Stochastic variational method with a correlated Gaussian basis

K. Varga [1,2,3] and Y. Suzuki [2]
[1] *RIKEN, Hirosawa, Wako, Saitama 351-01, Japan*
[2] *Department of Physics, Niigata University, Niigata 950-21, Japan*
[3] *Institute of Nuclear Research of the Hungarian Academy of Sciences, Debrecen, H-4001, Hungary*
(Received 27 July 1995)

Variational solutions are given for problems involving diverse fermionic and bosonic $N=2-7$-body systems. The trial wave functions are chosen to be combinations of correlated Gaussians, which facilitate a fully analytical calculation of the matrix elements. The nonlinear parameters of the trial function are selected by a stochastic technique. The method has proved efficient, accurate, and seems feasible for any few-body bound-state problems emerging in atomic or nuclear physics.

PACS number(s): 31.15.Pf, 21.45.+v

The solution of the many-body Schrödinger equation for bound states of more than two particles is generally difficult. To treat an N-body system one needs to cope with the large number of variables required to specify the wave function. By using $N-1$ relative coordinates to describe the system, for example, the discretization on a mesh with p points, or the expansion of the relative wave functions in terms of p suitable chosen functions, leads to $p^{(N-1)}$ numbers or basis functions, which becomes prohibitively large as the number of particles increases.

The variational foundation for the time-independent Schrödinger equation provides a solid and arbitrarily improvable framework for the solution of bound-state problems. The crucial point of the variational approach is the choice of the trial function. There are two widely applied strategies: (1) to select the most appropriate functional form to describe the short-range as well as long-range correlations and to compute the matrix elements by Monte Carlo technique, or (2) to use a number, possibly a great number, of simple terms, which facilitate the analytical calculation of the matrix elements. We follow the second course by using an expansion over a correlated Gaussian "basis" [1]. An N-particle basis function looks like

$$\Phi_{(LS)JM}(\mathbf{x},\underline{a})=\mathscr{A}\{e^{-1/2\mathbf{x}\underline{a}\mathbf{x}}[\theta_L(\mathbf{x})\phi_S]_{JM}\}, \qquad (1)$$

where $\mathbf{x}=\{\mathbf{x}_1,\ldots,\mathbf{x}_{N-1}\}$ is a set of Jacobi coordinates, $\underline{a}$ is a positive-definite, symmetric matrix of nonlinear parameters, specific to each basis element, $\theta_{LM_L}(\mathbf{x})$ is a vector-coupled product of solid spherical harmonics, ϕ_S is the spin function, and $\mathscr{A}$ is an antisymmetrizer (or, for bosons, a symmetrizer). The quantum numbers of the intermediate couplings are suppressed. Note that the form (1) encompasses Gaussian products, $\exp\{-\frac{1}{2}\Sigma_i a_i' x_i'^2\}$, of any sets of Jacobi coordinates $\mathbf{x}'$, thereby allowing for various correlations flexibly. The correlated Gaussian basis functions proved to be an accurate tool and is widely used in atomic and molecular physics [2–4].

The variational approximation, however, may run into difficulties for the following reasons: (i) when the nonlinear parameters are varied, it is difficult to optimize them, (ii) when they are not, then the number of terms required may be excessively large, and, in both cases, (iii) the properly symmetrized trial function becomes extremely involved. We show, however, that instead of performing an optimization, it is expedient to choose these parameter sets randomly and keep or discard them by trial and error. The original procedure of the stochastic variational method (SVM) proposed in [5] has recently been greatly developed and sussessfully applied to multicluster descriptions of light exotic nuclei, such as $^6\mathrm{He}=\alpha+n+n$, $^8\mathrm{He}=\alpha+n+n+n+n$, $^9\mathrm{Li}=\alpha+t+n+n$, and $^9\mathrm{C}=\alpha+^3\mathrm{He}+p+p$ [6,7]. By learning from these applications, we have now generalized and refined the method further. At this stage of maturity the method appears to be powerful and generally applicable in few-body physics.

Conventional methods [2,8] for the choice of Gaussian parameters lead to prohibitively large bases for more than three or four particles as shown above. However, due to the nonorthogonality of the basis functions, there are different sets of $\underline{a}$ that represent the wave function equally well. This enables one to select the most appropriate parameters randomly. As one more basis state always lowers the energy, its "utility" may be quantified by the energy gained by including it in the basis. We set up the basis stepwise by choosing $\underline{a}$ from a preset domain of the parameter space. In the first step we select a number of parameter sets $\underline{a}$ randomly, and we keep the one that gives the lowest energy. Next we generate a new random set and calculate the energy with this two-element basis. If the energy gain is larger than a preset value ϵ, then we admit this state to the basis, otherwise we discard it and try a new random candidate. A discarded state is not excluded from the calculation but can be tested again at a later stage. This process is repeated until the energy converges. The rate of convergence can be controlled by dynamically decreasing the value of ϵ during the search. This procedure is superior to earlier versions [5,6] and, although not a full optimization, results in very good and relatively small bases. A similar procedure, called "stochastic diagonalization" has been used to determine the smallest eigenvalue of extremely large matrices [9].

To keep the computational cost at minimum, the following scheme has been developed. With a $K\times K$ matrix diagonalized, the inclusion of the $(K+1)$th element results in a

matrix whose elements are only nonzero in the $(K+1)$th row and column and in the diagonal. The lowest eigenvalue of this simple matrix, the only one required for judging the utility of a candidate, is calculated by an explicit formula. When a suitable $(K+1)$th basis state has been found, the Hamiltonian matrix is to be rediagonalized, but that is also relatively simple if we take advantage of its special form. Thus the random selection procedure does not involve a great number of time-consuming diagonalizations. Most computing time is spent on the evaluation of the matrix elements.

We have used a systematic analytical method for evaluating matrix elements. This procedure is different from the conventional way of evaluating the matrix elements of the correlated Gaussians [2–4]. As the symmetrization postulate can be most easily imposed on single-particle coordinates, we start from a properly symmetrized product of single-particle functions. The calculation consists of three steps: (i) evaluation of the N-body matrix elements in a single-particle (SP) generator-coordinate (GC) representation, (ii) transformation from the SP GC's to Jacobi GC's, and (iii) integral transformation from the GC's to the parameters $\underline{a}$ of the correlated Gaussian basis. The N-body functions used in step (i) are Slater determinants (or, for bosons, ''Slater permanents'') of the SP functions

$$\phi(\mathbf{r}_i,\mathbf{s}_i)=(2\nu/\pi)^{3/4}\exp[-\nu(\mathbf{r}_i-\mathbf{s}_i)^2]\chi_{\sigma\tau}, \qquad (2)$$

where $\chi_{\sigma\tau}$ are the spin-isospin functions. The N-body matrix elements, given in closed analytic forms as functions of the GC's, are then subjected to orthogonal transformations in the second step. The dependence on the center-of-mass GC thus factors out, and, by omitting this factor, the center-of-mass motion itself is eliminated. The integral transformation between the Jacobi GC vectors and $\underline{a}$ is similar to that given by [10]. For the potential-energy matrix elements first a generic form is evaluated by replacing the spatial factor of the two-particle interaction with $\delta(|\mathbf{r}_j-\mathbf{r}_i|-r)$. The resulting expression consists of terms of the form of $D(r)\sim r^k e^{-pr^2}$, and from these the matrix element of any $V(r)$ is obtained via $\int_0^\infty D(r)V(r)dr$. This calculation scheme of matrix elements is a generalization of the techniques used in nuclear cluster models [10]. The details of the evaluation of the matrix elements will be given elsewhere [11]. The dependence of the matrix elements on $\underline{a}$ being known, one can organize the numerical calculations involved in the random search economically. A change of the value of $\underline{a}$ does not require recalculation of the whole matrix element, and a change of Jacobi coordinates $\mathbf{x}$ is also just a matter of setting $\underline{a}$. Once the matrix elements have been calculated for one value of $\underline{a}$, to calculate them for many more requires virtually no time. This organization is again an essential prerequisite of performing extensive calculations.

To make $\underline{a}$ positive definite, it is expressed as $\underline{a}=\underline{u}\,\underline{d}\,\underline{u}^t$, where $\underline{u}$ is an $(N-1)\times(N-1)$ orthogonal matrix containing $(N-1)(N-2)/2$ parameters and $\underline{d}$ is a diagonal matrix with $N-1$ positive parameters. Although no restriction on $\underline{u}$ is necessary, we found that those transforming $\mathbf{x}$ into other Jacobi coordinates are especially suitable, and used only such $\underline{u}$, so as to alternate the Jacobi coordinates in a random sequence.

TABLE I. Energies and rms radii of electron-positron systems treated as fermions (f) and as bosons (b). Atomic units are used.

System	Method	E	$\langle r^2\rangle^{1/2}$	K
(e^+,e^-) b,f	SVM	-0.25	1.732	10
	exact	-0.25	1.732	
$(2e^+,e^-)$ b,f	SVM	-0.262004	4.592	150
	Var. [12]	-0.26200507	4.594	700
$(2e^+,2e^-)$ b,f	SVM	-0.515989	3.608	300
	Var. [4]	-0.515980	3.600	300
$(3e^+,2e^-)$ f	SVM	no bound states found		1000
$(3e^+,2e^-)$ b	SVM	-0.5493	3.53	200
$(3e^+,3e^-)$ f	SVM	no bound states found		1000
$(3e^+,3e^-)$ b	SVM	-0.820	3.42	300
	Var. [13]	-0.789		5

In the following we show tables for the ground-state energies E and point-matter root-mean-square (rms) radii $\langle r^2\rangle^{1/2}$ calculated with the SVM for some few-body systems with different interactions. The basis dimensions K of the SVM listed in the tables are those beyond which the energies and the radii do not change in the digits shown. Each calculation was repeated several times to confirm the convergence. The average computational time is 10 min for a four-body and 2 h for a six-body calculation on the VPP500 computer at the Institute of Physical and Chemical Research (RIKEN).

As is shown in Table I, the method works for the pure Coulomb interaction. For the ground state of $(2e^+,e^-)$, our calculation reproduces the first six digits of the variational calculation of Ref. [12], and the rms radius also agrees with it. For the dipositronium molecule $(2e^+,2e^-)$ our result is slightly better than the energy calculated [3,4] with a trial function similar to that of Ref. [12], but now containing many more nonlinear parameters. This shows the powerfulness of the random selection of the parameters. We found no bound states for the $(3e^+,2e^-)$ and $(3e^+,3e^-)$ systems. The energy of $(3e^+,3e^-)$, for example, converges to the sum of the energy of a dipositronium molecule and of a positronium ($0.515989+0.25$ a.u.$=0.765989$ a.u.), with the rms radius growing excessively. The system of a negative and a positive positronium ion thus forms no bound state but dissociates into a dipositronium molecule and a positronium. This result suggests that the Coulomb force cannot bind more than four particles out of identical charged fermions and their antiparticles.

We repeated the same calculation by replacing the fermions with bosonic equivalents. On a different scale, these systems may be identified, e.g., by systems of π^- and π^+ with their strong interaction neglected [13]. Such bosons turn out to form bound states even for $N=5$. As may have been expected, the radius of the charged boson system decreases by increasing the number of particles.

In Table II we show results for bosonic and fermionic systems with a purely attractive Gm^2/r (''gravitational'') interaction. Self-gravitating boson systems have recently attracted some interest [14]. For these systems, both varia-

TABLE II. Energies and rms radii of "self-gravitating" m-particle–n-antiparticle systems $(m+,n-)$; f: fermions; b: bosons. VLB and VUB stand for the variational lower and upper bounds given in Ref. [14]. The units of the energy and length are $G^2m^5\hbar^{-2}$ and $G^{-1}m^{-3}\hbar^2$, respectively.

System	Method	E		$\langle r^2\rangle^{1/2}$	K
$(+,-)$ b,f	SVM	-0.25		1.732	10
	exact	-0.25		1.732	
$(2+,-)$ b,f	SVM	-1.072		1.304	15
	Var. [14]	-1.067			
$(2+,2-)$ b,f	SVM	-2.791		1.027	100
	VUB (VLB)	-1.951	(-3.00)		
$(3+,2-)$ f	SVM	-3.758		1.554	200
$(3+,2-)$ b	SVM	-5.732		0.844	200
	VUB (VLB)	-4.336	(-6.25)		
$(3+,3-)$ f	SVM	-6.409		1.621	300
$(3+,3-)$ b	SVM	-10.215		0.718	300
	VUB (VLB)	-8.130	(-11.25)		

tional lower and upper bounds are now available. In this case even the five-fermion system is bound. Thus the lack of bound states in five-electron-positron systems is a joint effect of the antisymmetry and of the repulsion between identical particles. As the force is attractive, the binding energy of the boson systems rapidly increases with the number of particles.

Finally, we mention an example involving an excited state. With $K=500$, the ground and first excited state of the $t+d+\mu^-$ system was put at -111.3640 and -100.9121 a.u., while the coupled rearrangement channel Gaussian basis variational (CRCGBV) method on a similar basis with $K=1442$ gave -111.364342 and -100.916421 a.u., respectively [15].

Various calculations have used the Malfliet-Tjon potential [16], which is sum of two Yukawa potentials, as a benchmark test to compare the accuracy and feasibility of the different methods of solution of the N-body Schrödinger-equation. Table III shows our results (SVM), together with results of others, for this potential to systems with $N=2$–7 nucleons. This agreement corroborates that the SVM is as accurate as the direct solution of the Faddeev-Yakubovsky (FY) and the Faddeev equations [17,18] or the method of the amalgamation of two-body correlations into multiple scattering (ATMS) [19] or the variational Monte Carlo (VMC) method [20]. The basis used in the CRCGBV method [8] is similar to that of the SVM but the Gaussian parameters follow geometric progressions. The fact that the basis size needed in the SVM is much smaller proves the efficiency of our selection procedure.

TABLE III. Energies and rms radii of N-nucleon systems interacting via the Malfliet-Tjon potential V [16].

N	Method	E (MeV)	$\langle r^2\rangle^{1/2}$ (fm)	K
2	Numerical	-0.4107	3.743	
	SVM	-0.4107	3.743	5
3	Faddeev [18]	-8.2527		
	SVM	-8.2527	1.682	80
4	ATMS [19]	-31.36		
	CRCGBV [8]	-31.357		1000
	FY [17]	-31.36		
	SVM	-31.360	1.4087	150
5	VMC [20]	-42.98 ± 0.16	1.51	
	SVM	-43.48	1.51	500
6 (^{6}He)	VMC [20][a]	-66.34 ± 0.30	1.50	
	SVM	-66.30	1.52	800
7 (^{7}Li)	SVM	-83.4	1.68	1300

[a]Calculated with Coulomb potential, the Coulomb contribution then subtracted perturbatively.

In summary, the method we have reported on is a combination of refined analytical techniques developed to calculate the matrix elements of the correlated Gaussian basis functions and the stochastic basis selection procedure and problem-conform numerical strategy. We have demonstrated its power in solving bound-state few-body problems. In none of the test cases has it proved to be inferior to any of the alternative methods, and it did not require excessive effort to reach with it the present-day record of precisely describing a six-body bound state. Since the calculations involved are almost completely analytical, it looks straightforward to go beyond the six-body problem, although, of course, the required basis size becomes excessive sooner or later. The method has turned out to be much more economical than similar non-stochastic methods, and its basis has proved very flexible in adapting itself to both Coulomb-interacting and nuclear sytems. The application of this method for more complex system is underway (see, for example [11]).

This work was supported by OTKA Grant No. T17298 (Hungary) and by a Grant-in-Aid for Scientific Research (Nos. 05243102 and 06640381) of the Ministry of Education, Science and Culture, Japan. K. V. gratefully acknowledges the hospitality of the RIKEN LINAC Laboratory and the support of the Science and Technology Agency of Japan. We thank Professor R. G. Lovas for a careful reading of the manuscript.

[1] S. F. Boys, Proc. R. Soc. London Ser. A **258**, 402 (1960); K. Singer, *ibid.* **258**, 412 (1960).

[2] S. A. Alexander, H. J. Monkhorst, and K. Szalewicz, J. Chem. Phys. **85**, 5821 (1986).

[3] D. B. Kinghorn and R. D. Poshusta, Phys. Rev. A **47**, 3671 (1993).

[4] P. M. Kozlowski and L. Adamowicz, Phys. Rev. A 1903 (1993).

[5] V. I. Kukulin and V. M. Krasnopol'sky, J. Phys. G **3**, 795 (1977)

[6] K. Varga, Y. Suzuki, and R. G. Lovas, Nucl. Phys. **A371**, 447 (1994).

[7] K. Varga, Y. Suzuki, and Y. Ohbayasi, Phys. Rev. C **50**, 189 (1994); K. Arai, Y. Suzuki, and K. Varga, *ibid.* **51**, 2488 (1995); K. Varga, Y. Suzuki, and I. Tanihata, *ibid.* **52**, 3013 (1995).

[8] M. Kamimura and H. Kameyama, Nucl. Phys. **A508**, 17c (1990).
[9] H. De Raedt and M. Frick, Phys. Rep. **231**, 109 (1993).
[10] M. Kamimura, Prog. Theor. Phys. Suppl. No. **62**, 236 (1977).
[11] K. Varga and Y. Suzuki, Phys. Rev. C **52**, 2885 (1995).
[12] A. Yeremin, A. M. Frolov, and E. B. Kutukova, Few-Body Systems **4**, 111 (1988); Y. K. Ho, J. Phys. B **16**, 1503 (1983); Phys. Rev. A **48**, 4780 (1993) and references therein.
[13] S. Fleck and J.-M. Richard, Few-body Systems **19**, 19 (1995).
[14] J. L. Basdevant, A. Martin, and J. M. Richard, Nucl. Phys. **B343**, 60 (1990).
[15] M. Kamimura, Phys. Rev. A **38**, 621 (1988).
[16] R. A. Malfliet and J. A. Tjon, Nucl. Phys. **A127**, 161 (1969).
[17] W. Glöckle and H. Kamada, Phys. Rev. Lett. **71**, 971 (1993); Nucl. Phys. **A548**, 205 (1992).
[18] N. W. Schellingerhout and L. P. Kok, Nucl. Phys. **A508**, 299c (1990).
[19] Y. Akaishi, in *International Review of Nuclear Physics* (World Scientific, Singapore, 1986), Vol. 4, p. 259.
[20] R. B. Wiringa (private communication).