tests on very large ODE for the

muonic helium atom show the principal feasibility of such extensions of our computations.

The application to physical problems is quite general. The input are masses and charges of the particles, and the rate of convergence depends on how much physical information is introduced via the parameters of the correlation function. We give general hints on how to choose these parameters. It is not necessary to use a variational principle to fix these parameters.

A nonlinear correlation function makes all observables (short and long ranged) as well as $\langle H \rangle$ converge at comparable rates. Also, the convergence to the correct limits, as the number of ODE is increased, is ensured.

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