last summation of Eq. (A1). The same methods are used to treat this state as in the preceding; we obtain $((\sqrt{t'q^{-1}(J_3T_3\alpha_3)}i''b(J_n''T_n''\alpha_n''))(J_4T_4\alpha_4)j_c^{4j_c+1}(j_c\frac{1}{2}))(J_5T_5\alpha_5),j''[J_eT_e\alpha_e)$

$$
= \left(\frac{a}{N-1}\right)^{1/2} \left(j'^{a-1}(J_3T_3\alpha_3), j'\left[j'^{a}(J_n'T_n'\alpha_n')\right)\n\times \left[\frac{2J_n+1}{2T_n+1}(2J_n+1)(2J+1)(2J_4+1)(2J_4+1)(2J_5+1)(2J_5+1)\right]^{1/2}\n\times W(J_n'J_n''j'J_4; J_eJ_3)W(T_n'T_n''\frac{1}{2}T_4; T_eJ_3)W(Jj_ej'J_5; J_eJ_4)W(T_{\frac{1}{2}}\frac{1}{2}T_5; T_eJ_4)
$$
\n(A6)

and

 $((\sqrt{3}/\sqrt{3}/T_n'\alpha_n')j''b^{-1}(J_3T_3\alpha_3)\sqrt{(J_4T_4\alpha_4)}j_c^{4j_c+1}(j_c\frac{1}{2}))(J_5T_5\alpha_5),j''[J_6T_6\alpha_6)]$

$$
= \left(\frac{b}{N-1}\right)^{1/2} \left(j''b^{-1}(J_{3}T_{3}\alpha_{3}),j''\left[j''b(J_{n}''T_{n}''\alpha_{n}'')\right)\right)
$$

× $\left[(2J_{n}''+1)(2T_{n}''+1)(2J+1)(2T+1)(2J_{4}+1)(2J_{5}+1)(2J_{5}+1)(2T_{5}+1)\right]^{1/2}$
× $W(J_{n}'J_{3}Jj''; J_{4}J_{n}'')W(T_{n}'T_{3}T_{\frac{1}{2}}; T_{4}T_{n}'')W(Jj_{c}j''J_{5}; J_{c}J_{4})W(T_{\frac{1}{2}}\frac{1}{2}T_{5}; T_{e}T_{4}).$ (A7)

PHYSICAL REVIEW VOLUME 147, NUMBER 3 22 JULY 1966

Direct Numerical Solution of the Three-Body Problem

S. ROSATI Istituto di Fisica dell'Università, Pisa, Italy and

Istituto Nazionale di Fisica Nucleare, Sezione di Pisa, Pisa, Italy

AND

M. BARBI Istituto di Fisica dell Vniversita, Pisa, Italy (Received 31 January 1966)

We discuss a numerical method to determine the binding energy and the wave function for a three-body system. Radial wave functions of the form $g_1(r_1)g_2(r_2)g_3(r_3)$ are used, r_1 , r_2 , and r_3 being the interparticle distances. The method is applied to He³ and $H³$ with central forces and hard core to show the accuracy and the speed of the calculation.

1. INTRODUCTION

HE study of the bound states of three particles is of great interest for molecular, atomic, and nuclear physics. Often only a knowledge of the binding energy is required but sometimes one needs also detailed information about the wave function. The variational method has been extensively applied to these problems with a radial trial function of the form $g_1(r_1)g_2(r_2)g_3(r_3)$, r_1, r_2 , and r_3 being the three interparticle distances. Such a radial function is appropriate to describe the correlation between the particles and at the same time has a reasonable asymptotic behavior. The complete wave function is obtained by taking a superposition of products of spin-orbital functions by a radial function of the above type. The disadvantage of the variational analysis is well known. The number of trial parameters and correspondingly the numerical calculations, increase rapidly with the accuracy required for the binding energy and, even more, for the details of the wave function. As an example, when potentials with hard core are considered, trial functions with a great flexibility are necessary to reproduce accurately the exact wave function just outside the hard core, where the potentials have large values. Austern and Iano' have proposed a type of trial functions which are constructed with particular attention in the region where the potentials have large values and go over into variational functions for larger distances. Such functions give excellent results for two-particle systems and can be at once extended to the cases of a larger number of particles by choosing the trial function, up to a certain interparticle separation, as a product of the solutions of a two-body Schrödinger equation. This method has been end sody sembanger equation. This method has been
successfully applied^{2,3} to particular states of three and

33, 259 (1964).
⁸ Y. C. Tang Tang, R. C. Herndon, and E. W. Schmid, Nucl. Phys. 65, 203 (1965); Phys. Rev. 134, B743 (1964).

 \overline{N} . Austern and P. Iano, Nucl. Phys. 18, 672 (1960).

P. H. Wackman and N. Austern, Nucl. Phys. 30, 529 (1962); K. W. Schrnid, Y. C. Tang, and R. C. Herndon, Nuovo Cimento

four-particle systems. However to determine the best values of the trial parameters it is necessary to repeat the same type of calculation many times and this results in a large computational time. Moreover, the radial functions used, $2,3$ also in the inner region, are not the best product functions one can realize.

Recently, there have been also some attempts to solve the few-body nuclear problem by direct numerica methods. Baker *et al.*,⁴ starting from the time-dependent Schrödinger equation and using the different time evolution of the various eigenfunctions, have studied the ground state of $H³$ for a central nucleon-nucleon potential without hard core. In a different approach, due to Kalos,⁵ the Schrödinger equation is transformed into an integral equation whose solution is searched by a Monte Carlo method.

On the other hand, a variational calculation can either be conducted by minimizing the energy with respect to the parameters of a trial wave function, or by solving the corresponding Euler-Lagrange equations. In this paper we illustrate the practicability of the latter method to get an exact numerical solution of the bound states of three particles using radial functions of a product form and the technique developed by Bodmer and Ali⁶ for states with $L=0$ and by Murphy and Rosati' for states with arbitrary spin and orbital angular momenta. AVe also give the results obtained for He³ and H³ with central forces and a radial function totally symmetrical or symmetrical only with respect to the two identical particles.

2. METHOD OF CALCULATION

In this paper we consider the case of three particles bound by central two-body forces. It is then appropriate to use the LS coupling scheme, and the wave function of a state with total angular momentum J and z component J_z is written as follows:

$$
\Psi_{(l_1, l_2)L, S}^{J, J_z} = \left[\sum_{L_z, S_z} C(LSJ, L_z S_z J_z) \phi_{(l_1, l_2)}^{L, L_z} \chi^{S, S_z} \right]
$$

$$
\times g_1(r_1) g_2(r_2) g_3(r_3), \quad (1)
$$

where $C(LSJ, L_zS_zJ_z)$ is a Clebsh-Gordan coefficient. The orbital function $\phi_{(l_1, l_2)} L, L_z$ is an eigenfunction of the angular momentum operators $I_1^2, I_2^2, I_1^2 = (I_1 + I_2)^2$ and L_z , where $\mathbf{l}_j = -i\hbar \mathbf{r}_j \times \nabla_{\mathbf{r}_j}$ $(j = 1, 2)$; χ^{S, S_z} is the corresponding function for the total spin S. It must be noticed that the dependence of the exact three-body wave function on the interparticle distances, will not in general be of the form $g_1(r_1)g_2(r_2)g_3(r_3)$, so that the function (1) can reproduce only approximately the exact solution. The problem is to choose $g_1(r_1)$, $g_2(r_2)$, and $g_3(r_3)$ in such a way to obtain the best approxima-

 6 A. R. Bodmer and S. Ali, Nucl. Phys. 56, 657 (1964).

tion. Let us define the functions

$$
\mathcal{L}_1(r_1,r_2,r_3) = \frac{1}{2L+1} \sum_{M=-L}^{L} |\phi_{(l_1,l_2)}|^{L,M} |^2, \qquad (2)
$$

and

$$
N_i(r_i) = \int d\tau^{(i)} \mathfrak{L}_1 \prod_{\substack{j=1,\\j\neq i}}^3 g_j^2(r_j), \quad (i=1, 2, 3).
$$
 (3)

In the last equation

$$
d\tau^{(i)} = \prod_{\substack{j=1,\\j\neq i}}^3 r_j dr_j,
$$

and the integration region satisfies the triangular inequalities between the coordinates r_1 , r_2 , and r_3 , i.e., $r_i+r_j\geq r_k$ with $i\neq j\neq k=1, 2, 3$. Together with $g_1, g_2,$ and g_3 it is convenient to introduce the functions

$$
f_i(r_i) = (r_i N_i)^{\frac{1}{2}} g_i(r_i) , \quad (i = 1, 2, 3).
$$
 (4)

It can be shown^{6,7} that the best solutions g_1 , g_2 , and g_3 are such that the corresponding functions f_1 , f_2 , and f_3 given by (4) satisfy two-body Schrodinger-type equations

$$
2K_i f_i'' + [E - v_i(r_i) - W_i(r_i)] f_i = 0, \quad (i = 1, 2, 3), \quad (5)
$$

where E is the total energy of the three-body system, $K_i = \frac{1}{4}h^2(m_j + m_k)/m_j m_k$ ($i \neq j \neq k = 1, 2, 3$), and $v_i(r_i)$ is the radial part of the potential acting between the particles of the *i*th pair. The effective potential for each pair of particles is $v_i(r_i)+W_i(r_i)$. Thus, the effect on any pair due to the presence of the third particle is represented by the "induced" potential $W_i(r_i)$ given by⁷

$$
W_i(r_i) = \frac{1}{N_i} \sum_{\substack{j=1 \ j \neq i}}^3 [K_j T_j + v_i^{(j)}] + \frac{v_i^{(L)}}{N_i}
$$

-
$$
K_i \left[\frac{1}{2} \left(\frac{N_i'}{N_i} \right)^2 - \frac{1}{2} \frac{N_i''}{N_i} - \frac{1}{r_i} \frac{N_i'}{N_i} + \frac{1}{2r_i^2} \right], \quad (6)
$$

with

$$
T_i^{(j)}(r_i) = \int d\tau^{(i)} \mathcal{L}_1 \left[(g'_j)^2 - g'_j{}'' g_j - \frac{2g'_j g_j}{r_j} \right] g_k^2,
$$

$$
v_i^{(j)}(r_i) = \int d\tau^{(i)} v_j(r_j) \mathcal{L}_1 \prod_{\substack{k=1,\\k \neq i}}^3 g_k^2(r_k), \qquad (7)
$$

$$
v_i^{(L)}(r_i) = \frac{1}{2} \int d\tau^{(i)} \mathcal{L}_3 \prod_{\substack{k=1, \\ k \neq i}}^3 g_k^2(r_k) ,
$$

and \mathfrak{L}_3 a certain function of the interparticle distances defined by Eq. (16) of Ref. 7; in the case $L=0$, we have $\mathfrak{L}_1=1$ and $\mathfrak{L}_3=0$ so that the induced centrifugal term $v_i^{(L)}$ is zero.

⁴ G. A. Baker, Jr., J. L. Gamel, B. J. Hill, and J. G. Wills, Phys. Rev. 125, 1754 (1962).

⁵ M. H. Kalos, Phys. Rev. 128, 1791 (1962).

⁷ J. W. Murphy and S. Rosati, Nucl. Phys. 63, 625 (1965).

FIG. 1.Integration path in the plane used in the calculation of the
function $F(r)$ de-
fined by Eq. (8).

In Refs. 6 and 8 one of Eqs. (5) has been solved exactly, the two other equations being satisfied approximately with trial functions g of a simple form which allow the integrals to be evaluated analytically. The eigenvalue, which is a function of the trial parameters, is then minimized.

Here we propose instead to solve numerically the system of three coupled integro-differential equations by means of an iteration procedure. Starting with two input functions $g_1^{(0)}(r_1)$ and $g_2^{(0)}(r_2)$ which reproduce reasonably well the exact corresponding radial functions, we calculate with (6) and (7) the potential term $W_3(r_3)$ of Eq. (5) $(i=3)$. The corresponding Schrödinger equation is then solved numerically to get the eigenvalue and the related eigenfunction. This eigenvalue gives a first estimate of the total three-particle energy. From the approximated eigenfunction, a function $g_3^{(1)}(r_3)$ can be derived with the help of Eq. (4). $g_3^{(1)}(r_3)$ is then used as input function together with one of the proceeding two, say $g_1^{(0)}(r_1)$, to obtain $g_2^{(1)}(r_2)$ and a second estimate of the total energy, and so on, until self-consistency among the three equations (5) is reached. Since Eqs. (5) have been derived from a minimum variational principle, the convergence of the procedure is ensured. As we shall see in the next section, in all the cases we have examined the procedure converges rapidly. Self-consistent solutions are obtained after 3-6 iterations, a very small number compared to the number of iterations which are required to obtain the best values of the trial parameters in a variational calculation.

For a numerical evaluation of the various quantities (7), the main problem we are faced with is the calculation of double integrals of the following form

$$
F(r) = \int_{a}^{\infty} ds \int_{M(a,|r-s|)}^{r+s} dt f(s,t), \qquad (8)
$$

where the function $f(s,t)$ vanishes when one of its arguments goes to infinity, in such a way as to have a finite integral; the constant a may or may not be zero (in what follows it will represent the radius of the hard core of the two-body forces), and $M(a, |r-s|)$ denotes the largest of the two quantities within the bracket. Et follows from (8) that

$$
G(r) = \frac{dF}{dr}
$$

=
$$
\int_{a}^{\infty} ds [f(s,r+s) + \theta(a,r-s)f(s,|r-s|)], \quad (9)
$$

with

$$
\theta(a,r-s) = 0 \quad \text{if} \quad |r-s| < a \n= -1 \quad \text{if} \quad r-s \ge a \n= 1 \quad \text{if} \quad r-s \le -a.
$$
\n(10)

The integration path for the integral (9) is shown in Fig. 1; to obtain $G(r)$ we have to add the integrals of $f(s,t)$ along the lines 1 and 3 of Fig. 1 and then subtract the integral along line 2:

$$
G(r) = \left[\int_{L_1} ds + \int_{L_2} ds - \int_{L_2} ds \right] f(s,t). \tag{11}
$$

As $F(0)=0$, we derive from (9)

$$
F(r) = \int_0^r G(r') dr'.
$$
 (12)

To get $F(r)$ from this relation it is necessary to know the function $G(r')$ also for values $r' \leq a$; this does not however require the knowledge of $f(s,t)$ in the regions where either s or t are smaller than a . Equations (11) and (12), as is more fully discussed in Appendix, can be used to calculate $F(r)$ by numerical integration.

3. NUMERICAL CALCULATIONS

We present now some of the results obtained by applying the method discussed in the preceding paragraph to the study of the $He³$ and $H³$ nuclei. We consider two-body charge-independent central potentials of the form

$$
V_{i,j} = \frac{1}{2} (1 + P_{i,j}) V_t(\vert \mathbf{x}_i - \mathbf{x}_j \vert) + \frac{1}{2} (1 - P_{i,j}) V_s(\vert \mathbf{x}_i - \mathbf{x}_j \vert), \quad (13)
$$

where $P_{i,j}$ is the spin-exchange operator. The most general wave function for the three-nucleon state with $L=0$ can be written as

$$
\Psi = u_S(r_1, r_2, r_3)X_A + u_A(r_1, r_2, r_3)X_S, \qquad (14)
$$

where X_A and X_B are spin functions antisymmetrical and symmetrical, respectively, in the spin coordinates of the two identical particles; the radial functions u_A and u_S have a similar symmetry property with respect to the spatial coordinates.

 8 L. Lovitch and S. Rosati, Nucl. Phys. 73, 648 (1965); S. Ali, J. W. Murphy, and A. R. Bodmer, Phys. Rev. Letters 15, 534 (1965).

TABLE I. Results obtained for the potential of Baker et al. (Ref. 4). n is the number of step-lengths h considered in the calculation of the various integrals.

h (F)	Step-length Number of step-lengths	F. (MeV)	Rms radius (F)	Еc (MeV)
0.25	60	-9.749	1.489	0.8878
0.20	75	-9.761	1.490	0.8876
0.15	100	-9.766	1.490	0.8875
0.10	150	-9.767	1.490	0.8875
0.05	300	-9.767	1.490	0.8875

The iteration procedure discussed in Sec. 2 has been applied to two special cases:

(A) The potential (13) is replaced by an "effective" spin-independent potential $\frac{1}{2}[V_i(r_i)+V_s(r_i)], i=1,2,3$ (the radial wave function is in this case totally symmetrical).

(8) The wave function (14) is approximated by

$$
\Psi = g_1(r_1) g_2(r_2) g_2(r_3) X_A , \qquad (15)
$$

 r_1 being the distance between the two identical particles.

First of all we consider the potential of Baker et al.⁴

$$
V_t(\mathbf{r}) = V_s(\mathbf{r}) = V_0 \exp[-(\mathbf{r}/b)^2], \quad (16)
$$

with $V_0 = -51.5$ MeV and $b = 1.60$ F. The lack of spin dependence ensures that the radial eigenfunction is totally symmetrical, so that in this case the functions g_1 and g_2 in (15) are equal. In Table I the results obtained for the binding energy and the rms radius of the triton and the Coulomb energy E_c of the He³ nucleus are given for diferent values of the step-length $h⁹$. The calculated numbers are given with four figures to show how large the step-length h or how small the number n of steps can be chosen; this is important because the computing time increases approximately as n^2 . It may be worthwhile to notice that the deviations arising for the largest values of h given in Table I, are partly due to the use of a large step-length in the solution of the two-body Schrödinger equation; this could be avoided by interpolating other values of the potential on the values directly calculated. However, at least in this case, the question is unimportant because the total computing time is only a few seconds for $h=0.25$ and not more than a minute for $h=0.05$. With the same two-body potential but a different method of calculation, Baker et al.⁴ obtained $E=-9.42$ MeV, Example 1. Baker et al. botained $E = -9.42$ MeV
Kalos⁵ $E = -9.47$ MeV and Tang *et al.*³ an upper bound $E_u = (-9.74 \pm 0.05)$ MeV which is quite close to our estimate.

Also the radial functions obtained for each value of h given in Table I are essentially coincident and, as a consequence, the results for E_c and the radius are nearly independent on h . The Coulomb energy E_c has been calculated by first-order perturbation neglecting the proton radius.

' All the numerical calculations have been performed on the IBM 7090 computer of Pisa University.

Let us now consider the case of an exponential radial dependence of the potentials

$$
V_t(r) = \infty, \qquad (r < a)
$$

= $V_{0t} \exp[-\sigma_t(r-a)], \quad (r > a)$

$$
V_s(r) = \infty, \qquad (r < a)
$$

= $V_{0s} \exp[-\sigma_s(r-a)]. \quad (r > a)$ (17)

For hard core $a=0$, the results depend smoothly on the step length h as in the preceeding case. We give (first and second line of Table II) the results obtained for the spin-dependent potential used by Rarita and Present
in a study of the two-, three-, and four-body problems,¹⁰ in a study of the two-, three-, and four-body problems, having the following parameter values:

$$
V_{0t} = -123.56 \text{ MeV}, \quad V_{0s} = -70.429 \text{ MeV}, \quad (18)
$$

$$
\sigma_t = \sigma_s = 1.156 \text{ F}^{-1}.
$$

When we consider a completely symmetrical radial function it is not necessary to specify the potential for neutron-proton states with odd orbital angular momentum. The situation is different when two of the ^g functions in (15) are different and we assume, for simplicity, that the potential in the odd states is still given from (13) and (17). With a potential having a different space-exchange character (for example Majorana type) the total three-body energy can change' by about 0.1 MeV. However it is possible to modify the procedure so as to treat correctly all the cases; the difference would be the appearance of an inhomogenous term in Eq. (5) which would not however essentially modify the procedure.

For potentials with a nonzero hard core the situation is a little different. If a constant step-length h is used in all the calculations, values $h=0.05$ F are required to get results with three significant figures. This is due to the fact that the radial solutions for potentials with hard core contain components which vary faster than the components due to the potentials with $a=0$. The best way to treat this situation is to use a small steplength in the region where the rapidly varying components are important, and then change it to a larger one. A similar procedure may be quite useful when a long computational time becomes a problem.

We present in Table II some of the results obtained

¹⁰ W. Rarita and R. D. Present, Phys. Rev. 51, 788 (1937).

FIG. 2. The full lines reproduce the $\frac{g_1}{g_2}$ and $\frac{g_2}{g_2}$ of a partially symmetrical three-body radial func tion while the dashed line refers to the case of a completely symmetrical radial function. r (Fermi) 02 1 7

for potentials of the form (13), (17). The computing time for each case (B) has been ²—4 min; about ¹ min for each case (A). In Fig. 2 we have plotted the radial functions calculated for an exponential potential with $a=0.2$ F. g corresponds to case (A), g_1 and g_2 to case (B). The normalization is $\int_0^{\infty} [g(r)]^2 r dr = 1$. As can be seen from the curves, the functions obtained in the two cases are considerably diferent though they give essentially the same binding energy.

4. CONCLUSIONS

This investigation shows that for a three-body system it is possible to obtain an exact numerical evaluation of radial functions of a product form. The accurate wave functions can be used to calculate other quantities more sensitive than the binding energy to the behavior of the radial functions in the external region. For example they can be used to determine the nuclear radii and the form factors. The technique we have discussed allows a greater precision than the usual variational method and requires a shorter computing time. This last point is especially important if we want to study the properties of $H³$ and $He³$ with a nucleon-nucleon potential more realistic than the one here considered. As an example, if the potentialcontains a tensor part, we must take for the wave function a superposition of terms with different angular momenta, and the calculations increase rapidly with the number of terms. However, the method here applied to $L=0$ states can be extended to these more involved cases, the computing time being still reasonable. Numerical calculations on this subject and on the structure of three-particle molecules are now in progress.

ACKNOWLEDGMENTS

We are much indebted to Professor L. A. Radicati for his interest in this work and for many helpful comments.

^A useful discussion with Dr. L. Lovitch and Dr. L. E. Picasso is also acknowledged.

APPENDIX

We discuss here a possible way of calculating the function $F(r)$ defined by (8), for a set of equally spaced values $r_k = a + kh$, $k = 0, 1, \dots, n$. Let us suppose that the function $f(s,t)$ of Eq. (8) has been tabulated for the values $(s_i = a + ih, t_i = a + jh), i, j = 0, 1, \dots, n$; moreover, let $f(s,t)$ be essentially zero outside the above region in the (s,t) plane. We take the quantity a to be a multiple of the step-length h so that the same is true a multiple of the step-length *n* so that the same is true
also for $(r_k + s_i)$ and $|r_k - s_i|$: this reduces the number of points in the (s,t) plane where the function $f(s,t)$ must be known to numerically perform the integrations of Eq. (10) .

First of all from (12) we calculate $G(r_k)$, $k=0,1,\dots,n$ by means of an accurate numerical integration formula. Then we evaluate (for all possible values of k) the integral

$$
\int_{r_{k-1}}^{r_k} G(r') dr'
$$

approximating $G(r')$ by the polynomial interpolating the values $G(r_{k-p}), G(r_{k-p+1}), \cdots, G(r_{k+p}),$ with p an integer. Finally, $F(r_i)$ is obtained as

$$
F(r_i) = \sum_{k=1}^i \int_{r_{k-1}}^{r_k} G(r') dr'.
$$

This method of calculation has been tested in a number of cases. Quite accurate results have been obtained using (i) a seven-point Bode integration formula¹¹ to calculate $G(r)$, and (ii) an eight-point Lagrangian interpolation formula" to calculate the integral of $G(r)$ on the interval (r_{k-1}, r_k) . As an example, for $f(s,t) = (s-a)^{l}(t-a)^{m} \exp[-(s+t)]$, l and m integers, with $h=0.1$ and a number $n=100$ of step-lengths for each of the variables r , s , and t , the results are obtained in the main to an accuracy of 10^{-5} , and the computing time turns out to be a fraction of a second.

¹¹ See, for example, *Handbook of Mathematical Functions*, edited by M. Abramowitz and I. A. Stegun (U. S. Department of Commerce, National Bureau of Standards, Washington, D. C., 1965), Appl. Math. Ser.