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# Monte-Carlo Solution of Schrödinger's Equation*

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A new Monte-Carlo method is presented for the calculation of the ground-state wavefunction and energy value of the many-body Schrödinger equation. Several refinements to the iterative scheme, including the use of variational wavefunctions to improve the energy estimate and a variance reducing technique, are also discussed. The method allows for a straightforward treatment of repulsive potentials. It is applied to several problems including the three-nucleon problem with simple two-body forces.

## 1. INTRODUCTION

In a recent paper [1] we reported on a new numerical method for obtaining solutions to the Schrödinger equation, based on the consideration of the operator $\exp(-\beta H)$, where $H$ is the Hamiltonian for the system and $\beta$ is a real parameter. By obtaining an approximate closed form for the coordinate space representation of this operator, we were able to reduce the problem to that of an integral eigenvalue equation, which we then solved by numerical quadratures. One of the salient features of the method is the very easy extension to systems with many spatial variables, but the numerical solution of the resulting multidimensional integral equations by quadratures is not feasible even with the present generation of modern digital computers. On the other hand, the evaluation of multidimensional integrals can be quite conveniently handled by Monte Carlo methods, and in this paper we present such a method designed to provide estimates for the ground-state energy and the corresponding wavefunction of a many-particle system.

Monte-Carlo methods have in fact been used extensively in the calculation of the ground-state energy and wavefunction for the Schrödinger equation [2–11, 16, 17]. Metropolis and Ulam [2] replaced the original differential equation by a difference equation whose solution is obtained by a random walk on the lattice defined by the difference scheme. Donsker and Kac [3] and Fortet [4] used a

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method based on the Wiener process and estimated the value of a Wiener or path integral [5, 6]. The value obtained can then be related to the value of the ground-state wavefunction at the point corresponding to the start of the path. A similar procedure is followed by Lawande, Jensen, and Sahlin [7], who have used the Monte-Carlo method to project out the ground-state contribution to the statistical density matrix and hence find a distribution approximating the square of the ground-state wavefunction. A different approach has been taken by Kalos [8, 9], who has written the Schrödinger equation as an integral equation whose eigenvalue is related to the strength of the potential. He then used a Monte-Carlo procedure to iterate the kernel of this integral equation to obtain a sequence of points which are distributed according to a density function equal to the ground-state wavefunction. Kostin and Steiglitz [10] related the solution of the Schrödinger equation to that of a Boltzmann transport equation and estimated the solution of this equation stochastically.

In this paper, we present a new Monte-Carlo method for the calculation of the ground-state wavefunction and energy value of the Schrödinger equation, based on the iteration scheme proposed in Ref. [1]. The relation between this method and the evaluation of path integrals was discussed in Ref. [1]. The result is a set of points distributed according to the ground-state wavefunction weighted by a function which can be chosen to minimize the variance associated with the scheme. It is shown how the approximate wavefunction obtained by this method can be used to find estimates of the corresponding energy value. The method is applied to several problems which have been chosen to enable us to compare the results with those obtained by other techniques.

## 2. The Monte-Carlo Method

The formal expressions derived in our earlier work [1] carry over in a quite straightforward manner for the solution of the Schrödinger equation with $n$ particles. In this case we look for the lowest eigenvalue and corresponding eigenfunction of the operator, $H = -\sum_{i=1}^{n} (\partial^2/\partial \mathbf{x}_i^2) + V(\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_n)$, where for convenience we have taken units such that $\hbar^2/2m = 1$. For simplicity we have also assumed the system to consist of like particles; there is no essential complication if particles of different mass are also included.

Taking $H_0 = -\sum_{i=1}^{n} (\partial^2/\partial \mathbf{x}_i^2)$, it has been shown quite generally that the operator $e^{-\beta H}$ can be approximated for small $\beta$ as

$$e^{-\beta H} \approx e^{-\frac{1}{2}\beta V} e^{-\beta H_0} e^{-\frac{1}{2}\beta V}, \tag{2.1}$$

with an error of order $\beta^3$. Moreover, if $E_0$ and $\psi_0(\mathbf{X})$ $(\mathbf{X} = \{\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_n\})$

represent the ground-state energy and wavefunction for the Hamiltonian $H$, then it has been shown that $\psi_0(\mathbf{X})$ satisfies the integral equation

$$e^{-\beta E_0}\psi_0(\mathbf{X}) = \int d\mathbf{Y}\, \langle \mathbf{X} \mid e^{-\beta H} \mid \mathbf{Y} \rangle\, \psi_0(\mathbf{Y}), \tag{2.2}$$

where for small $\beta$ we may replace the kernel by the approximation

$$\langle \mathbf{X} \mid e^{-\beta H} \mid \mathbf{Y} \rangle \approx e^{-\frac{1}{2}\beta V(\mathbf{X})} \frac{1}{(4\pi\beta)^{3n/2}} \exp\left[-\frac{(\mathbf{X}-\mathbf{Y})^2}{4\beta}\right] e^{-\frac{1}{2}\beta V(\mathbf{Y})}. \tag{2.3}$$

Using this expression in an iterative procedure based on Eq. (2.2) will give an energy $E_0(\beta)$ and a wavefunction $\psi_0(\mathbf{X}; \beta)$ which have the property that

$$\psi_0(\mathbf{X}; \beta) \to \psi_0(\mathbf{X})$$

and

$$E_0(\beta) \to E_0 \tag{2.4}$$

as $\beta \to 0$.

A Monte-Carlo technique for finding the ground state for operators of this type has been developed by Kalos [8, 9]; however, his original method [8] was confined to considering positive kernels only (which corresponds to attractive potentials), and the extension to repulsive potentials [9] complicates the sampling procedure. The method proposed in this section has none of these complications since the kernel used in Eq. (2.3) is always nonnegative (even in the presence of a hard core).

To describe the procedure expressed by Eq. (2.4) more precisely, we define a sequence of approximations to the ground-state wavefunction, $\psi^{(N)}(\mathbf{X}; \beta)$, where

$$\psi^{(N+1)}(\mathbf{X}; \beta) = \int e^{-\frac{1}{2}\beta V(\mathbf{X})} \frac{1}{(4\pi\beta)^{3n/2}} \exp\left[-\frac{(\mathbf{X}-\mathbf{Y})^2}{4\beta}\right] e^{-\frac{1}{2}\beta V(\mathbf{Y})} \psi^{(N)}(\mathbf{Y}; \beta)\, d\mathbf{Y}. \tag{2.5}$$

Now under quite general conditions, we have that [1]

$$\lim_{N\to\infty} \psi^{(N+1)}(\mathbf{X}; \beta) = e^{-\beta E_0(\beta)} \psi^{(N)}(\mathbf{X}; \beta)$$

and

$$\lim_{N\to\infty} \psi^{(N)}(\mathbf{X}; \beta) = \text{const}\ \psi_0(\mathbf{X}; \beta). \tag{2.6}$$

The Monte-Carlo technique employed to perform these iterations can be described as follows. Let

$$\chi^{(N)}(\mathbf{X}) = e^{\frac{1}{2}\beta V(\mathbf{X})} \psi^{(N)}(\mathbf{X}; \beta),$$

and write Eq. (2.5) as

$$\chi^{(N+1)}(\mathbf{X}) = \int \frac{1}{(4\pi\beta)^{3n/2}} \exp\left[-\frac{(\mathbf{X}-\mathbf{Y})^2}{4\beta}\right] e^{-\beta V(\mathbf{Y})}\chi^{(N)}(\mathbf{Y})\, d\mathbf{Y}. \tag{2.7}$$

We now select a set of $M^{(0)}$ $3n$-dimensional points $\{\mathbf{Y}_1, \mathbf{Y}_2, ..., \mathbf{Y}_{M^{(0)}}\}$ which are distributed according to an arbitrary density function $\chi^{(0)}(\mathbf{Y})$. Convergence will be improved if this approximates the function $e^{\pm\beta V(\mathbf{Y})}\psi_0(\mathbf{Y}; \beta)$, but this is not essential. Then we can construct a new set of points distributed according to $e^{-\beta V(\mathbf{Y})}\chi^{(0)}(\mathbf{Y})$ by replacing each point $i(1 \leqslant i \leqslant M^{(0)})$ in our original set by $m_i$ points at the same position. The integer $m_i$ is chosen so that

$$m_i = [ce^{-\beta V(\mathbf{Y}_i)}] + 1$$

if the fractional part of $ce^{-\beta V(\mathbf{Y}_i)}$ is greater than a random number chosen from a uniform distribution between 0 and 1, and

$$m_i = [ce^{-\beta V(\mathbf{Y}_i)}]$$

otherwise. Here $c$ is an arbitrary constant which determines the number of points in the new distribution and square brackets are used to denote the integral part of their contents. The value $c$ can be adjusted in the course of the computation to stabilize the number of points near some predetermined number so that the storage space in the computer is not overloaded. Suppose that $M^{(1)} = \sum_{i=1}^{M^{(0)}} m_i$ is the number of points thus generated. These are then distributed according to $e^{-\beta V(\mathbf{Y})}\chi^{(0)}(\mathbf{Y})$. We now add to each component of each of the $M^{(1)}$ points a different random number $\xi_{i\alpha}$ picked from a normal distribution with zero mean and variance $2\beta$, i.e.,

$$X_{i\alpha} = Y_{i\alpha} + \xi_{i\alpha}; \qquad i = 1,..., M^{(1)}; \qquad \alpha = 1,..., 3n. \tag{2.8}$$

Then using the convolution theorem governing the composition of random variables [11], the new set of points $\{\mathbf{X}_1, ..., \mathbf{X}_{M^{(1)}}\}$ are distributed according to $\chi^{(1)}(\mathbf{X})$, where

$$\chi^{(1)}(\mathbf{X}) = \int \frac{1}{(4\pi\beta)^{3n/2}} \exp\left[-\frac{(\mathbf{X}-\mathbf{Y})^2}{4\beta}\right] e^{-\beta V(\mathbf{Y})}\chi^{(0)}(\mathbf{Y})\, d\mathbf{Y}. \tag{2.9}$$

This corresponds to one iteration of the integral operator in Eq. (2.7). We can continue this procedure to obtain, after $N$ steps, $\chi^{(N)}(X)$, and so if $N$ is large enough, we will have a set of $M^{(N)}$ points distributed according to $\chi_0(\mathbf{X}) = e^{\pm\beta V(\mathbf{Y})}\psi_0(\mathbf{X}; \beta)$. The ground-state eigenvalue can be obtained by continuing the

iteration procedure past the point at which the distribution of points has converged to the ground state. Then Eq. (2.9) becomes

$$e^{-\beta E_0(\beta)}\chi_0(\mathbf{X}) = \int \frac{1}{(4\pi\beta)^{3n/2}} \exp\left[-\frac{(\mathbf{X}-\mathbf{Y})^2}{4\beta}\right] e^{-\beta V(\mathbf{Y})}\chi_0(\mathbf{Y})\, d\mathbf{Y}, \quad (2.10)$$

so that each iteration reproduces $\chi_0(\mathbf{X})$ but with a different sample of points. If the integral in Eq. (2.10) extends over all space we may obtain an expression for the ground-state energy value by integrating the last equation with respect to $\mathbf{X}$. We then have

$$e^{-\beta E_0(\beta)} = \frac{\int e^{-\beta V(\mathbf{X})}\chi_0(\mathbf{X})\, d\mathbf{X}}{\int \chi_0(\mathbf{X})\, d\mathbf{X}}, \quad (2.11)$$

and so $E_0(\beta)$ can be estimated by sampling the function $e^{-\beta V(\mathbf{X})}$ over a set of points distributed according to $\chi_0(\mathbf{X})$. Thus

$$e^{-\beta E_0(\beta)} \approx \frac{1}{M}\sum_{i=1}^{M} e^{-\beta V(\mathbf{X}_i)} \quad (2.12)$$

if we have $M$ points in the corresponding sample. This estimate can be improved by taking the average of Eq. (2.12) over many iterations. If $\beta$ is chosen small enough then $E_0(\beta) \approx E_0$ and so we have an estimate for the ground-state energy value.

## 3. The Use of Variational Wavefunctions

Although the iterative procedure based on Eq. (2.7) converges to the ground-state wavefunction for all potentials, the use of Eq. (2.11) as an estimator for the ground-state energy value will lead to erroneous results in some instances. The difficulty arises from the fact that Eq. (2.11) is obtained by an integration over all space. Clearly, there will be some situations (e.g., potentials with hard-core interactions) where the basic iteration equation applies over only a restricted domain of the configuration space variable $\mathbf{X}$, and we will be unable to use this expression. This problem can be overcome, and, indeed, we can obtain more accurate results for smooth potentials, by making use of the information obtained about the ground-state wavefunction by variational and other methods.

Let us suppose that an approximate wavefunction $\phi(\mathbf{X})$, which is continuous (with continuous first and piecewise continuous second derivatives) and satisfies the appropriate boundary conditions, has been obtained in analytic form. Then

both $\phi(\mathbf{X})$ and $H\phi(\mathbf{X})$ can be expanded in terms of the eigenfunctions, $\psi_s(\mathbf{X})$, of the original Schrödinger equation,

$$\phi(\mathbf{X}) = \sum_s a_s \psi_s(\mathbf{X}) \tag{3.1}$$

and

$$H\phi(\mathbf{X}) = \sum_s a_s E_s \psi_s(\mathbf{X}). \tag{3.2}$$

If we know the exact ground-state wavefunction, $\psi_0(\mathbf{X})$, then the energy can be obtained by using the orthogonality properties of the functions $\psi_s(\mathbf{X})$, i.e.,

$$E_0 = \frac{\int \psi_0(\mathbf{X})\, H\phi(\mathbf{X})\, d\mathbf{X}}{\int \psi_0(\mathbf{X})\, \phi(\mathbf{X})\, d\mathbf{X}}. \tag{3.3}$$

Now we can evaluate the above integrals, at least to an accuracy of order $\beta^3$, by using a set of points distributed according to $\chi_0(\mathbf{X}) = e^{\frac{1}{2}\beta V(\mathbf{X})}\psi_0(\mathbf{X}; \beta)$, obtained by using the iterative procedure based on Eq. (2.7). For small $\beta$, $\psi_0(\mathbf{X}; \beta) = \psi_0(\mathbf{X}) + O(\beta^3)$. Thus

$$\begin{aligned} E_0 &= \frac{\int \chi_0(\mathbf{X})\, e^{-\frac{1}{2}\beta V(\mathbf{X})} H\phi(\mathbf{X})\, d\mathbf{X}}{\int \chi_0(\mathbf{X})\, e^{-\frac{1}{2}\beta V(\mathbf{X})} \phi(\mathbf{X})\, d\mathbf{X}} + O(\beta^3) \\ &\approx \frac{\sum_{i=1}^{M} e^{-\frac{1}{2}\beta V(\mathbf{X}_i)} \{H\phi\}(\mathbf{X}_i)}{\sum_{i=1}^{M} e^{-\frac{1}{2}\beta V(\mathbf{X}_i)} \phi(\mathbf{X}_i)}, \end{aligned} \tag{3.4}$$

if there are $M$ points in the sample.

Although Eq. (3.3) is an exact result for all functions $\phi(\mathbf{X})$ with the appropriate continuity and boundary properties, the variance associated with the Monte-Carlo estimate Eq. (3.4) is affected by its choice. In general the closer $\phi(\mathbf{X})$ approximates the ground-state wavefunction $\psi_0(\mathbf{X})$ the smaller is the corresponding variance.

## 4. An Application

To illustrate the method we have calculated the ground-state energy for a system of $n$ equal particles in one dimension, which interact pairwise via inverse cube ("centrifugal potential") and linear ("harmonic oscillator potential") forces. The value of this particular example lies in the fact that it is a relatively nontrivial $n$-body problem for which an explicit analytic solution has been found [12, 13].

The Schrödinger equation for this problem is

$$\left\{-\sum_{i=1}^{n}\frac{\partial^2}{\partial x_i^2}+\frac{1}{2}\omega^2\sum_{i<j}(x_i-x_j)^2+g\sum_{i<j}(x_i-x_j)^{-2}\right\}\psi(x_1,\ldots,x_n)$$
$$=E\psi(x_1,\ldots,x_n). \tag{4.1}$$

Following the analysis of Calogero, the solution for the ground-state wavefunction (in the restricted region $x_1 \leqslant x_2 \leqslant \cdots \leqslant x_n$) and energy is found in terms of the variables

$$Z=\prod_{i<j}(x_i-x_j) \tag{4.2}$$

and

$$r^2=\frac{1}{n}\sum_{i<j}(x_i-x_j)^2.$$

It can be written as

$$\psi_0(x_1,\ldots,x_n)=Z^{a+\frac{1}{2}}\exp\left[-\frac{1}{2}\omega\sqrt{\frac{n}{2}}\,r^2\right]$$

and

$$E_0=\omega\sqrt{\frac{n}{2}}\left[n^2-1+\left(a-\frac{1}{2}\right)n(n-1)\right], \tag{4.3}$$

where $a=\frac{1}{2}(1+2g)^{1/2}$ with $g>-\frac{1}{2}$ to avoid the singularity at the origin introduced with two-body collapse [14]. As expected from the nature of the centrifugal forces, this wavefunction has the property of approaching zero when any two of the particles come together. Coupled to the one-dimensional nature of the problem, this property prevents particles overtaking one another, so that (as Calogero has observed [13]) the solution can be quite adequately described by considering only the restricted region of configuration space. The solution for the whole space can then be easily constructed with the appropriate statistics from the function $\psi_0(x_1,\ldots,x_n)$ [12]. As far as the calculation of the ground-state energy is concerned, however, it is sufficient to carry out the Monte-Carlo procedure in the restricted region.

In choosing the function $\phi(x_1, x_2,\ldots,x_n)$ to be used in calculating the energy in the Monte-Carlo method, it is most important that we satisfy the boundary condition as $(x_i-x_j)\to 0$. However, it is also necessary that the function we choose should be as simple as possible, in order to reduce the amount of computa-

tion. By demanding that each point $\mathbf{X}_i = \{x_1, ..., x_n\}_{(i)}$, in the sample belong to the restricted region of configuration space, it is clearly only necessary to satisfy the above boundary condition for neighbouring particles. Thus we have taken

$$\phi(x_1, ..., x_n) = \prod_{i=1}^{n-1} \phi(r_{i,i+1}) \tag{4.4}$$

where $r_{i,i+1} = x_{i+1} - x_i$, and $\phi$ must satisfy the boundary conditions $\phi(x_{i,i+1}) \to 0$ as $r_{i,i+1} \to 0, \infty$. A convenient form for the function $\phi$ is

$$\phi(r_{i,i+1}) = r_{i,i+1} e^{-\gamma r_{i,i+1}^2}, \tag{4.5}$$

where $\gamma$ is a parameter which can be chosen to reduce the variance.

With this particular form for $\phi(\mathbf{X})$, the function $H\phi$ needed in the expression Eq. (3.3) is easily found as

$$H\phi = 2 \sum_{i=2}^{n-1} \left\{\frac{1 - 2\gamma r_{i-1,i}^2}{r_{i-1,i}}\right\}\left\{\frac{1 - 2\gamma r_{i,i+1}^2}{r_{i,i+1}}\right\} \phi + 8\gamma \sum_{i=1}^{n-1} \left\{\frac{3}{2} - \gamma r_{i,i+1}^2\right\} \phi$$

$$+ \frac{1}{2} \omega^2 \sum_{i<j} (x_i - x_j)^2 \phi + g \sum_{i<j} (x_i - x_j)^{-2} \phi. \tag{4.6}$$

To commence the iteration process it is necessary to construct an initial distribution of sample points. Although it is not vital, at least as far as the final result is concerned, for this to be a very good approximation to the function $\chi_0(\mathbf{X})$, the choice will affect the amount of computation necessary for the distribution to converge to a given statistical uncertainty. In our calculations we have begun with a sample of one hundred points $\mathbf{X}_i$ distributed according to the formula

$$\begin{aligned} X_{i\alpha} &= \kappa(\alpha - n/2 - 1 + \tfrac{1}{2}\eta_{i\alpha}) \qquad \text{for } n \text{ odd} \\ &= \kappa(\alpha - n/2 - \tfrac{1}{2} + \tfrac{1}{2}\eta_{i\alpha}) \qquad \text{for } n \text{ even} \end{aligned} \tag{4.7}$$

with $1 \leqslant i \leqslant 100$, $1 \leqslant \alpha \leqslant n$. Here $\kappa$ is a parameter describing the separation of the particles and $\eta_{i\alpha}$ is a random number picked from a normal distribution with zero mean and variance one.

Now with a reasonably large value of $\beta$ (0.05), this distribution was iterated in such a fashion that the sample size increased to approximately five hundred points. This merely involves selecting an appropriate value of $c$ ($c \approx 1.2$ will allow for this to occur in approximately ten iterations without overloading the storage capacity). The value of $c$ was then fixed so that the sample size stabilized at this number of points ($c \approx 1.0$). After collecting the results for several hundred itera-

tions with this value of $\beta$ (the distribution would have converged well before this number of iterations), we repeated iterating with $\beta$ reduced to 0.025. With only 500 points this procedure can only be repeated usefully for a certain range of values of $\beta$. Eventually, if the value of $\beta$ is too small, the Monte-Carlo method becomes insensitive to the potential term, $e^{-\beta V(\mathbf{X}_i)} \approx 1 - \beta V(\mathbf{X}_i)$, since on the average only the fraction $\beta V$ of the total number of points in the sample are affected by the potential. Any further reduction in the value of $\beta$ must be accompanied by a corresponding increase in the number of sample points. Thus after further reducing the value of $\beta$ to 0.01 we increased the sample size to 1000 points to improve the results. Of course this will eventually provide a limit to the accuracy of the calculations; however, for most cases, this will not concern us too much since the errors involved in the basic approximation to the Green's function can easily be kept smaller than the statistical error involved with the Monte-Carlo method. It is interesting to note the analogous difficulty which arose with the application of finite-difference methods [1]; there, any reduction in $\beta$ must be accompanied by an increase in the number of grid points for the accurate numerical evaluation of the integrals.

TABLE I

A Typical Set of Monte-Carlo Estimates[a] for the Ground-State Energy of a System with Nine Particles when $\omega = 0.25$ and $g = 1.5$.

| $\beta$ | $M$ | $E_v$ | $E_{mc}$ |
|---|---|---|---|
| 0.05 | 500 | $61.15 \pm 0.04$ | $60.13 \pm 0.08$ |
| 0.025 | 500 | $61.56 \pm 0.04$ | $61.11 \pm 0.11$ |
| 0.01 | 500 | $61.42 \pm 0.03$ | $61.12 \pm 0.15$ |
| 0.01 | 1000 | $61.51 \pm 0.03$ | $61.31 \pm 0.10$ |

[a] The approach towards the exact value (61.51828) is noticeable in the estimates $E_{mc}$. Notice also, the greatly improved value for $\beta = 0.05$ using the variational estimate against the usual Monte-Carlo average. As the distribution improves for smaller $\beta$ this difference becomes less significant. Each set of one hundred iterations with approximately 500 sample points took approximately 6 min to compute on a CDC 6400 computer.

The results obtained for the case $n = 9$ are illustrated in Table I. Each result represents the mean over 100 iterations (each involving approximately $M$ sample points) taken at a stage when the distribution had appeared to have converged for that value of $\beta$. We have presented here both estimates for the energy value: $E_{mc}$ calculated using Eq. (2.12) and $E_v$ using Eq. (3.4). The estimate Eq. (2.12) is permissible in this case (even though we have used a restricted region of configuration space in the calculations) since the equation (2.9) is valid over the whole space.

Of course in the discussion of any Monte-Carlo procedure some estimate of

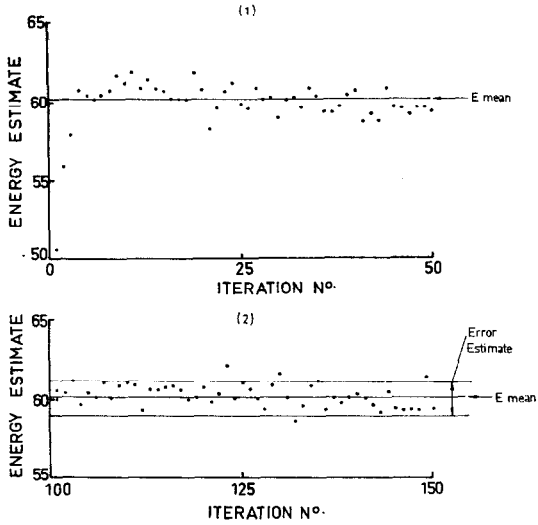


FIG. 1. Graphs showing the results of successive energy estimates plotted against iteration number. Both sets were taken with $\beta = 0.05$ and a sample size of 500 points.

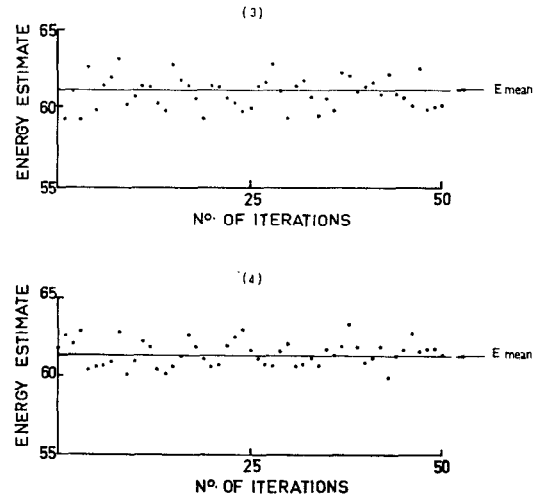


FIG. 2. Sucessive energy estimates plotted against the number of iterations for two different values of $\beta$. (3) $\beta = 0.025$; (4) $\beta = 0.01$. These plots illustrate the correlations between successive estimates which are particularly pronounced in curve (4).

the statistical uncertainty plays an important role. In the present case, however, this needs a little explanation. In normal Monte-Carlo work (e.g., in the estimation of the value of some integral) the procedure may be repeated several times to

obtain different estimates for the quantity desired. If a different set of sampling points is taken for each calculation, one would expect the distribution of Monte-Carlo estimates to be random, so that an estimate of the error can be given from the variance associated with their distribution. It is usual, for example, to calculate the standard error in the mean value and quote this as the error in the calculated value. In our calculations however, the successive estimates for the energy values are correlated to some extent as we illustrate in Figs. 1 and 2. In the first of these diagrams we have traced the values of the estimate $E_{\mathrm{mc}}$ for the first 50 iterations (1) and from the 150-th to the 200-th iteration (2) with $\beta = 0.05$ and $M \approx 500$. One particularly noticeable feature is the very fast convergence illustrated in Fig. 1(1). In Fig. 2 we have given samples of two sets of 50 iterations taken with different values of $\beta$ ($\beta = 0.025$ in (3) and $\beta = 0.01$ in (4)) after convergence was reached, showing that the correlations get more pronounced as $\beta$ is decreased. This correlation between successive estimates arises because successive sample points differ only by the addition of a small random number (see Eq. (2.8)), which on the average becomes smaller as $\beta$ is decreased.

From plots such as these we can tell quite easily when the iteration procedure has converged, and also obtain some feeling for the errors involved by drawing in bounds as we have done in Fig. 1(2). Because of the correlations a straightforward variance calculation is likely to be misleading; however, if we take a number of estimates, large enough so that the correlations extend over a small fraction of this sample, then a calculation of the variance does given an indication of the statistical uncertainty. We have presented this with each estimate.

In Table II we compare the analytic values of the ground state energy with the Monte-Carlo estimates for a range of values of $n$. A noticeable feature of the

TABLE II

A Comparison of the Monte-Carlo Estimates[a] with the Exact Values for the Ground-State Energy for the System with $n$ Particles

| $n$ | $\gamma$ | Exact value | $E_{\mathrm{v}}$ | $E_{\mathrm{mc}}$ |
|---|---|---|---|---|
| 3 | 0.15 | 3.36804 | $3.35 \pm 0.004$ | $3.35 \pm 0.02$ |
| 5 | 0.2 | 13.43968 | $13.40 \pm 0.006$ | $13.37 \pm 0.04$ |
| 7 | 0.25 | 32.27179 | $32.40 \pm 0.01$ | $32.34 \pm 0.09$ |
| 9 | 0.025 | 61.51828 | $61.51 \pm 0.03$ | $61.31 \pm 0.10$ |
| 11 | 0.3 | 102.60284 | $102.55 \pm 0.04$ | $102.31 \pm 0.14$ |

[a] Each estimate represents an average of 100 Monte-Carlo iterations. The iterations were performed with a sample of approximately 1000 points and $\beta = 0.01$. With $n = 11$ each set of 100 iterations takes typically 15 min computing time on a CDC 6400 computer.

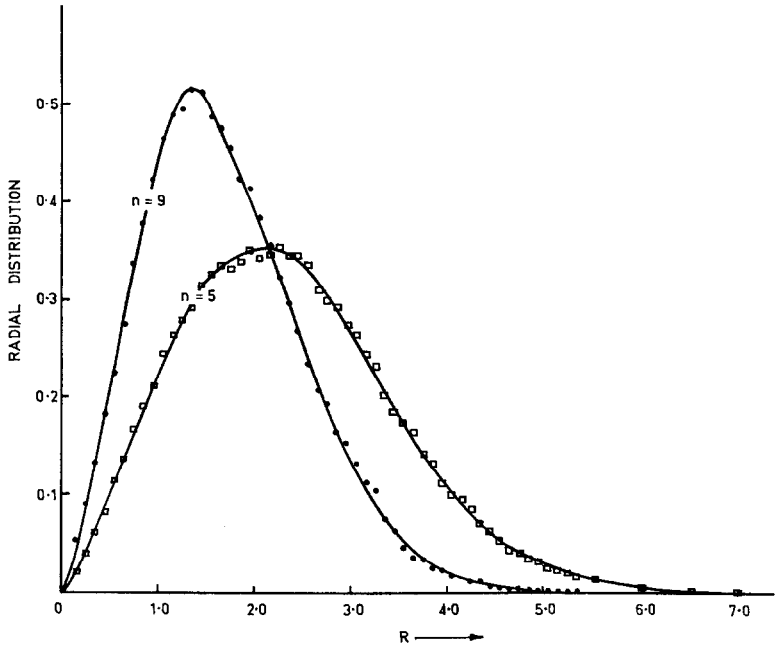


FIG. 3. The radial distribution function for two neighbouring particles in a set of five and nine particles in one dimension. The function is weighted by the factor $e^{\frac{1}{2}\beta V}$. The histograms (represented by the points) were normalized to 100 points, distributed in the region $0 < R < 10$ in equal intervals of 0.1. The solid lines are drawn in as an approximate best fit to the histogram. The Monte-Carlo calculations were performed with $\beta = 0.01$ and approximately 1000 sample points.

calculations is the small error associated with the estimates $E_V$. One should not be too concerned about the apparent inconsistency in the estimates $E_V$, which do not all satisfy $E_V - \Delta E_V < E_{\text{exact}} < E_V + \Delta E_V$. For a particular value of $\beta$ this would not necessarily be true unless $\beta$ is sufficiently small. We should also point out that the value $E_V$ for a given $\beta$ also depends upon the parameter $\gamma$, since this will determine the amount of admixture of higher states (see Eq. (3.1)). In general the value of $\gamma$ must be found by trial-and-error tactics, if it is not possible to gain some information about the wavefunction from some other means. Since this example was taken to illustrate the method we did not consider this point too seriously and so we did not use an optimum value of $\gamma$ for each $n$.

Finally, in Fig. 3 we illustrate the type of distribution obtained for the quantity $R = r_{12}$, which represents the probability for two neighbouring particles to be separated by a distance $R$.

## 5. Improved Variance

In Monte-Carlo work it is always important to use as much information about the functions being integrated as can be obtained. In our particular case each iteration involves an integral over an approximation to the wavefunction. Often we will have some prior knowledge about the general form of this function; for example, we may know its asymptotic form for large distances or its behaviour near the origin. Even if the form is not known beforehand, it can always be found using the methods of the last sections. In this section we show how this knowledge can be used to obtain estimates for $E_0$ with smaller variances than those associated with the estimator given in Eq. (2.12).

To see how that can be done, we first multiply the basic equation Eq. (2.5) by a function $f(\mathbf{X})$ and consider the resultant equation as one which we can iterate to find the functions $\chi^{(N)}(\mathbf{X})$ defined by

$$\chi^{(N)}(\mathbf{X}) = f(\mathbf{X})\, \psi^{(N)}(\mathbf{X}; \beta) \qquad (N = 0, 1, 2, \ldots). \tag{5.1}$$

Thus

$$\chi^{(N+1)}(\mathbf{X}) = \int d\mathbf{Y}\, f(\mathbf{X})\, e^{-\frac{1}{2}\beta V(\mathbf{X})} \frac{1}{(4\pi\beta)^{3n/2}} \exp\left[-\frac{(\mathbf{X}-\mathbf{Y})^2}{4\beta}\right] \times e^{-\frac{1}{2}\beta V(\mathbf{Y})} f^{-1}(\mathbf{Y})\, \chi^{(N)}(\mathbf{Y}). \tag{5.2}$$

Now

$$\begin{aligned} \lim_{N\to\infty} \chi^{(N+1)}(\mathbf{X}) &= e^{-\beta E_0(\beta)} \chi^{(N)}(\mathbf{X}) \\ &= \text{const}\, f(\mathbf{X})\, \psi_0(\mathbf{X}; \beta), \end{aligned} \tag{5.3}$$

and integrating Eq. (5.2) over all $\mathbf{X}$,

$$e^{-\beta E_0(\beta)} = \int d\mathbf{Y} \left\{ \int d\mathbf{X}\, f(\mathbf{X})\, e^{-\frac{1}{2}\beta V(\mathbf{X})} \frac{1}{(4\pi\beta)^{3n/2}} \exp\left[-\frac{(\mathbf{X}-\mathbf{Y})^2}{4\beta}\right] \right\} \times \frac{e^{-\frac{1}{2}\beta V(\mathbf{Y})} f^{-1}(\mathbf{Y})\, f(\mathbf{Y})\, \psi_0(\mathbf{Y}; \beta)}{\int d\mathbf{X}\, f(\mathbf{X})\, \psi_0(\mathbf{X}; \beta)}. \tag{5.4}$$

Thus, by generating a set of points $\mathbf{Y}_i$ distributed according to $\chi^{(N)}(\mathbf{X})$ we obtain the following Monte-Carlo estimate:

$$e^{-\beta E_0(\beta)} \approx \frac{1}{M} \sum_{i=1}^{M} \left\{ \int d\mathbf{X}\, f(\mathbf{X})\, e^{-\frac{1}{2}\beta V(\mathbf{X})} \frac{1}{(4\pi\beta)^{3n/2}} \exp\left[-\frac{(\mathbf{X}-\mathbf{Y}_i)^2}{4\beta}\right] \right\} \times e^{-\frac{1}{2}\beta V(\mathbf{Y}_i)} f^{-1}(\mathbf{Y}_i) \tag{5.5}$$

When $f(\mathbf{X})$ is actually equal to $\psi_0(\mathbf{X}; B)$ there will be a zero variance for this expression since the term inside the summation is a constant. Since we are trying to find $\psi_0(\mathbf{X}; \beta)$ this does not appear to be a very useful result. However, a small variance would be expected if we choose for $f(\mathbf{X})$ a function which is a reasonable approximation to $\psi_0(\mathbf{X}; \beta)$. This is not the only restriction on $f(\mathbf{X})$, however, for we have to be able to perform the integrations over $\mathbf{X}$ in Eq. (5.5). In practice these two restrictions require that $f(\mathbf{X})\, e^{-\frac{1}{2}\beta V(\mathbf{X})}$ be of Gaussian form. (An expression involving a sum of Gaussians would also be permissible.) So let us choose

$$f(\mathbf{X}) = \exp[\tfrac{1}{2}\beta V(\mathbf{X}) - \mathbf{X}^2/\alpha^2], \tag{5.6}$$

where $\alpha$ is a range parameter which can be chosen to make $f(\mathbf{X})$ approximate $\psi_0(\mathbf{X}; \beta)$. The strong damping of $\chi(\mathbf{X})$ for large $\mathbf{X}$ now has the effect of increasing the sample size at small distances. With this choice we can rewrite the equation describing the iteration procedure, Eq. (5.2), as

$$\begin{aligned}\chi^{(N+1)}(\mathbf{X}) = \int d\mathbf{Y}\, \frac{1}{(4\pi\beta\sigma)^{3n/2}} \exp\left[-\frac{(\mathbf{X}-\mathbf{Y})^2}{4\beta\sigma}\right] \\ \times\, \sigma^{3n/2} \exp\left[\frac{4\beta\sigma\mathbf{Y}^2}{\alpha^4} - \beta V(\mathbf{Y})\right] \chi^{(N)}(Y),\end{aligned} \tag{5.7}$$

where $\sigma = \alpha^2/(\alpha^2 + 4\beta)$.

To iterate this equation stochastically, we use a similar procedure to that outlined in Section 2. We start with an arbitrary set of points distributed according to $\chi^{(0)}(\mathbf{Y})$, construct a set of points $\{\mathbf{Y}_1, \ldots, \mathbf{Y}_{M^{(1)}}\}$ distributed according to $\exp[4\beta\sigma\mathbf{Y}^2/\alpha^4 - \beta V(\mathbf{Y})]\, \chi^{(0)}(\mathbf{Y})$, and then form the new points

$$\begin{aligned} X_{i\alpha} &= \sigma Y_{i\alpha} + \xi_{i\alpha}\,; \\ i &= 1, \ldots, M^{(1)}; \qquad \alpha = 1, \ldots, 3n, \end{aligned} \tag{5.8}$$

where the $\xi_{i\alpha}$ are selected from a normal distribution with zero mean and variance $2\beta\sigma$. Note that we have multiplied each $Y_{i\alpha}$ by $\sigma$ before adding the $\xi_{i\alpha}$. The new points $\{\mathbf{X}_1, \ldots, \mathbf{X}_{M^{(1)}}\}$ will now be distributed according to $\chi^{(1)}(\mathbf{X})$ as given by Eq. (5.7). The process is repeated until it converges to the ground state, i.e., until we obtain a set of points distributed according to $\chi_0(\mathbf{X}) = f(\mathbf{X})\, \psi_0(\mathbf{X}; \beta)$. Now for smooth potentials we can estimate $e^{-\beta E_0(\beta)}$ by integrating Eq. (5.7) (cf. Eq. (5.4)) to obtain

$$\begin{aligned} e^{-\beta E_0(\beta)} &= \frac{\int d\mathbf{X}\, \sigma^{3n/2} \exp[4\beta\sigma\mathbf{X}^2/\alpha^4 - \beta V(\mathbf{X})]\, \chi_0(\mathbf{X})}{\int d\mathbf{X}\, \chi_0(\mathbf{X})} \\ &\approx \frac{1}{M} \sum_{i=1}^{M} \sigma^{3n/2} \exp\left[\frac{4\beta\sigma\mathbf{X}_i^2}{\alpha^4} - \beta V(\mathbf{X}_i)\right], \end{aligned} \tag{5.9}$$

if there are $M$ points in the sample. Alternatively, we can use the variational form Eq. (3.4), which now becomes

$$E_0 = \frac{\int d\mathbf{X}\, \chi_0(\mathbf{X}) f^{-1}(\mathbf{X})\, H\phi(\mathbf{X})}{\int d\mathbf{X}\, \chi_0(\mathbf{X}) f^{-1}(\mathbf{X})\, \phi(\mathbf{X})} \approx \frac{\sum_{i=1}^{M} f^{-1}(\mathbf{X}_i)\{H\phi\}(\mathbf{X}_i)}{\sum_{i=1}^{M} f^{-1}(\mathbf{X}_i)\, \phi(\mathbf{X}_i)}. \tag{5.10}$$

## 6. The Three-Body Problem

The calculation of the ground-state energy for a system of three particles interacting with realistic two-particle forces is of fundamental interest in physics. Undoubtedly the most popular numerical method for the solution of the problem involves the variational approach, viz. the minimization of an expression for the energy by the variation of certain parameters describing an assumed form for the appropriate wavefunction, or alternatively the solution of the corresponding Euler–Lagrange equations. The result of such a calculation is a value for an upper (and lower) bound to the actual energy. Although the accuracy afforded by this method is excellent, the calculations are often lengthy (perhaps a few hours) in terms of the computer time required. The approach which we have advanced in this work gives results with an accuracy of about 0.1 MeV for computing times measured in fractions of an hour.

For a system of three particles the starting point for our calculation is the partial differential equation

$$\left\{ -\sum_{i=1}^{3} \frac{\hbar^2}{2m_i} \frac{\partial^2}{\partial \mathbf{X}_i^2} + \sum_{i<j} V(|\mathbf{r}_{ij}|) \right\} \Psi(\mathbf{X}_1, \mathbf{X}_2, \mathbf{X}_3, \beta) = -\frac{\partial \Psi}{\partial \beta}(\mathbf{X}_1, \mathbf{X}_2, \mathbf{X}_3, \beta), \tag{6.1}$$

where the $\mathbf{X}_i$ are the coordinates of the three particles (of mass $m_i$) and $\mathbf{r}_{ij} = \mathbf{X}_i - \mathbf{X}_j$. The centre-of-mass motion can easily be separated by performing the following transformation to the coordinates $\mathbf{q}_i$, defined by

$$\mathbf{q}_1 = \frac{2}{\hbar} \frac{m_1\mathbf{X}_1 + m_2\mathbf{X}_2 + m_3\mathbf{X}_3}{(2M)^{1/2}},$$

$$\mathbf{q}_2 = \frac{2}{\hbar} \left(\frac{m_2 m_3}{2m}\right)^{1/2} (\mathbf{X}_2 - \mathbf{X}_3),$$

and

$$\mathbf{q}_3 = \frac{2}{\hbar}\left(\frac{m_1}{2mM}\right)^{1/2}(m_2\mathbf{X}_2 + m_3\mathbf{X}_3 - m_1\mathbf{X}_1), \tag{6.2}$$

where $M = m_1 + m_2 + m_3$ and $m = m_2 + m_3$. The Jacobian for this transformation is easily found to be

$$\frac{\partial(\mathbf{X}_1, \mathbf{X}_2, \mathbf{X}_3)}{\partial(\mathbf{q}_1, \mathbf{q}_2, \mathbf{q}_3)} = \left(\frac{\hbar^6}{2^3 m_1 m_2 m_3}\right)^{3/2}.$$

The value of this transformation is that the relative coordinates

$$\mathbf{r}_{23} = \frac{\hbar}{2}\left(\frac{2m}{m_2 m_3}\right)^{1/2}\mathbf{q}_2,$$

$$\mathbf{r}_{31} = \frac{\hbar}{2}\left[\left(\frac{2M}{mm_1}\right)^{1/2}\mathbf{q}_3 - \left(\frac{2m_2}{mm_3}\right)^{1/2}\mathbf{q}_2\right],$$

and

$$\mathbf{r}_{21} = \frac{\hbar}{2}\left[\left(\frac{2M}{mm_1}\right)^{1/2}\mathbf{q}_3 + \left(\frac{2m_3}{mm_2}\right)^{1/2}\mathbf{q}_2\right], \tag{6.3}$$

are functions of the variables $\mathbf{q}_2$ and $\mathbf{q}_3$ only. Integrating over the centre-of-mass coordinates ($\mathbf{q}_1$), we see that the ground-state wavefunction $\psi_0(\mathbf{q}_2, \mathbf{q}_3)$ satisfies the integral equation (corresponding to Eq. (2.2)),

$$e^{-\beta E_0}\psi_0(\mathbf{q}_2, \mathbf{q}_3) = \int d\mathbf{p}_2 \int d\mathbf{p}_3\, e^{-\frac{1}{2}\beta v(\mathbf{q}_2,\mathbf{q}_3)} \times \frac{1}{(4\pi\beta)^3}\exp\left[-\frac{(\mathbf{q}_2 - \mathbf{p}_2)^2 - (\mathbf{q}_3 - \mathbf{p}_3)^2}{4\beta}\right] e^{-\frac{1}{2}\beta v(\mathbf{p}_2,\mathbf{p}_3)} \times \psi_0(\mathbf{p}_2, \mathbf{p}_3), \tag{6.4}$$

where

$$v(\mathbf{q}_2, \mathbf{q}_3) = \sum_{i<j} V(|\mathbf{r}_{ij}|).$$

In terms of the harmonic oscillator approximation (see Appendix), the kernel of this integral equation is replaced by the better approximation

$$e^{-\frac{1}{2}\beta u(\mathbf{q}_2,\mathbf{q}_3)}\frac{1}{(4\pi\gamma)^3}\exp\left[-\frac{(\mathbf{q}_2 - \mathbf{p}_2)^2 - (\mathbf{q}_3 - \mathbf{p}_3)^2}{4\gamma}\right] e^{-\frac{1}{2}\beta u(\mathbf{p}_2,\mathbf{p}_3)}, \tag{6.5}$$

where

$$u(\mathbf{q}_2, \mathbf{q}_3) = v(\mathbf{q}_2, \mathbf{q}_3) + \frac{\omega}{\beta}[\tanh(\beta\omega) - \beta\omega](\mathbf{q}_2^2 + \mathbf{q}_3^2), \tag{6.6}$$

and $\gamma = \sinh(2\omega\beta)/2\omega$. In these expressions, the value of $\omega$ is to be determined independently to reduce the approximations involved in the replacement of the exact Green's function. Introducing the factor

$$f(\mathbf{q}_2, \mathbf{q}_3) = \exp[\tfrac{1}{2}\beta\, u(\mathbf{q}_2, \mathbf{q}_3) - (\mathbf{q}_2^2 + \mathbf{q}_3^2)/\alpha^2]$$

to reduce the variance (see Section 5), the basic equation we must iterate becomes

$$e^{-\beta E_0}\chi_0(\mathbf{q}_2, \mathbf{q}_3) = \int d\mathbf{p}_2 \int d\mathbf{p}_3 \frac{\sigma^3}{(4\pi\gamma\sigma)^3} \exp\left[-\frac{(\mathbf{q}_2 - \sigma\mathbf{p}_2)^2 - (\mathbf{q}_3 - \sigma\mathbf{p}_3)^2}{4\gamma\sigma}\right]$$
$$\times \exp\left[\frac{4\gamma\sigma(\mathbf{p}_2^2 + \mathbf{p}_3^2)}{\alpha^4}\right] - \beta u(\mathbf{p}_2, \mathbf{p}_3)\, \chi_0(\mathbf{p}_2, \mathbf{p}_3), \tag{6.7}$$

where $\sigma = \alpha^2/(\alpha^2 + 4\gamma)$ and

$$\chi_0(\mathbf{q}_2, \mathbf{q}_3) = e^{\pm\beta u(\mathbf{q}_2, \mathbf{q}_3) - (\mathbf{q}_2^2 + \mathbf{q}_3^2)/\alpha^2}\psi_0(\mathbf{q}_2, \mathbf{q}_3). \tag{6.8}$$

*The three-nucleon problem*

As an example we consider the following simplified model of the triton; three identical particles interacting via the central two-body (spin-independent) potential

$$V(r) = -51.5 \exp\left(-\frac{r^2}{b^2}\right) \text{MeV} \tag{6.9}$$

with $b = 1.6$ F. Such a potential has been used by Baker, Gammel, Hill, and Wills [15] in their numerical calculations and yields the result $E_0 = -9.42$ MeV for the ground state (a spherically symmetric $s$ state). Kalos [8] used a Monte-Carlo iterative method which finds the strength of the potential needed to produce a particular ground-state energy. He found $E_0 = -9.47 \pm 0.4$ MeV. Herndon and Tang [17], using a five-parameter variational wavefunction, obtained an upper and lower bound to the ground-state energy such that $-9.75 \pm 0.04 > E_0 > -9.99 \pm 0.05$. This, along with the calculations of Rosati and Barbi [18] and Banville and Kunz [20], are the most accurate calculations made with this potential.

Before we can apply the method described in the previous sections for the solution of Eq. (6.7), we must select an approximate solution $\phi(\mathbf{X}_1, \mathbf{X}_2, \mathbf{X}_3)$ to use in calculating the estimate for the energy in Eq. (5.10), and values for the parameters $\omega$ and $\alpha$. The approximate variational wavefunction was taken to be of the product form (cf. Ref. [19])

$$\phi(\mathbf{X}_1, \mathbf{X}_2, \mathbf{X}_3) = \rho(r_{21})\, \rho(r_{31})\, \rho(r_{23}). \tag{6.10}$$

With this particular form the function $H\phi$ needed in the expression Eq. (5.10) can easily be found using the following relation for the kinetic energy operator [19]:

$$\begin{aligned} T &= -\frac{\hbar^2}{2m}\sum_{i=1}^{3}\frac{\partial^2}{\partial \mathbf{X}_i^2} \\ &= -\frac{\hbar^2}{m}\sum_{\text{cyclic}}\left[\frac{\partial^2}{\partial r_{23}^2}+\frac{2}{r_{23}}\frac{\partial}{\partial r_{23}}+\cos\theta_1\frac{\partial^2}{\partial r_{31}\,\partial r_{21}}\right], \end{aligned} \tag{6.11}$$

where $\cos\theta_1 = (r_{31}^2 + r_{21}^2 - r_{23}^2)/2r_{31}r_{21}$, and $\sum_{\text{cyclic}}$ means the sum over all cyclic permutations of the indices 1, 2, 3. It is

$$\begin{aligned} H\phi &= (T+V)\,\phi \\ &= -\frac{\hbar^2}{m}\sum_{\text{cyclic}}\left\{\rho(r_{21})\,\rho(r_{31})\,\rho''(r_{23})+\frac{2}{r_{23}}\rho'(r_{23})+\rho(r_{23})\,\rho'(r_{21})\,\rho'(r_{31})\cos\theta_1\right\} \\ &\quad +\sum_{\text{cyclic}} V(r_{23})\,\rho(r_{21})\,\rho(r_{31})\,\rho(r_{23}). \end{aligned} \tag{6.12}$$

The function $\rho(r)$ was taken to have the form

$$\rho(r) = e^{-(\eta_1 r)^2} - \kappa e^{-(\eta_2 r)^2}. \tag{6.13}$$

This particular approximation has been used by Herndon and Tang [17] in their variational calculations and the optimum values for the parameters $\eta_1$, $\eta_2$, and $\kappa$ were found to be $\eta_1 = 0.228$ F, $n_2 = 0.565$ F, and $\kappa = 1.06$.

According to the discussion on the harmonic oscillator approximation in the Appendix, a value of $\omega$ is given by minimizing (with respect to $\omega$) the expression

$$\epsilon(\omega) = \int \Phi_0(\mathbf{q}_2, \mathbf{q}_3)\, H\Phi_0(\mathbf{q}_2, \mathbf{q}_3)\, d\mathbf{q}_2\, d\mathbf{q}_3, \tag{6.14}$$

where $\Phi_0(\mathbf{q}_2, \mathbf{q}_3)$ is the ground-state harmonic oscillator wavefunction,

$$\Phi_0(\mathbf{q}_2, \mathbf{q}_3) = \left(\frac{\omega}{\pi}\right)^{3/2}\exp\left[-\frac{\omega}{2}(\mathbf{q}_2^2 + \mathbf{q}_3^2)\right]. \tag{6.15}$$

In their variational calculations, Herndon and Tang [17] have already considered this task. Their results yield the value $\omega = 0.16$ (corresponding to the variational estimate $E_0 < -6.39$ MeV).

Finally, we must select a value for $\alpha$ to minimize the variance in the Monte-Carlo estimates. The basic requirement is that the function $\phi$ be chosen to mimic the

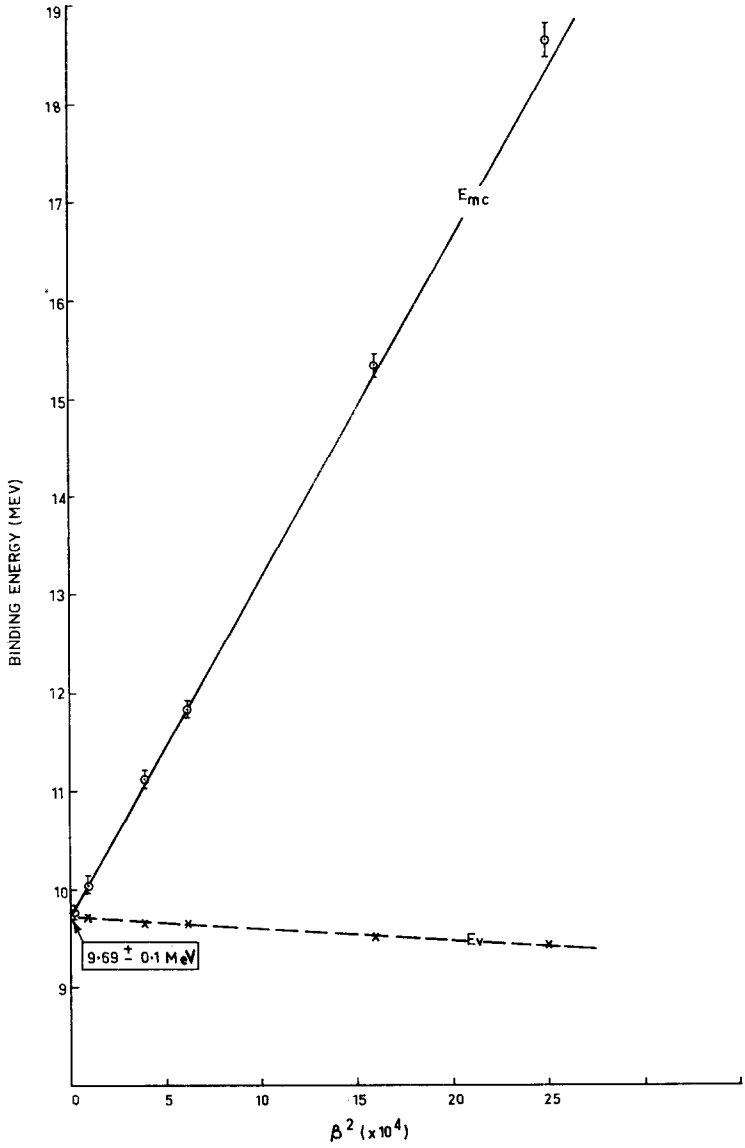


FIG. 4. The variation in the estimate for the binding energy of the ground state of the triton as a function of $\beta^2$. A least mean squares fit to the values of $E_{mc}$ with $\beta \leqslant 0.025$ gives an extrapolated result (for $\beta = 0$) of $E_0 = -9.69 \pm 0.1$ MeV.

ground-state wavefunction. From a practical point of view, the collection of statistics from only a few iterations of the Monte-Carlo process (over a range of values of $\alpha$) will quickly suggest a suitable value. In the cases we have tried, we have found that the results were not very sensitive to variations in the value of $\alpha$, provided $\alpha$ is chosen greater than the range of the ground-state wavefunction. For very small values of $\beta$, the expression (6.8) for $\phi$ is of Gaussian form and hence $\alpha$ is related to the value of $\omega$ through $\alpha = \sqrt{2/\omega}$.

The Monte-Carlo calculations were performed in the same way as has already been described in Section 4. An initial distribution for the solution $\chi_0(\mathbf{q}_2, \mathbf{q}_3)$ can easily be generated using a Gaussian of the form Eq. (6.15) for the function $\psi_0(\mathbf{q}_2, \mathbf{q}_3)$. Then, for small $\beta$, $\chi_0(\mathbf{q}_2, \mathbf{q}_3)$ has the form of a normal distribution with mean zero and variance $(\omega + 2/\alpha^2)^{-1/2}$. An initial set of 100 points with this distribution is then iterated until a sufficiently large sample is obtained. Iterations are repeated until convergence appears for this value of $\beta$. The value of $\beta$ is then reduced and we continue in this fashion until no significant improvement is obtained with a further reduction in $\beta$. At this stage it is necessary to increase the sample size for the reasons already stated in Section 4. An example of the sort of results obtained is given in Table III. These results have been plotted against $\beta^2$ in Fig. 4 to illustrate the trend as $\beta$ is decreased. From the extrapolation of these calculations for $E_{\mathrm{mc}}$, this method suggests the value $E_0 = -9.69 \pm 0.10$ MeV for the ground-state energy value. Although this result is an improvement over

TABLE III

Monte-Carlo Estimates[a] for the Ground-State Energy Value of the Triton

| | | Energy estimates (MeV)[b] | |
|---|---|---|---|
| $\beta$ | $M$ | $E_{\mathrm{v}}$ | $E_{\mathrm{mc}}$ |
| 0.05 | 600 | $-9.44 \pm 0.01$ | $-18.64 \pm 0.16$ |
| 0.04 | 600 | $-9.50 \pm 0.01$ | $-15.33 \pm 0.13$ |
| 0.025 | 600 | $-9.63 \pm 0.02$ | $-11.85 \pm 0.09$ |
| 0.02 | 600 | $-9.63 \pm 0.02$ | $-11.12 \pm 0.09$ |
| 0.01 | 600 | $-9.70 \pm 0.02$ | $-10.04 \pm 0.09$ |
| 0.005 | 600 | $-9.61 \pm 0.02$ | $-9.55 \pm 0.08$ |
| 0.005 | 1900 | $-9.70 \pm 0.02$ | $-9.77 \pm 0.06$ |

[a] Each calculation represents the mean of 300 iterations, each performed with approximately $M$ sample points. For each calculation we have also presented the standard error in the mean value. A noticeable feature is the great improvement provided by the variation calculation ($E_{\mathrm{v}}$) over the Monte-Carlo average ($E_{\mathrm{mc}}$) for large values of $\beta$. With $M \approx 600$, each 100 iterations takes approximately 5 min on the CDC 6400 computer.

[b] For comparison, the variational result is $-9.78$ MeV [17, 20].

the results of Kalos [8], and in good agreement with the variational calculations [18, 19, 20], it is rather apparent that an extremely large sample is required to obtain really accurate results. To illustrate this breakdown in the method we have included some results using only 600 sample points for $\beta = 0.005$ in Table III. As we can see from the table there is an improvement as the sample size is increased to 1900 points; however, as each iteration with this number of points takes approximately 10 secs on the CDC 6400 computer, and it is necessary to iterate several hundred times to obtain good statistics, we did not feel that any further decrease in $\beta$ would be justified. The two particle distribution function (weighted by the factors $e^{\frac{1}{2}\beta u(q_2,q_3)-(q_2^2+q_3^2)/\alpha^2}$) can be calculated by compiling a histogram of the values of the quantity $r_{12}$ during the course of the computation. A typical example is drawn in Fig. 5 for $\beta = 0.005$.

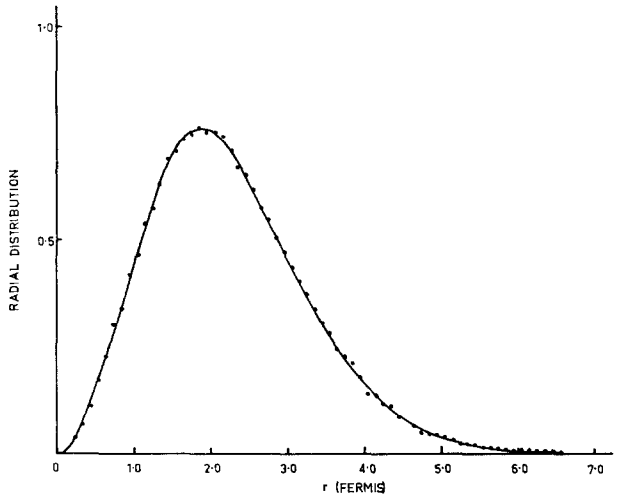


FIG. 5. The (normalized) two-particle distribution function (weighted by the factor $e^{\frac{1}{2}\beta u(q_2,q_3)-(q_2^2+q_3^2)/\alpha^2}$ for the ground state of the triton. The Monte-Carlo calculations were performed with $\beta = 0.005$ and approximately 1900 sample points. The rapid approach to zero for large distances is a consequence of the Gaussian weighting factor, which was introduced in an attempt to reduce the variance in the energy value estimates.

## DISCUSSION

We have discussed a possible method for the numerical solution of the many-body Schrödinger equation and described the computational procedures required for a solution by Monte-Carlo methods. For well-behaved potentials this procedure is very simple and we can find quite reasonable first estimates to the energy and

wavefunction of the ground state without a great deal of computation. These results require no knowledge of the form of the wavefunction; however, increased accuracy has been obtained by an importance sampling technique using prior knowledge of the wavefunction obtained by variational methods. Such experiments are likely to be of considerable value, for example, where one does not require a very great accuracy in the results or, on the other hand, needs a good first approximation to commence (say) a variational calculation.

## APPENDIX. The Harmonic Oscillator Approximation

The basic approximation Eq. (2.2) is valid for many different divisions of $H$ into $H_0$ and $V$, and there will be certain divisions for which the errors made are smaller than those where $H_0$ is defined as in Section 2. One useful division results from defining $H_0 = -\partial^2/\partial \mathbf{x}^2 + \omega^2 \mathbf{x}^2$, so that $V(\mathbf{x})$ is replaced by $U(\mathbf{x}) = V(\mathbf{x}) - \omega^2 \mathbf{x}^2$ and $\omega$ is a parameter which can be chosen so that the variation in $U(\mathbf{x})$ is small. Now from Ref. [1],

$$\langle \mathbf{x} \mid e^{-\beta H_0} \mid \mathbf{x}' \rangle = \left[\frac{\omega}{2\pi \sinh(2\omega\beta)}\right]^{3/2} \times \exp\left\{-\frac{\omega}{2}\coth(2\omega\beta)(\mathbf{x}^2 + \mathbf{x}'^2) + \omega \operatorname{cosech}(2\omega\beta)\, \mathbf{x} \cdot \mathbf{x}'\right\},$$

and the kernel Eq. (2.4) can be easily shown to reduce to one of the form in Eq. (6.5). Moreover if the variation in $U(\mathbf{x})$ is small we would expect the harmonic oscillator wavefunction (for that particular value of $\omega$) to be a good approximation to the wavefunction of the corresponding Schrödinger equation; Eq. (6.14) follows immediately. A more complete discussion of these ideas, together with some results illustrating their value, will be presented in the near future.

## References

1. R. Grimm and R. G. Storer, *J. Comp. Phys.* **4** (1969), 230.
2. N. Metropolis and S. M. Ulam, *J. Amer. Statist. Assoc.* **44** (1949), 247.
3. M. D. Donsker and M. Kac, *J. Res. Nat. Bur. Standards* **44** (1950), 551.
4. R. Fortet, *J. Res. Nat. Bur. Standards* **48** (1952), 68.
5. R. P. Feynman and A. R. Hibbs, "Quantum Mechanics and Path Integrals," McGraw-Hill, New York, 1965.
6. S. G. Brush, *Rev. Mod. Phys.* **33** (1961), 79.
7. S. V. Lawande, C. A. Jensen, and H. L. Sahlin, *J. Comp. Phys.* **3** (1969), 416; **4** (1969), 451.
8. M. H. Kalos, *Phys. Rev.* **128** (1962), 1791.
9. M. H. Kalos, *J. Comp. Phys.* **2** (1967), 257.

10. M. D. KOSTIN AND K. STEIGLITZ, *Phys. Rev.* **159** (1967), 27.
11. W. FELLER, "An Introduction to Probability Theory and its Application," Vol. II, Wiley, New York, 1966.
12. F. CALOGERO, *J. Math. Phys.* **10** (1969), 2191.
13. F. CALOGERO, *J. Math. Phys.* **10** (1969), 2197.
14. L. D. LANDAU AND E. M. LIFTSHITZ, "Quantum Mechanics," Chapter 5, Pergamon, London, 1958.
15. R. A. BAKER, J. L. GAMMEL, B. J. HILL, AND J. G. WILLS, *Phys. Rev.* **125** (1962), 1754.
16. Y. C. TANG, R. C. HERNDON, AND E. W. SCHMID, *Phys. Rev. B* **134** (1964), 743; *Nucl. Phys.* **65** (1965), 203.
17. R. C. HERNDON AND Y. C. TANG, *Methods Comp. Phys.* **6** (1966), 153; *Nucl. Phys. A* **93** (1967), 692.
18. S. ROSATI AND M. BARBI, *Phys. Rev.* **147** (1966), 730.
19. D. H. HOMAN AND L. P. KOK, *Nucl. Phys. A* **117** (1968), 231.
20. M. BANVILLE AND P. D. KUNZ, *Can. J. Phys.* **44** (1966), 2095.