Monte Carlo Calculations of the Ground State of Three- and Four-Body Nuclei

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By means of a suitable Green's function, the Schrödinger equation for the few-body nuclear problem is written as an integral equation. In this equation, the binding energy of the ground state is assumed known and the strength of potential required to give this energy is an eigenvalue to be determined. A random walk can be devised whose collision density satisfies the same integral equation. The simulation of this random walk therefore permits an exact numerical solution by Monte Carlo methods. The calculation has been carried out with pairwise potentials of square, Gauss, and exponential shape.

I. INTRODUCTION

THE integration of the N-body wave equation for the ground state of an atom or nucleus is clearly a very difficult, perhaps impossible, problem. An exact numerical solution would be very desirable, but it seems difficult even with the help of modern high-speed digital computers. It is the purpose of this paper to propose a specific Monte Carlo method, to show how it may be applied to the simplest possible nuclear problem, and to give some numerical results.

It is well known that from a purely numerical point of view, Monte Carlo methods may be more efficient than standard finite difference methods for the solution of many dimensional problems.[1] The literature contains some references to the solution of partial differential equations including the Schrödinger equation[2] by Monte Carlo methods. These have involved first making finite difference approximations and then introducing a random walk on a lattice. It seemed more natural and promising to look for an integral equation formulation of the Schrödinger equation and attempt its solution by Monte Carlo methods. Since this integral equation contains the appropriate boundary conditions, it evades the difficulty in numerical solution which lies in getting the right behavior at infinity. We shall see that it is also makes unnecessary the reduction to center-of-mass system.

Monte Carlo methods are best used in dealing with problems in which the solutions and intermediate quantities obtained are positive. It is desirable, therefore, that the kernel of the integral equation be positive if this can be arranged. The operator $(-\nabla^2+1)$ has a Green's function which is positive definite. This operator occurs if the binding energy of the system is assumed known—or else taken as a unit of energy—and the strength of a potential of some given shape is left to be determined. In applications to the calculations of ground-state nuclear wave functions this is most appropriate since the binding energy is known better than the nuclear forces.

[1] G. Goertzel and M. H. Kalos, in *Progress in Nuclear Energy* (Pergamon Press, New York, 1958), Series I, Vol. 2, p. 315.
[2] N. Metropolis, in *Symposium on Monte Carlo Methods*, edited by H. A. Meyers (John Wiley & Sons, Inc., New York, 1956), p. 29. G. W. King, IBM Seminar on Scientific Compulation, November, 1949 (unpublished).

II. THE INTEGRAL EQUATION

Let the coordinates of the N particles be $\mathbf{x}_1$, $\mathbf{x}_2$, $\cdots\mathbf{x}_N$. The Schrödinger equation is

$$-\sum_i \frac{\hbar^2}{2M_i}\nabla_i^2\psi(\mathbf{x}_1,\cdots\mathbf{x}_N)+V(\mathbf{x}_1,\cdots\mathbf{x}_N)\psi(\mathbf{x}_1,\cdots\mathbf{x}_N) =E\psi(\mathbf{x}_1,\cdots\mathbf{x}_N). \quad (1)$$

Suppose that the energy is fixed to be

$$E=-B. \quad (2)$$

Let

$$\mathbf{r}_i=(2M_iB/\hbar^2)^{1/2}\mathbf{x}_i, \quad (3)$$

and

$$V(\mathbf{x}_1,\mathbf{x}_2,\cdots,\mathbf{x}_N)=-\lambda BW(\mathbf{r}_1,\mathbf{r}_2,\cdots,\mathbf{r}_N). \quad (4)$$

The last equation introduces the eigenvalue λ, the strength of the potential (in terms of B) required to bind the system. For convenience let us denote by the $3N$ dimensional vector $\mathbf{R}$, the entire set of 3 dimensional vectors $(\mathbf{r}_1,\cdots,\mathbf{r}_N)$. With these changes, the Schrödinger equation is written simply

$$(-\nabla^2+1)\psi(\mathbf{R})=\lambda W(\mathbf{R})\psi(\mathbf{R}); \quad (5)$$

The Laplace operator on the left-hand side of (5) is understood to be carried out in $3N$ dimensions.

Equation (5) is to be transformed into an integral equation by the use of a Green's function for the operator $(-\nabla^2+1)$:

$$(-\nabla_R^2+1)G(\mathbf{R}_0,\mathbf{R})=\delta(\mathbf{R}-\mathbf{R}_0). \quad (6)$$

To find a suitable G, we impose the boundary condition that the wave function ψ be square integrable as a function of all $3N$ coordinates. This implies that as a function of R, $G(\mathbf{R}_0,\mathbf{R})$ must go to zero at infinity. Since the boundary condition singles out no direction (in configuration space), G must fall off in the same way in all directions and is therefore a function of $|\mathbf{R}-\mathbf{R}_0|$. By transforming Eq. (6) into appropriate spherical coordinates, it is easy to show that

$$G(\mathbf{R}_0,\mathbf{R})= [1/(2\pi)^{3N/2}][K_{3N/2-1}(|\mathbf{R}-\mathbf{R}_0|)/|\mathbf{R}-\mathbf{R}_0|^{3N/2-1}], \quad (7)$$

where $K_\nu(z)$ is the Bessel function of imaginary argument.[3] This conclusion may also be drawn from the

[3] G. N. Watson, *Treatise on the Theory of Bessel Functions* (Cambridge University Press, New York, 1945), 2nd ed., p. 78.

general integral representation[4] of the Green's function of $(-\nabla^2+1)$ and an explicit contour integration.

With the Green's function given by Eq. (7), the Schrödinger equation is written in integral form

$$\psi(\mathbf{R})=\lambda\int d\mathbf{R}'\,G(\mathbf{R}',\mathbf{R})W(\mathbf{R}')\psi(\mathbf{R}'). \tag{8}$$

This Green's function guarantees that the internal wave function is square integrable. However, there remains the question whether, having fixed the total energy of the system to be $-B$, any energy is associated with the center of mass in the final solution. Nothing depends explicitly upon the coordinates of the center of mass, so that it is natural to ignore their values. This means precisely that in obtaining all answers of interest—the eigenfunctions and eigenvalues—we integrate over the values of the center-of-mass coordinates. We shall now show that the result of this integration, or "projection" on to the space of internal coordinates, yields a correct internal wave function with energy $-B$.

First we note that the isolation of purely internal coordinates may be accomplished by a unitary transformation (i.e., a rotation in $3N$-dimensional space):

$$\mathbf{q}_1=N^{-1/2}\sum_{j=1}^{N}\mathbf{r}_j, \tag{9}$$

$$\mathbf{q}_i=[i(i-1)]^{-1/2}\sum_{j=1}^{i-1}(\mathbf{r}_j-\mathbf{r}_i), \qquad i=2,3,\cdots,N, \tag{10}$$

$$\sum\mathbf{r}^2=\mathbf{q}_1^2+\sum_{i>1}\mathbf{q}_i^2.$$

We may introduce into Eq. (8) a specific integral representation[5] of the K_ν function to obtain

$$\psi(\mathbf{q}_1,\mathbf{q}_i)=(4\pi)^{-3N}\lambda\int_0^\infty\tau^{-3N}d\tau\int d\mathbf{q}_1'\int d\mathbf{q}_2'\cdots\int d\mathbf{q}_N'\times\exp\left[-\tau-\frac{1}{4\tau}|\mathbf{q}_1-\mathbf{q}_1'|^2-\frac{1}{4\tau}\sum_{i>1}|\mathbf{q}_i-\mathbf{q}_i'|^2\right]\times W(\mathbf{q}_i')\psi(\mathbf{q}_1',\mathbf{q}_i'). \tag{11}$$

If we integrate over $\mathbf{q}_1$, we obtain

$$\varphi(\mathbf{q}_i)=\int d\mathbf{q}_1\,\psi(\mathbf{q}_1,\mathbf{q}_i)=(4\pi)^{-3N+3}\lambda\int_0^\infty\tau^{-3N+3}d\tau\int d\mathbf{q}_2'\cdots\int d\mathbf{q}_N'\times\exp\left[-\tau-\frac{1}{4\tau}\sum|\mathbf{q}_i-\mathbf{q}_i'|^2\right]W(\mathbf{q}_i')\varphi(\mathbf{q}_i'). \tag{12}$$

[4] P. M. Morse and H. Feshbach, *Methods of Theoretical Physics* (McGraw-Hill Book Company, New York, 1953), Part I, Chap. 7.
[5] Reference 3, p. 183.

TABLE I. Potential depths required to bind the triton.

Well shape	Range b/R_t	Range b (10^{-13} cm)	Well depth V_0/B_t	Well depth V_0 (MeV)	s
Square	1.35	2.11	3.17	26.9	1.17
	1.5477	2.42	2.49	21.1	1.21
	2.0	3.13	1.71	14.5	1.39
Gauss	1.35	2.11	6.60	56	1.09
	1.5477	2.42	5.44	46.2	1.18
	2.0	3.13	3.67	31.2	1.33
Exponential	1.5477	2.42	17.5	149	1.16
	2.0	3.13	11.6	98	1.28
	3.0	4.69	6.09	52	1.51
	4.0	6.25	4.30	37	1.90

This equation is the correct internal wave equation which could have been obtained directly. Note that the Green's function is the same as in Eq. (11) except that $3N$-3 replaces $3N$.

More generally, we may project out whichever coordinates are relevant to $W(R)$. For this reason, if a computation is set up for a four-body problem, a two- or three-body problem may also be solved if W is made to depend only on the appropriate number of relative coordinates. The ability to do an otherwise soluble two-body problem provides a useful numerical check.

III. ITERATION OF THE INTEGRAL EQUATION

Equation (8) may be solved by iteration: Suppose ψ_0 is a given function and let λ_0 be any constant. Put

$$\psi_1(\mathbf{R})=\lambda_0\int d\mathbf{R}'\,G(\mathbf{R}',\mathbf{R})W(\mathbf{R}')\psi_0(\mathbf{R}'),$$
$$\psi_{n+1}(\mathbf{R})=\lambda_0\int d\mathbf{R}'\,G(\mathbf{R}',\mathbf{R})W(\mathbf{R}')\psi_n(\mathbf{R}'). \tag{13}$$

Write the last equation symbolically as

$$\psi_{n+1}(\mathbf{R})=\lambda_0\mathcal{S}\psi_n(\mathbf{R}). \tag{14}$$

Suppose ψ_0 is expanded in the eigenfunctions $\psi^{(k)}$ of the operator $\mathcal{S}$

$$\psi_0=\sum C_k\psi^{(k)}, \tag{15}$$

and that $\lambda^{(k)}$ is the eigenvalue of $\psi^{(k)}$.

$$\psi^{(k)}=\lambda^{(k)}\mathcal{S}\psi^{(k)}. \tag{16}$$

Then

$$\psi_1=\lambda_0\sum C_k\psi^{(k)}/\lambda^{(k)}, \tag{17}$$

$$\psi_n=\sum C_k\psi^{(k)}(\lambda_0/\lambda^{(k)})^n. \tag{18}$$

As the interation proceeds, the $\psi^{(k)}$ for which $|\lambda^{(k)}|$ is smallest gives the largest contribution to ψ_n, providing, of course, that C_k is not zero for that k. If

$$\lambda_0=\lambda\equiv[|\lambda^{(k)}|],$$

then the iteration becomes stable. If $\lambda\neq\lambda_0$, then although the shape of ψ reproduces itself the size of ψ grows or decays according as λ_0 is greater or less than λ.

The state $\psi^{(k)}$ for which $|\lambda|$ is smallest is the state bound with the weakest potential, i.e., the ground state.

IV. MONTE CARLO SOLUTION OF THE INTEGRAL EQUATION

Each iteration of Eq. (13) may be interpreted as a step of a continuous random walk. Let a population of points $\mathbf{R}_1, \cdots, \mathbf{R}_M$ be chosen so that the expected number per unit volume in configuration space is $\psi_n(\mathbf{R})$. For each of these, compute $\lambda_0 W(\mathbf{R}_m)$. Then let ϵ_m be an integer chosen at random so that its mean value is $\lambda_0 W(\mathbf{R}_m)$.[6] For each point R_m, pick ϵ_m new points $\mathbf{R}$ according to the probability distribution function[7] $G(\mathbf{R}_m,\mathbf{R})$. When we average over the distributions of ϵ_m and of $\mathbf{R}_m$, the expected number of points so chosen, per unit volume at $\mathbf{R}$, is

$$\int G(\mathbf{R}',\mathbf{R})\lambda_0 W(\mathbf{R}')\psi_n(\mathbf{R}')=\psi_{n+1}(\mathbf{R}). \quad (19)$$

Since the result is a set of points whose distribution is $\psi_{n+1}(\mathbf{R})$, a repetition of the procedure generates ψ_{n+2}.

The random walk may be carried out to many steps; if λ_0 is chosen too large or too small the population of points will fall to zero or grow beyond the capacity of a computer. It is convenient to choose only a few or even just one point from ψ_0 and use the first part of the calculation for the purpose of iterating to the ground-state wave function, and also to build up a population of useful size. The latter is done by temporarily setting λ_0 sufficiently large.

When many iterations have been carried out and the ground state is isolated, more steps of the random walk must be generated in order to provide good statistics in estimating λ, ψ itself or any quantities to be derived from ψ.

In the calculations carried out so far, only the value of λ required to bind the system has been calculated. An estimate of λ may be derived by integrating (5) over all configuration space.

$$\int \psi(\mathbf{R})dR=\lambda\int W(\mathbf{R})\psi(\mathbf{R})d\mathbf{R}. \quad (20)$$

Now ψ is the density with which points are generated in the random walk. Suppose that after the iteration settles down to the ground state, the points $\mathbf{R}_1$, $\mathbf{R}_2$, $\cdots \mathbf{R}_I$ occur. Then the Monte Carlo estimate of λ is

$$\lambda=(I/\sum W(\mathbf{R}_i)). \quad (21)$$

[6] This is easily done for instance by computing the integer and fractional parts of $\lambda_0 W$. ϵ_m is the integer part plus, with probability equal to the fractional part, one more.

[7] G is a displacement kernel. To generate a point $\mathbf{R}_n$, it is necessary to pick a displacement vector $\mathbf{R}_n-\mathbf{R}_m$ according to Eq. (7). The procedure for doing this is explained in detail in the Appendix.

TABLE II. Potential depths required to bind the alpha nucleus.

Well shape	Range b/R_α	Range b (10^{-13} cm)	Well depth V_0/B_α	Well depth V_0 (MeV)	s
Square	2.0	1.71	1.17	33.1	0.95
	3.0	2.57	0.67	19.0	1.22
	4.0	3.42	0.48	13.6	1.56
Gauss	2.0	1.71	2.55	72.2	0.92
	3.0	2.57	1.40	39.6	1.14
	4.0	3.42	0.97	27.4	1.40
Exponential	2.0	1.71	9.0	255	0.99
	3.0	2.57	4.27	121	1.06
	4.0	3.42	2.94	83	1.30

Future calculations will be carried out so as to determine also information about the wave function itself.

V. RESULTS AND DISCUSSION

Calculations have been carried out with pair forces derivable from square, Gauss, and exponential wells.[8] The numerical results for three- and four-body problems are given in Tables I and II. The widths of the wells are specified by the intrinsic range parameter, b, of Blatt and Jackson.[9] The depths of the wells are given in units of the binding energy and in MeV. The binding energy of the triton was assumed to be 8.49 MeV. From this the unit of length

$$R_t=\hbar(2MB_t)^{-1/2}$$

turns out to be 1.56×10^{-13} cm. The binding energy of the alpha was taken as 28.3, so that $R_\alpha=0.856\times10^{-13}$ cm. Finally the well depth parameter[9] s is tabulated. Note that for a square well

$$s=(4/\pi^2)(MV_0/\hbar^2)b^2=(2/\pi^2)(b/R)^2(V_0/B). \quad (22)$$

For a Gauss well of the form

$$V=-V_0\exp[-(1.4354r/b)^2],$$
$$s=0.09043(b/R)^2(V_0/B). \quad (23)$$

The exponential well has the form

$$V=-V_0\exp[-3.5412r/b],$$

and

$$s=0.02758(b/R)^2(V_0/B). \quad (24)$$

The numerical results for well depth are estimated to have an error, mostly statistical, of about 1%. One problem, for the three-body Gauss well at a range $b=1.5477$ corresponds exactly to a calculation performed recently by Baker et al.[10] They carried out a

[8] A preliminary account of this work was published in the *Proceedings of the Rutherford Jubilee International Conference*, edited by J. B. Birks (Academic Press Inc., New York, 1962). The numerical results quoted there for the square well are, however, incorrect owing to an error in the computer code.

[9] J. M. Blatt and J. D. Jackson, Phys. Rev. **76**, 18 (1949).

[10] G. A. Baker, Jr., J. L. Gammel, B. J. Hill, and J. G. Wills, Phys. Rev. **125**, 1754 (1962).

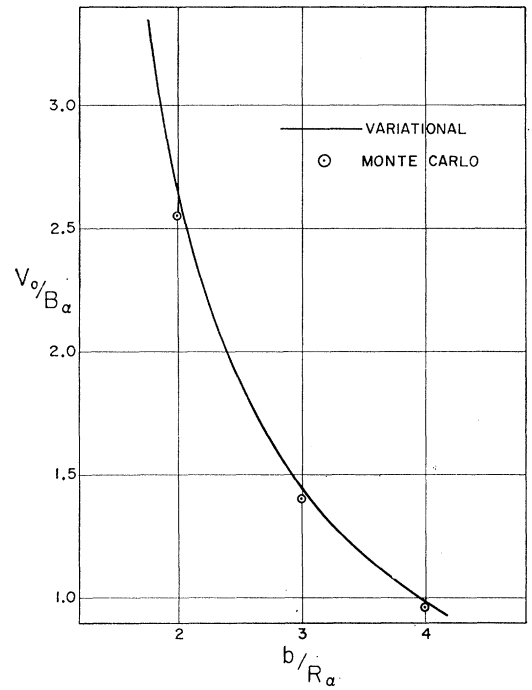

FIG. 1. Depth of Gauss well required to bind alpha particle as given by variational and by Monte Carlo methods.

numerical integration of the three-body problem using Gauss potentials. The results for which they quote a numerical value ($V_0=+51.5$ MeV, $B=9.416$ MeV) gives an eigenvalue $V/B=5.47$, in very good agreement with the Monte Carlo result of 5.44.

It is interesting to compare the numerical results with those from a simple variational calculation. For a Gauss well and a trial function in the form of a Gaussian function of relative coordinates, a variational calculation is straightforward to carry out. General formulas for this treatment of the few-body problem have been given by Laskar.[11] A calculation of this kind gives $B=6.9$ MeV for the three-body problem mentioned above. If variational calculations are made of the binding energy, and the results converted to give V_0/B as a function of b/R, the disagreement appears much smaller. Figure 1 shows a curve prepared in this way from the variational method together with the Monte Carlo results for the four-body Gauss problems.

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[11] William Laskar, Ann. Phys. (New York) **17**, 436 (1962).

APPENDIX

An essential step of the calculation is the generation of components of a $3N$-dimensional vector, $\mathbf{R}$, distributed according to

$$p(\mathbf{R})d\mathbf{R}=[1/(2\pi)^{3N/2}][K_{3N/2-1}(R)/R^{3N/2-1}]d\mathbf{R}. \quad \text{(A1)}$$

We write

$$d\mathbf{R}=R^{3N-1}d\mathbf{\Omega}dR,$$

where $\mathbf{\Omega}$ is a unit vector. Then it becomes necessary to pick a length R from the distribution

$$p_R(R)=\frac{2^{3N/2-1}\Gamma[(3N-1)/2]}{\Gamma(1/2)\Gamma(3N-1)}R^{3N/2}K_{3N/2-1}(R) \quad \text{(A2)}$$

and to generate components of an isotropic unit vector $\mathbf{\Omega}$.

As is conventional in Monte Carlo calculations, we assume that a supply of random or pseudo-random numbers, ξ, equidistributed in the range (0,1) is available. We will show that if $\xi_0, \xi_1, \xi_2, \cdots, \xi_{3N}$ are such numbers and if

$$u=-\ln(\xi_1\xi_2\cdots\xi_{3N}), \quad 0\leqslant u<\infty \quad \text{(A3)}$$

and

$$v=(1-\xi_0^{2/(3N-1)})^{1/2}, \quad 0\leqslant v\leqslant 1, \quad \text{(A4)}$$

then

$$R=uv \quad \text{(A5)}$$

has the distribution given by (A2).

First we state two laws of the composition of random variables.[12] Let x and y be random variables on the range $(0,\infty)$ distributed as $f(x)$ and $g(y)$, respectively. Let

$$z=x+y,$$
$$w=xy.$$

Then the probability distribution functions (p.d.f.) of z and w are, respectively,

$$h(z)=\int_0^z f(x)g(z-x)dx, \quad \text{(A6)}$$

$$j(w)=\int_0^\infty f(x)g(w/x)dx/x. \quad \text{(A7)}$$

Now let

$$\eta_i=-\ln\xi_i;$$

$$u_n=-\sum_{i=1}^n \ln\xi_i=\sum_{i=1}^n \eta_i. \quad \text{(A8)}$$

The p.d.f. of η is such that

$$p_\eta(\eta)d\eta=p(\xi)d\xi=d\xi, \quad \text{(A9)}$$

$$p_\eta(\eta)=d\xi/d\eta=e^{-\eta}, \quad 0\leqslant 0<\infty. \quad \text{(A10)}$$

[12] H. Kahn, Atomic Energy Commission Report AECU-3259, April, 1954 (unpublished), pp. 16, 17.

The p.d.f. of u_n is

$$p_n(u)=\frac{u^{n-1}}{(n-1)!}e^{-u}, \quad 0\leqslant u<\infty. \tag{A11}$$

This result is easily proved by induction. It is immediate for $n=1$. Then by (A6)

$$p_{n+1}(u)=\frac{1}{(n-1)!}\int_0^u x^{n-1}e^{-x}e^{-(u-x)}dx \tag{A12}$$

$$=(1/n!)u^n e^{-u}.$$

The p.d.f. of v is given by

$$p_v(v)dv=-d\xi.$$

$$p_v(v)=|d\xi/dv|.$$

But (A4) may be inverted to give

$$\xi=(1-v^2)^{(3N-1)/2}, \tag{A13}$$

so that

$$p_v(v)=[(3N-1)/2]2v(1-v^2)^{(3N-3)/2}. \tag{A14}$$

Finally, from Eq. (A7) we find that

$$p_R(R)=\frac{(3N-1)}{(3N-1)!}\int_0^1 v(1-v^2)^{(3N-3)/2} \times(R/v)^{3N-1}e^{-R/v}dv/v. \tag{A15}$$

Putting $t=1/v$, the last equation becomes

$$p_R(R)=\frac{R^{3N-1}}{(3N-2)!}\int_1^\infty (t^2-1)^{(3N-3)/2}e^{-tR}dt. \tag{A16}$$

One of the integral representatives of the K_ν function given by Watson[13] shows that the last expression is identical with (A2).

A straightforward way of generating isotropic components $\omega_1, \cdots\omega_{3N}$ of a unit vector $\mathbf{\Omega}$ is to pick a point at random in the $3N$-dimensional unit hypercube. If this point lies inside the enclosed hypersphere, then it may be used to define the components ω. Because the ratio of the volume of sphere to cube is very small, this method seems rather inefficient. A satisfactory but less direct method consists in picking a vector $(\zeta_1,\zeta_2,\cdots,\zeta_{3N})$ from the $3N$-dimensional Gaussian

$$\exp(-\zeta_1^2-\zeta_2^2-\cdots-\zeta_{3N}^2),$$

and then set

$$\omega_i=\zeta_i(\sum \zeta_j^2)^{-1/2}.$$

To pick from the Gaussian it seems best to generate pairs of variables (ζ_1,ζ_2) distributed in a two-dimensional Gaussian

$$p(\zeta_1,\zeta_2)d\zeta_1 d\zeta_2=\frac{1}{\pi}\exp(-\zeta_1^2-\zeta_2^2)d\zeta_1 d\zeta_2.$$

With the change of variable

$$\zeta_1=\zeta\cos\phi,$$

$$\zeta_2=\zeta\sin\phi,$$

$$p(\zeta,\phi)=\frac{1}{\pi}\zeta\exp(-\zeta^2),$$

from which it follows that

$$\zeta=(-\ln\xi)^{1/2}.$$

The angle ϕ is equidistributed in $(0,2\pi)$.

[13] Reference 3, p. 172.