Solution of few-body problems with the stochastic variational method: I. Central forces

K. Varga$^{1,2}$ and Y. Suzuki$^2$

$^1$Institute of Nuclear Research, Hungarian Academy of Sciences, (ATOMKI), H-4001 Debrecen, Hungary

$^2$Department of Physics, Niigata University, Niigata 950-21, Japan

Abstract

This paper presents a fortran program to solve diverse few-body problems with the stochastic variational method. Depending on the available computational resources the program is applicable for $N = 2 – 3 – 4 – 5 – 6 – ...$-body systems with $L = 0$ total orbital momentum. The solution with the stochastic variational method is “automatic” and universal. One defines the system (number of particles, masses, symmetry, interaction, etc.) and the program finds the ground state energy and wave function. The examples include nuclear (alpha particle: four-body, $^6$He: six-body), atomic ($td\mu^-$ and $e^+e^-e^+e^-$) and subnuclear (the nucleon and the delta in a nonrelativistic quark model) systems. The solutions are accurate for excited states as well, and even the Efimov-states can be studied. The program is available from the author (e-mail:varga@rikaxp.riken.go.jp).

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I. INTRODUCTION

The solution of few-body problems is an important basic problem of physics. One encounters few-body problems from celestial to quark level in atomic, chemical, nuclear or subnuclear physics. In recent years, due to the intense experimental, theoretical and technological interest in mesoscopic scale systems in solid state physics (few ions in a trap, few electrons in a quantum dot, etc.) the traditional domain of application is greatly enlarged.

In the last few years we have elaborated a powerful technique, the stochastic variational method (SVM) [3,2,1], which is proved to be especially suitable for solution of diverse few-body problems. The stochastic variational method optimizes the variational basis in a random trial and error procedure. The basis selection is free from any bias, keeps the dimension of the basis low, and lastly but most importantly, provides a very accurate solution. The method can be used with different type of bases. The correlated Gaussian basis [4] seems to be particularly suitable for description of \( N = 2 - 8 \) particle systems, while for larger number of particles displaced Gaussian or harmonic oscillator bases can be applied.

The method is a natural extension of the rigorous few-body (\( N = 3, 4 \)) techniques [5-11] to larger systems of strongly correlating particles and offers a wide range of applications.

The aim of this paper is to present a computer code for solution of few-body problems with the stochastic variational method on correlated Gaussian bases. The particles can interact via different central (Coulomb, Yukawa, Gauss or power law or other numerically given) potentials. The interaction may contain spin-isospin dependent operators. The program is general: the number of particles is in principle arbitrary, in practice it is limited by the speed and the memory of the available computer. The method can be used to get very accurate solution for smaller systems or to find an approximate upper bound for larger systems. One can treat bosons and fermions.

The applicability of the program is shown with various examples, including nuclear, Coulombic and quark systems. The accuracy of the solutions are tested by comparing the results to those of the literature. An example of the Efimov-states [12] shows that the method gives precise energies for ground and excited states.

The plan of the paper is as follows. In section 2 we outline the method. In section 3 we show the calculation of the matrix elements. The fortran code is described in section 4. Examples are presented in section 5. The papers ends with a brief summary.

II. THE STOCHASTIC VARIATIONAL METHOD

Let’s consider an \( N \)-particle system, where the \( i \)th particle with mass \( m_i \), spin \( s_i \), isospin \( t_i \) and charge \( z_i \) is placed at the position \( \mathbf{r}_i \). The positions of the particles can be more conveniently described by introducing a set of relative (Jacobi) coordinates \( \mathbf{x} = (\mathbf{x}_1, ..., \mathbf{x}_{N-1}) \) and the coordinate of the centre of mass \( \mathbf{x}_N \). The object of this paper is to solve the many-body Schrodinger-equation

\[
\mathcal{H}\Psi = E\Psi \quad (\mathcal{H} = \sum_{i=1}^{N} \frac{\mathbf{p}_i^2}{2m_i} - T_{cm} + \sum_{i<j}^{N} V_{ij})
\]

for central two-body interactions \( V_{ij} \).
In our variational approach the basis functions are assumed to have the form

\[ \psi_{SMST M_T}(x, A) = \mathcal{A}\{G_A(x)\chi_{SM_S}\eta_{T M_T}\}, \quad G_A(x) = e^{-\frac{1}{2}x^TAx}, \quad (2) \]

where the operator \( \mathcal{A} \) is an antisymmetrizer, \( \chi_{SM_S} \) is the spin function, and \( \eta_{T M_T} \) is the isospin function of the system (for Coulombic system this latter can be suppressed). The diagonal elements of the \((N-1) \times (N-1)\) dimensional symmetric, positive definite matrix \( A \) corresponds to the nonlinear parameters of an Gaussian expansion, and the off diagonal elements connect the different relative coordinates representing the correlations between the particles. This trial function, the correlated Gaussian basis, is widely used in physics [4,13,14], although the applications are mostly restricted to three and four particle systems.

The above form assumes orbital angular momentum \( L = 0 \).

In the variational method the wave function of the system is expanded as

\[ \Psi = \sum_{i=1}^{K} c_i \psi_{SMST M_T}(x, A_i), \quad (3) \]

and an upper bound for the ground state energy of the system is given by the lowest eigenvalue of the generalized eigenvalue problem

\[ HC = E_K BC, \quad (4) \]

where

\[ H_{ij} = \langle \psi_{SMST M_T}(x, A_i)|H|\psi_{SMST M_T}(x, A_j) \rangle, \quad B_{ij} = \langle \psi_{SMST M_T}(x, A_i)|\psi_{SMST M_T}(x, A_j) \rangle \]

(5)

The adequate choice of the nonlinear parameters (the elements of the \((N-1) \times (N-1)\) matrix \( A \)) is crucial. If these parameters are properly optimized, the variational solution gives very precise energies. Although several ways for the choice of elements of \( A \) have been suggested, there is no safe recipe available. While the numerical optimization would be in principle the method of choice, in practice there are several difficulties to face. The most serious ones amongst these are probably the large number of parameters to be optimized and the nonorthogonality of the basis states. Due to the nonorthogonality, none of the parameter sets is indispensable, and several different choices can represent the wave functions equally well. This property makes the optimization tedious but offers the possibility of random selection of the nonlinear parameters.

In the stochastic variational method the most suitable parameters are selected as follows: (1) several sets of \((A^1_1, ..., A^n_K, n = 1, ..., \mathcal{N})\) are generated randomly, (2) by solving the eigenvalue problem the corresponding energies \((E^1_K, ..., E^n_K)\) are determined, (3) the parameter set \((A^1^n, ..., A^n_K)\) belonging to the lowest energy \( E^n_K \) are chosen as basis parameters.

The bottleneck of the above procedure is that it assumes a full diagonalization to solve the eigenvalue problem and beyond a certain dimension it becomes too computer time consuming. In practical implementation it is more advantageous to fix \((A_1, ..., A_{K-1})\) and change only \( A_K \). In this case only one row (column) of the matrices \( H \) and \( B \) has been changed,
and no diagonalization is needed but one can utilize the formulae of ref. [3]. Moreover, as by increasing the number of basis states the energy decreases \((E_{K+1} \leq E_K)\), we found it advantageous to increase the dimension of the basis after selecting the most suitable \(A_K^n\) amongst the random candidates. This step ensures that the energy \(E_K^n\), belonging to a new, randomly selected \((A_K^n)\) basis state, is lower than the energy \(E_{K-1}\) on the previously found basis, and provides a convenient selection criteria. The steps of the most economical way is therefore:

(i) several sets of \((A_K^n, n = 1, \ldots, \mathcal{N})\) are generated randomly,
(ii) by solving the eigenvalue problem the corresponding energies \((E_1^K, \ldots, E_N^K)\) are determined,
(iii) the parameter \((A_K^n)\) belonging to the lowest energy \(E_n^K\) chosen as a basis parameter and by adding it to the previous basis states the parameters of the new basis become \((A_1, \ldots, A_{K-1}, A_K = A_K^n)\),
(iv) the basis dimension is increased to \(K + 1\).

III. MATRIX ELEMENTS

One of the main advantages of the correlated gaussian basis is that its matrix elements can be easily calculated analytically. We list these matrix elements in the following.

The overlap of the correlated Gaussians takes the simple form:

\[
\langle G_A | G_{A'} \rangle = \left( \frac{(2\pi)^{N-1}}{\det(A + A')} \right)^{\frac{3}{2}}.
\]  

(6)

The matrix element of the kinetic energy between the correlated Gaussians reads as:

\[
\langle G_A | \sum_{i=1}^{N} \frac{p_i^2}{2m_i} - T_{cm} | G_{A'} \rangle = \langle G_A | G_{A'} \rangle \left( 3\text{Tr}(\Lambda A) - 3\text{Tr}(A + A')^{-1}(A'\Lambda A') \right),
\]  

(7)

where \(\Lambda\) is an \((N-1) \times (N-1)\) diagonal matrix

\[
\Lambda = \begin{pmatrix}
\frac{h^2}{2\mu_1} & 0 & \cdots & 0 \\
0 & \frac{h^2}{2\mu_2} & \cdots & \vdots \\
\vdots & \ddots & \ddots & \vdots \\
0 & \cdots & 0 & \frac{h^2}{2\mu_{N-1}}
\end{pmatrix},
\]  

(8)

and the reduced masses are given by

\[
\mu_i = \frac{m_{i+1}m_{12\cdots i}}{m_{12\cdots i+1}} \quad (i = 1, \ldots, N-1), \quad \text{and} \quad \mu_N = m_{12\cdots N},
\]  

(9)

with \(m_{12\cdots i} = m_1 + m_2 + \cdots + m_i\).

To avoid the dependence of the matrix elements of the two-body interaction on the specific form of the potential, it is advantageous to express the potential in the form

\[
V(r_i - r_j) = \int dr V(r) \delta(r_i - r_j - r).
\]  

(10)
To calculate the matrix elements of the potential we first express the relative distance vector $r_i - r_j$ by the Jacobi coordinates. The Jacobi coordinates are defined as

$$x_i = \sum_{j=1}^{N} U_{ij} r_j,$$

with

$$U = \begin{pmatrix}
-1 & 1 & 0 & \ldots & 0 \\
\frac{m_1}{m_{12}} & -\frac{m_2}{m_{12}} & 1 & \ldots & 0 \\
\vdots & \vdots & \ddots & \ddots & \vdots \\
-\frac{m_1}{m_{12\ldots N-1}} & -\frac{m_2}{m_{12\ldots N}} & \ldots & \ldots & 1 \\
\frac{m_1}{m_{12\ldots N}} & \frac{m_2}{m_{12\ldots N}} & \ldots & \ldots & \frac{m_N}{m_{12\ldots N}}
\end{pmatrix},$$

The relative distance vector between two particles then can be written as

$$r_i - r_j = \sum_{k=1}^{N-1} B_{ijk} x_k, \quad B_{ijk} = U_{ik}^{-1} - U_{jk}^{-1}.$$  

By using this expression the matrix element of the potential is given by:

$$\langle G_A | \delta(r_i - r_j - r) | G_{A'} \rangle = \langle G_A | G_{A'} \rangle \left( \frac{1}{2\pi p_{ij}} \right)^{\frac{3}{2}} e^{-\frac{r^2}{2p_{ij}}}$$

where

$$p_{ij} = \sum_{k=1}^{N-1} \sum_{l=1}^{N-1} B_{ijk}(A + A')_{ki}^{-1} B_{ijl}.$$  

By integrating eq. (14) over $r$ one can recover the norm of the wave function. To calculate the matrix element of the potential one has to multiply eq. (14) by the radial form $V(r)$ and integrate over $r$:

$$\langle G_A | V_{ij} | G_{A'} \rangle = \int dr V(r) \langle G_A | \delta(r_i - r_j - r) | G_{A'} \rangle = \langle G_A | G_{A'} \rangle v(p_{ij}),$$

where

$$v(p_{ij}) = \left( \frac{1}{2\pi p_{ij}} \right)^{\frac{3}{2}} \int dr V(r)e^{-\frac{r^2}{2p_{ij}}}$$

In the applications the two-body interaction is expressed as

$$V_{ij} = \sum_{i=1}^{N_a} \left( \sum_{k=1}^{N_i} V_i^k(|r_i - r_j|) \right) \mathcal{O}_i,$$

where the operators ($\mathcal{O}_1, \ldots, \mathcal{O}_4$) are the Wigner, Majorana, Bartlett and Heisenberg operators.
If the radial part can be given in the form

$$V_{ki}(r) = r^n e^{-ar^2 + br}(n \geq -2), \quad (19)$$

then the integration can be calculated analytically by using the formula

$$\int_0^\infty dr r^n e^{-ar^2 + br} = \frac{1}{2} (-1)^n \sum_{k=0}^{n} \frac{n!}{(n-k)!k!} f(k) g(n-k), \quad (20)$$

$$f(k) = \left( \frac{1}{2p} \right)^{k/2} \frac{k!}{i!(k-2i)!} q^{k-2i} p^i \quad (21)$$

$$g(0) = \text{erfc}(y), \quad g(k) = (-1)^k \frac{2}{\sqrt{\pi}} \left( \frac{1}{2\sqrt{p}} \right)^k H_{k-1}(y), \quad (k > 1), \quad y = \frac{q}{2\sqrt{p}}. \quad (22)$$

In other cases one has to rely on a numerical integration. To calculate the matrix elements, the function $v(p)$ has to be evaluated many times for many different values of $p$. Both the analytical and the numerical evaluation takes some time on the computer. This part of the computation can be made faster, however, noticing that $v(p)$ is a rather simple smooth function of $p$ and it can be easily interpolated. To this end, for a given potential we tabulate $v(p)$ at certain representative values of $p$ and during the computation of the matrix elements $v(p)$ is interpolated in the necessary points. The precision of the interpolation can be easily controlled.

IV. SYMMETRIZATION

The antisymmetrizer $A$ is defined as

$$A = \sum_{i=1}^{N!} p_i P_i, \quad (23)$$

where the operator $P_i$ changes the particle indices according to the permutation $(p_1^i, \ldots, p_N^i)$ of the numbers $(1, 2, \ldots, N)$, and $p_i$ is the parity of that permutation. The effect of this operator on the set of position vectors $(r_1, \ldots, r_N)$ is

$$P_i(r_1, \ldots, r_N) = (r_{p_1^i}, \ldots, r_{p_N^i}) \quad (24)$$

By representing the permutations by the matrix

$$(C_i)_{kj} = 1 \quad \text{if} \quad j = p_k^i \quad \text{and} \quad (C_i)_{kj} = 0 \quad \text{otherwise}, \quad (25)$$

(for example, if $N = 3$ the permutation $(3 1 2)$ is represented by

$$C = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}. \quad (26)$$
while for \((1\ 2\ 3)\) \(C\) is a unit matrix, the effect of the permutation operator on the single particle coordinates

\[ P_i(r_1, ..., r_N) = C_i(r_1, ..., r_N). \]  

(27)

By using eqs. (11) and (27) the permutation of the relative coordinates is expressible as

\[ \mathcal{P}_i x = P_i x, \]  

(28)

where \(P_i\) is an \((N - 1) \times (N - 1)\) matrix obtained by omitting the last row and column (corresponding to the permutation invariant center-of-mass coordinate) of the \(N \times N\) matrix \(U^T C_i U\).

The correlated Gaussian function, after permutation takes the form:

\[ \mathcal{P}_i G_A(x) = G_{P_i^T A P_i}(x). \]  

(29)

This simple transformation property under permutation is particularly useful in calculating the matrix elements of the antisymmetrized basis functions.

In the spin-isospin space the permutation operator interchanges the indexes the single particle spin-isospin functions and can be easily evaluated.

V. PROGRAM DESCRIPTION

A. Fortran code

To prepare the data for the calculation, the main program calls the following subroutines:

- \textbf{input data}: This subroutine reads the input files described in the previous subsection.
- \textbf{cm_rel_tr}: This subroutine is responsible for the separation of the relative and centre-of-mass coordinates.
- \textbf{me_spiso}: The overlap of the spin-isospin part, and the \(P_i\) matrices are calculated in this segment.

The matrix elements of the kinetic energy and potential energy are calculated in the subroutines \textbf{vkin_ene} and \textbf{vpot_ene} by using the formulae (7) and (16). The overlap of the basis states, given by eq. (6), is computed in \textbf{vove_mat}. The subroutine \textbf{mat_elem} prepares the matrices \(H\) and \(B\) of eq. (4).

The parameters of the basis states can be selected in three ways. The first (s1) is a direct calculation on a given basis, the second (s2) and third (s3) are two versions of the stochastic selection of the basis states.

- (s1) One can use predefined basis. In this case, the parameters of the basis has to be written in the file “fbs.res”. The first line of this file defines the number of basis states \(K\). In the next lines the parameters of the basis are listed. Each line contains the corresponding nonlinear parameters \((A_k)_{ij} \ (k = 1, ..., K)\).
- (s2) One can select the parameters randomly and set up the basis step by step increasing the dimension, as described by (i)-(ii)-(iii)-(iv). This is a rather automatic procedure, the only
thing one has to define before starting is the interval from which the uniformly distributed random numbers are generated.

(S3) One can select the basis states through the steps (i)-(ii)-(iii), on a fixed basis dimension $K$. Before starting this procedure, one has to give initial values of the nonlinear parameters. Then a basis state, say the last one (the $K$th) is subjected to the procedure (i)-(ii)-(iii). If a better new parameter set is found, then the $K$th state is substituted by the new parameters. This procedure is repeated several times cyclically for the other elements of the basis as well. We refer to this step as refinement because in this way we can further improve a basis. Particularly, the bases, selected in the (s1) or the (s2) manner can be refined with this method.

The subroutines \texttt{preset, svm1, svm2} corresponds to the three possibilities above. To select amongst the three possibilities the value of ico should be set to 1, 2 or 3.

One does not need to solve the whole eigenvalue problem in each time when a basis parameter is changed. The program utilizes the simplifications described in ref. \[3\].

The function \(v(p)\) in eq. (17) can be calculated in three ways.

(p1) One can numerically integrate over the radial coordinate in eq. (17) for given values of \(p\) and tabulate the function \(v(p)\). This tabulation can be done before the real calculation is started. During the basis selection, one needs the value of \(v(p)\) at arbitrary values of \(p\) and these values will be approximated by interpolation.

(p2) If the potential is linear combination of terms like in eq. (18) one can use the analytical formula (19).

(p3) In this case we numerically integrate over the radial variable in eq. (17) for each value of \(p\) that appear during the basis selection. The difference between this case and the first one is that as the actual value of \(p\) is available only during the basis selection process, this numerical integration can only be done then.

The order of the above three possibilities reflects their speeds. The first way is the fastest by far, but it accumulates the inaccuracies of the numerical integration and interpolation. In most of the practical cases these inaccuracies can be kept under control. The second case is slower but it is exact for Coulomb, linear, harmonic oscillator, Gaussian and Yukawa potentials. The third case is quite slow. The recommended way is to use the first possibility for the basis selection. Once the selection is finished, the chosen basis can be considered as a predefined basis and one can rerun the calculation on that basis recalculating the matrix elements by the (p1) or (p2) method. The accuracy of the numerical integration is controlled by the variable \(eps\). To check the accuracy of the numerical integration one may rerun the calculation for different values of \(eps\).

To select amongst (p1)-(p2)-(p3) one has to create a file “pot.inp” and write a number “ipcon” (ipcon=1,2 or 3) into its first line. In the case (p2) one should write the parameters of the potentials into the file “pot.inp” as well. The number of the linear combinations of terms like eq. (17) should be written into the second line. It is to be followed by the coefficient of the linear combination, and the parameters \(a, b, n\) of the terms in the successive lines, in turn. In the cases (p1) and (p3), the radial form of the potential should be defined in the subroutine “pot” by the user. The value of “pot” should be equal to the value of the two-body potential at the radial distance “x”. 

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B. Selection of nonlinear parameters

The Jacobi coordinates are convenient, because the kinetic energy can be expressed simply (eq. (1)). The choice of the nonlinear parameters, however, is simpler in a coordinate system, where the interparticle distances \( r_i - r_j \) are used. The basis function in that system takes the form:

\[
\exp\{-\sum_{i<j} \alpha_{ij} (r_i - r_j)^2\}.
\]

The elements of \( A \) in \( G_A(x) \) can be expressed by \( \alpha_{ij} \) using an appropriate linear transformation. The advantage of \( \alpha_{ij} \) is that it is more directly connected to the interparticle distances and it can be more uniformly used. In the practical applications \( \alpha_{ij} \) are generated as random numbers from the \([b_{\text{min}}, b_{\text{max}}]\) interval. The elements of \( A \) are then expressed by using the values of \( \alpha_{ij} \).

Although one can choose the elements of \( A \) (through \( \alpha_{ij} \)) independently of each other randomly, we have found that it is slightly more advantageous to follow the following way. At first, one generates random values for each element. Then the first element of the matrix changed randomly \( K_0 \) times. The best (giving the lowest ground state energy) parameter is selected and fixed. The second element is fixed in the same way and this process is continued till the last element. This procedure is then repeated \( M_0 \) times. This selection requires \( N_0 \times M_0 \) evaluations. Only one element of the matrix of the nonlinear parameters is changed in each step and that leads to the possibility of fast evaluation.

C. Input data

The input data specifies the system and the interaction. One has to define the number of particles, the spins, isospins, charges and masses. The spin and isospin states are represented by integers, the 'down' state is coded as 1 and the 'up' state is coded as 2. The input data is read from the input file “fbs.inp”. The first line defines the number of particles \( N \), the second line lists the masses of particles \((m_1, \ldots, m_N)\), the third line gives the charges \((z_1, \ldots, z_N)\), the fourth the isospins \((t_1, \ldots, t_N)\). The spin part of the system can be given as linear combination of spin states. The next line contains the number of linear combinations, and the succeeding lines give the linear combination coefficients and the spin states. The following line should contain the value of \( \hbar^2/m \), an initial (negative integer) number for the random number generator and the control parameters \( ico \) and \( ibf \). The first parameter selects the method of basis optimization \((s1),(s2)\) or \((s3)\), while the second defines the symmetry of identical particles \((ibf=1\text{ for fermions and }ibf=2\text{ for bosons})\). The next line gives \( M_0, K_0 \) and \( K \). The program generates random numbers for a given nonlinear parameter, say \( A_{11} \) \( K_0 \) times, and once the best parameters for all \( A_{ij} \) has been found this random selection is repeated \( K_0 \) times.

In the fortran program, the parameter “mmbas” and ”mmpar” defines the maximum number of basis states and the maximum number of particles, respectively.
D. Output data

The main results of the calculation are the energies of the ground and excited states and the wave function. The energies are written in the file “ener.dat”. The basis dimension, the coefficients of the wave function of the ground state and the nonlinear parameters of the basis are in the file “fbs.res” after the calculation is finished.

VI. EXAMPLES

In this part we show a few examples for the application of the program. The computational time varies for different cases and strongly depends on the basis size and on the number of particles.

A. The $td\mu^-$ and the positronium molecule

This example includes a three- and a four-body system with Coulomb interaction. The $td\mu^-$ molecule is a bound system of two positively and a negatively charged particles with unequal masses. This system attracted considerable attention in connection with the muon catalysed fusion [15]. The input parameters (the input files) are shown in Table I. Atomic units are used. The isospin quantum number is not necessary in these systems so it just stands for distinguishing of the particles with different charges. The matrix elements of the Coulomb-potential can be analytically calculated and thus the second way (p2) is used.

One can start the calculation by a step-by-step random selection of the basis states (s2-type, $ico=2$). The first four digits of the ground state energy can be reproduced on a basis size of $K = 50$ (see Table II.). To improve the energy on this basis size further, one is to restart the calculation with a refinement circle (s3-type, $ico=3$). By repeating the refinement three times, the fifth digits of accuracy can be reached. By increasing the basis size more accurate result can be found in need. The energies in the tables are written into the output file ”ener.dat”.

One can solve the two-body problem as well. The above example can be recalculated for two-body case ($t\mu^-$), by changing the number of particles to 2 in the input file. One immediately arrives at the energy of the ($t\mu^-$) threshold (-99.64 a.u.).

The next example is the positronium molecule, the $e^+e^-e^+e^-$ Coulomb four-body system. This system has been subject of quite a few study, but accurate calculations have become available only recently [3,13,14]. In this case we have four particles with equal masses and a nonadiabatic treatment is necessary. The spins of the particles are coupled to $S = 0$. This spin coupling leads to a more symmetric system and the convergency is much faster. Due to the mass difference between the particles in this and in the previous case, the interval of the random numbers are to be chosen differently. The input files are in Table III. The basis selection follows the same way as in the previous example and the results are compared in Table IV. to those of other calculations. To increase the accuracy further one has to use a larger basis. It is remarkable that this calculation, after refining cycles, gives very close results on a basis dimension of $K = 50$ to that of refs. [1,13,14] with $K = 300$ Correlated Gaussians.
To see the tremendous effect of the spin coupling on the convergence one may try to rerun the same calculation with using only one of the spin configurations.

B. The alpha particle and the $^6$He

In this subsection we describe the application of the program for nuclear systems with a simple central interaction. A four- and a six-body system (the alpha particle and $^6$He) are chosen as example.

In the first example of this subsection the ground state energy of the alpha particle is calculated with the central, spin-isospin independent Malfleit-Tjon V [14] (MTV) interaction. The input is given in Table V. The spin coupling is the same as in the case of the positronium molecule. Although the potential matrix elements are analytical as before, the first representation (p1) is suggested as an illustrative example. To this end one has to write a function (in fortran) “pot(r)” which defines the MTV potential. The program runs faster with this choice and the accuracy is still appropriate for nuclear systems. The results are compared to other calculations in Table VI.

The next example is a six-body system. Usually only the Quantum Monte Carlo [5,10] methods are capable of going beyond four particles. In this example we try to solve the $^6$He with the central, spin-isospin dependent Minnesota potential [17]. The potential, though again analytical, is used in numerical form as a fortran function. To illustrate another option, this example uses a predefined basis ($ico=1$, $s1$-type). The predefined basis is to be included in the file “fbs.res”. (The program package contains this file under the name “fbs1.res”.)

C. The nucleon and the delta in a nonrelativistic quark model

In this example the SVM is used to solve the nonrelativistic three-quark problem. The nonrelativistic three-quark model of baryons has a long history (see e.g. refs. [18-21]). Many of the properties of the baryons are quite successfully explained in this framework [18,19,21]. In this section we solve the three-body Schrödinger with a one-gluon exchange potential [20]

$$V_{ij} = \frac{1}{2} \left( -\frac{\kappa}{r_{ij}} + \frac{r_{ij}}{a} - D + V_0 e^{-r_{ij}/r_0} \sigma_i \cdot \sigma_j \right)$$

(31)

for the nucleon and the delta. The parameters of the potential is taken from ref. [20]. The three-quark problem with this potential has been studied in the framework of the Faddeev-equations in ref. [21]. We use the same parameters and compare our results to theirs.

The potential has no dependence on color degrees of freedom therefore the antisymmetric color part of the wave function can be factorized and the spin-flavor-space part of the wave function must be symmetric (the control parameter “ibf” should be set to 2). The input files for the nucleon and the delta differ in the spin- and isospin- (flavor) part (see Table ). The potential is given in a numerical form (ipcon=1). The quark masses is taken to be 337 MeV like in ref. [21].

Due to the confining potential the basis size required for a reasonably accurate solution is very small. After suitable modifications of the symmetrization of the wave function the program can be used to calculate other baryons as well [22].
D. The Efimov states

The last example shows the application for Efimov states [12]. A three-body system with short range forces may have several bound states. If the two-body subsystem have just one bound state whose energy is (close to) zero, the three-particle can interact at long distances and an infinite number of bound state may appear in the three-body system. These "Efimov states" are extremely interesting from both experimental and theoretical points of view because of their distinct properties. These states are very loosely bound and their wave functions extend far beyond those of normal states. By increasing the strength of the two-body interactions these states disappear.

A three-boson system is considered, for simplicity. In this case we have three spinless identical particles with a symmetrized spatial wave function. The potential between the particles is taken as a the Pösch-Teller interaction because this potential is analytically solvable for the two-body case, and therefore the two-body binding energy can be easily set to zero. A spatially very extended basis is needed to represent the weakly bound states. In this case we use a predefined basis (s1). The predefined basis is created by using only the diagonal elements of the matrix $A$. These diagonal elements are taken as geometric progression:

$$(A_k)_{11} = \frac{1}{(a_0 q_0(i-1))^2} \quad (A_k)_{22} = \frac{1}{(a_0 q_0(j-1))^2} \quad (i = 1, ..., n, \quad j = 1, ..., n, \quad k = (n-1)i + j).$$

(32)

This construction defines an $n \times n$ dimensional basis. The parameters are chosen as $n = 20, a_0 = 0.1, x_0 = 2.4$. (This predefined basis can be found in the file “fbs2.res”.) To try this example one has to use the potential function "pot" with the Pösch-Teller potential [23]:

$$V(r) = \frac{625.972}{\sinh(1.586 \cdot r)^2} - \frac{1251.943}{\cosh(1.586 \cdot r)^2}.$$  

(33)

The result of this calculation is given in Table XI. One can find the first three Efimov states with this basis size. The ratios of the energies of the bound states follow the $E_{i+1}/E_i = \exp\{-2\pi\}$ rule [12]. By increasing the basis size one can reveal more bound excited states. Note that the value of $a_0 x_0^n$ roughly corresponds to the spatial extension of the basis. The present basis in this example goes out up to $a_0 x_0^n = 0.1 \times 2.4^9 = 1674990$ (fm). This extension is necessary to get the third bound state. As a comparison, to calculate the ground state energy ($-4.81$) it is enough to choose $n = 7$ and the basis covers only the $[0, 10]$ (fm) interval. The root mean square radii of the ground state is about 1.5 fm, while that of the first excited state is about 6000 fm. These facts illustrate the tremendous spatial extension of the Efimov states.

VII. SUMMARY

A fortran program is presented which solves the few-particle Schrödinger- equation by using the stochastic variational method. The usefulness and applicability of the method is
illustrated on various examples. The program can be used to solve diverse few-body problems. The stochastic variational method selects the most important basis states and keeps the basis size low even for six-body problems. The solution with the SVM is “automatic” and universal. One defines the system (number of particles, masses, symmetry, interaction, etc.) and the program finds the ground state energy and wave function. The refining steps [24,25] applied here increase the accuracy further. The number of particles can be easily increased up to a certain (computer dependent) limit. The program can be used without the SVM, by using a predefined basis as well.

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# TABLES

## TABLE I. Input files for the $td\mu$ system.

|        | fbs.inp | pot.inp |
|--------|---------|---------|
| 3      | number of particles | 2 | $\frac{\hbar^2}{m}$, $\text{iran}$, $\text{ico}$, $\text{ibf}$ |
| 206.786,5496.918,3670.481 | masses of particles | 1,0,-14491,2,1 | $M_0, K_0, K$ |
| $-1,1,1$ | charges of particles | 5,100.50 | $b_{\min}, b_{\max}$ |
| 1 | isospins | 0.000001,0.1 |
| $1.,1,2,1$ | number of spin configurations | | |
| $1.0,-14491,2,1$ | coefficient,spins | | |
| 5,100,50 | | | |
| 0.000001,0.1 | | | |

## TABLE II. Results for the $td\mu$ system. (In atomic units.)

| Energy | basis selection |
|--------|-----------------|
| $-111.291$ a.u. ($K = 50$) | (s2)-type |
| $-111.342$ a.u. ($K = 50$) | (s2)-type followed by an (s3)-type |
| $-111.360$ a.u. ($K = 50$) | (s2)-type followed by 3 times (s3)-type |
| $-111.36444$ a.u. ($K = 200$) | ref. [25] |
| $-111.36451$ a.u. ($K = 1442$) | ref. [15] |
TABLE III. Input files for the positronium molecule.

| fbs.inp | pot.inp |
|---------|---------|
| 4       | 2       |
| 1,1,1,1,1. | 1,0,0,0.1,15. |
| 1,1,−1,−1 | 1.0,−14491,2 |
| 1,1,2,2 | 5,25,50 |
| 4       | 0,1,15. |
| 1,1,2,1,2 | h^2/m, iran, ico, ibf |
| -1,1,2,2,1 | M_0, K_0, K |
| -1,2,1,1,2 | b_{\text{min}}, b_{\text{max}} |
| 1,2,1,2,1 |

TABLE IV. Results for the positronium molecule. (Atomic units are used.)

| Energy     | basis selection                                      |
|------------|------------------------------------------------------|
| −0.51548 a.u. (K = 50) | (s2)-type                                             |
| −0.51575 a.u. (K = 50) | (s2)-type followed by an (s3)-type                   |
| −0.51586 a.u. (K = 50) | (s2)-type followed by 3 times (s3)-type              |
| −0.51600 a.u. (K = 300) | refs. [1,13,14]                                       |
### TABLE V. Input files for the alpha particle.

| fbs.inp |             |
|---------|-------------|
| number of particles | 4           |
| masses of particles | 1,1,1,1    |
| charges of particles | 1,1,2,2    |
| isospins | 4           |
| number of spin configurations | 1,1,2,1,2 |
| coefficient, spins | -1,1,2,2,1 |
| -1,2,1,1,2 |            |
| 1,2,1,2,1 |             |
| $41.47, -14491, 2$ | $h^2/m, \text{iran, ico, ibf}$ |
| $5,25,50$ | $M_0, K_0, K$ |
| $0,1,15.$ | $b_{\text{min}}, b_{\text{max}}$ |

| pot.inp |             |
|---------|-------------|
| ipcon |             |
| $N_0, N_t$ |             |
| parameters of the potential | 0,0,0,0,0 |

### TABLE VI. Results for the alpha particle. (In MeV.)

| Energy | basis selection |
|--------|-----------------|
| $-31.30 \ (K = 100)$ | (s2)-type |
| $-31.32 \ (K = 100)$ | (s2)-type followed by an (s3)-type |
| $-31.33 \ (K = 100)$ | (s2)-type followed by 3 times (s3)-type |
| $-31.36 \ (K = 150)$ | ref. [3] |
### TABLE VII. Input files for the $^6$He.

| fbs.inp       |                  |                  |                  |                  |
|--------------|------------------|------------------|------------------|------------------|
| 6            | 1.,1.,1.,1.,1.,1. | 1,1,1,1,1,1,1,1,1 | 1,1,2,2,2,2,2,2 | 1               |
|              | 1,1,1,1,1,1,1,1,1 | 1,1,1,1,1,1,1,1,1 | 1,1,1,1,1,1,1,1,1 | 1,1,1,1,1,1,1,1,1 |
|              | 41.47,−14491,2   | 5,25,50          | 0,1,1,5          |                 |
|              |                  |                  |                  |                  |
| pot.inp      | 1                | ipcon            |                  |                  |
|              | 1,1              | No, Nt           |                  |                  |
|              | 0,0,0,0,0        |                  |                  |                  |

### TABLE VIII. Results for the $^6$He. (In MeV.)

| Energy      | basis selection |
|-------------|-----------------|
| −30.00 ($K = 100$) | (s1)-type        |
| −30.07 ($K = 300$) | ref. [3]        |

### TABLE IX. Input files for the nucleon and the delta particle.

| fbs.inp (nucleon) |                  |                  |                  |                  |
|-------------------|------------------|------------------|------------------|------------------|
| 3                 | 1.,1.,1          | 1,1,1,1          | 1,2,2            | 1,1,2,1          |
|                   |                 | 1,1,1           | 1,2,2            | 2 |                   |
|                   | 1,1,1,1,1,1,1,1,1 | 1,1,1,1,1,1,1,1,1 | 1,1,2,2,2,2,2,2 | 1,1,1,1,1,1,1,1,1 |
|                   | 115.54,−14491,2,2 | 5,25,50          | 0,1,1,8,0        |                 |
|                   |                  |                  |                  |                  |
| fbs.inp (delta, spin-isospin part only) |                  |                  |                  |                  |
| 1,1,1            |                 |                  |                  |                  |
| 1               |                  |                  |                  |                  |
| 1,1,1,1          |                  |                  |                  |                  |
### TABLE X. Results for nucleon and delta (in MeV) (3*337 MeV is added).

| Energy       | basis selection |
|--------------|-----------------|
| Nucleon      |                 |
| 1021 (K = 10)| (s2)-type       |
| 1024         | ref. [21]       |
| delta        |                 |
| 1330 (K = 5) | (s2)-type       |
| 1330         | ref. [21]       |

### TABLE XI. Input files for the Efimov states.

**fbs.inp (nucleon)**

- 3: number of particles
- 1., 1., 1.: masses of particles
- 1, 1, 1: charges of particles
- 1, 1, 1: isospins
- 1: number of spin configurations
- 1., 1, 1, 1: coefficient, spins
- 41.47, −14491, 1, 2: $\hbar^2/m, \text{iran, ico, ibf}$
- 5, 25, 50: $M_0, K_0, K$
- 0, 1, 15.: $b_{\text{min}}, b_{\text{max}}$

**pot.inp**

- 1: ipcon
- 1, 1: $N_o, N_t$
- 0, 0, 0, 0: parameters of the potential

**output: ener.dat**

- dimension: 400
- energy(1): −4.81
- energy(2): $−8.77 \times 10^{-3}$
- energy(3): $−1.50 \times 10^{-5}$