Variational Monte Carlo for Microscopic Cluster Models

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We examine the application of the Variational Monte Carlo (VMC) method to a cluster model for halo nuclei. Particular attention is paid to the error estimate in the presence of correlations in the underlying random walk. We analyse the required steps for a reliable application of the VMC in the case of a complicated many-body problem such as the direct solution of the nuclear hamiltonian with realistic interactions. We also examine the possibility of variance reduction through the ‘zero variance principle’, paying particular attention to the complexity of the many-body problem.

Keywords: Variational; Monte Carlo; correlations; realistic interactions; variance reduction

1. Introduction and Objectives

One of the great difficulties in nuclear physics, is the numerical solution of the many-body Schrödinger equation with a complicated state-dependent two-body potential. Although the theoretical background is fairly simple, a numerical evaluation of the matrix elements is required, due to the complexity of the many-body integrals. The variational Monte Carlo (VMC)\(^1,2\) is a well known method that can be used to numerically evaluate expectation values, particularly when the number of variables is large, such as in the many-body problem.

Our interest lies in the nuclear many-body problem and in particular in the area of light halo nuclei. Of particular importance is the presence of correlations which result from the nucleon-nucleon interaction. For this reason we require a direct solution of the Schrödinger equation. The final wavefunction is constructed by correlating a starting wavefunction that describes a simple non-interacting system, i.e., a product wavefunction or Slater determinant. The full wavefunction is then given by the action of a correlation operator on this
starting function. The exact form of such a wavefunction is provided by the Coupled Cluster method (CCM) \(^3,4\). In our approximation the correlation operator is composed of the product of linear and non-linear parts. The linear part (where the coefficients are determined from the eigenvalue problem) describes the long-range behaviour of the system and can be obtained by retaining only the linear terms in the CCM expansion of the wavefunction. The non-linear part is a Jastrow-type correlation operator \(^6,7\) that includes the short-range correlations appropriate to the short-range behaviour of the nuclear force. This central operator is parametrised in terms of a number of parameters that appear non-linearly in the variational principle.

One important issue in light nuclei is translational invariance, which can drastically effect the expectation value if not properly taken into account. For this reason the correlation operators depend on the inter-particle distances only and are thus invariant under translations. Since the physical picture of simple halo nuclei can be assumed to be that of an alpha-particle (or a number of alpha-particles) accompanied by a number of weakly-bound nucleons, we can use as a starting function the uncorrelated product of the alpha-particle(s) wavefunction(s) with the valence nucleon(s) ones. The alpha-particle wavefunction \(^5\) is obtained by correlating a starting function which is the product of harmonic oscillator wavefunctions. This can be separated into relative and centre-of-mass parts and can thus preserve translational invariance. The additional nucleons in the starting function are then assigned coordinates relative to the alpha-particle(s) centre(s)-of-mass and the formulation thus preserves translational invariance. A number of additional non-linear variational parameters enter the starting function that are related to the average separation between the individual constituents. Apart from the right quantum numbers the antisymmetry condition implementing the Pauli exclusion principle must be imposed. We make use of a scalar correlation operator that is invariant under any exchange of particle labels and thus all symmetry requirements reside in the starting function.

Therefore, a variational solution of the many-body problem can result in a large parameter space, where the expectation value of the Hamiltonian involves a large number of complicated integrals. The VMC is an efficient method that can be used for the ‘statistical’ evaluation of such expectation values. More sophisticated methods that have been successfully applied in the nuclear many-body problem are the Diffusion Monte Carlo (DMC) \(^8\) and Green’s function Monte Carlo (GMC) methods \(^9,10,11,12\). These are rather complicated methods that can provide statistically exact estimates for the expectation value of a Hamiltonian provided a starting wavefunction (usually obtained with VMC) is provided. However, the complexity of the many-body problem restricts for the time being the application of such methods up to medium-mass nuclei and for simple configurations and is not always easy to apply to halo nuclei. Although these methods are accurate they can only provide the numerical value of the expectation value and the particular structure provided by the wavefunction is not obvious. On the other hand the VMC provides an approximation to the expectation value (according to the choice for the trial wavefunction) and can serve as a starting point for further investigation. This way the structure required for the best description of the physical system in question can be easily identified.

The complexity of the many-body problem requires special attention rather than a naive
application of the VMC method. This is mainly due to the presence of correlations in
the random walk underlying the method. Apart for complicating the error estimate, such
correlations can impose limitations on the applicability of the VMC method. In this paper
we provide a detailed examination of the VMC method as applied to a realistic nuclear
many-body problem. We investigate the presence of correlations and the technical issues
involved in the evaluation of a reliable error estimate. We shall make use of a number
of statistical concepts, most of which can easily be found in the literature such as 1. In
addition we describe a possible variance reduction technique that potentially can be used
to improve the performance of VMC.

2. The Variational Problem

The basic equation in the VMC is the time-independent Schrödinger equation,
\[ H(x)\Psi(x) = E\Psi(x), \]
where in general we approximate \( \Psi(x) \) as
\[ \Psi(x) = \sum_n C_n f_n(x). \]
The wavefunction is expanded in terms of a set of normalizable trial functions linear in the
coefficients \( \{C_n\} \) and \( H \) is the hamiltonian. In general, \( x \) denotes the set of coordinates
appropriate for the many-body hamiltonian. However, for simplicity spin-isospin degrees
of freedom are ignored here. Multiplying equation (1) on the left by the complex conjugate
wavefunction and integrating over the appropriate variable, the equation takes the form
\[ \sum_n C_n^* \left( \int f_n^* H f_n d\Omega \right) C_n = E \sum_n C_n^* \left( \int f_n^* f_n d\Omega \right) C_n \]
where \( d\Omega \) is the volume element. The above equation can now be written as
\[ E = \frac{\sum_n C_n^* \mathcal{H}_{kn} C_n}{\sum_n C_n^* \mathcal{N}_{kn} C_n}, \]
where \( \mathcal{H}_{kn} \) and \( \mathcal{N}_{kn} \) represent the Hamiltonian and overlap matrix elements with
\[ \mathcal{H}_{kn} = \int f_n^* H f_n d\Omega, \]  \[ \mathcal{N}_{kn} = \int f_n^* f_n d\Omega. \]
The variational principle states that if \( E_0 \) represents the exact lowest eigenvalue of the
particular Hamiltonian then any estimate, \( E \), for \( E_0 \) obtained from (4) will be an upper
bound of \( E_0 \). Using this fact a particular form for \( \Psi(x) \) may be optimised by varying the
adjustable parameters to minimise the expectation value of (4). The best approximation to
the true lowest eigenvalue is obtained by the variation of the coefficients \( C_n \). This leads to a set of coupled equations of the form

\[
\sum_n \mathcal{H}_{kn} C_n - E \sum_n N_{kn} C_n = 0,
\]

that constitute a generalised eigenvalue problem. Once the matrix elements are known, solution of the eigenvalue problem is straightforward.

### 2.1. Error estimate

The matrix elements entering the eigenvalue problem will be evaluated numerically (as discussed in the next section), leading to an error in the estimated eigenvalue. In case where an error estimate for individual matrix elements exists, the total error for the eigenvalue problem of (7) can be obtained from the linear perturbation of the eigenvalue problem

\[
\sum_n (\mathcal{H}_{kn} + \delta \mathcal{H}_{kn}) (C_n + \delta C_n) = (E + \delta E) \sum_n (N_{kn} + \delta N_{kn}) (C_n + \delta C_n),
\]

where \( \delta E \) is the unknown error. Multiplying on the right by the same eigenvector and keeping only first order terms leads to

\[
\delta E = \frac{1}{C_k N_{kn} C_n} (C_k \delta \mathcal{H}_{kn} C_n - EC_k \delta N_{kn} C_n),
\]

with summation convention implied. If the Hamiltonian and overlap matrix elements were independent of each other the right hand side of the above equation could have been taken in quadrature giving a value for the maximum possible error, \( \Delta E \), that is the required error for the numerical calculation:

\[
\Delta E = \frac{1}{C_k N_{kn} C_n} \sqrt{(C_k \Delta \mathcal{H}_{kn} C_n)^2 + (EC_k \Delta N_{kn} C_n)^2}.
\]

However, the above equation can lead to an incorrect error estimate since in reality the errors in the Hamiltonian and overlap matrix elements are likely to be correlated (depending on the method used for their evaluation). A way of dealing with this problem is through the covariance matrix, which can be used to define a set of uncorrelated (independent) observables whose errors can be added in quadrature. The elements of the covariance matrix are \( \text{cov}(B_z B_{z'}) \), defined as

\[
\text{cov}(B_z B_{z'}) = \langle B_z B_{z'} \rangle - \langle B_z \rangle \langle B_{z'} \rangle,
\]

with \( B_z \in \{ \{ \mathcal{H}_z \}, \{ N_z \} \} \), while the angular brackets denote an expectation value. This gives a real symmetric matrix of the form

\[
C = \begin{pmatrix}
\sigma^2(H_{11}) & \cdots & \text{cov}(H_{11}H_{nn}) & \text{cov}(H_{11}N_{11}) & \cdots & \text{cov}(H_{11}N_{nn}) \\
\vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\
\text{cov}(H_{nn}H_{11}) & \cdots & \sigma^2(H_{nn}) & \text{cov}(H_{nn}N_{11}) & \cdots & \text{cov}(O_{nn}N_{nn}) \\
\text{cov}(N_{11}H_{11}) & \cdots & \text{cov}(N_{11}H_{nn}) & \sigma^2(N_{11}) & \cdots & \text{cov}(N_{11}N_{nn}) \\
\vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\
\text{cov}(N_{nn}H_{11}) & \cdots & \text{cov}(N_{nn}H_{nn}) & \text{cov}(N_{nn}N_{11}) & \cdots & \sigma^2(N_{nn}) \\
\end{pmatrix}
\]
with dimensions $(2n^2) \times (2n^2)$, where $n \times n$ is the dimension of the Hamiltonian and overlap matrices. The diagonal elements correspond to the variance of the Hamiltonian and overlap matrix elements $\sigma^2$ that is discussed later. Diagonalising the covariance matrix is equivalent to obtaining a new set of uncorrelated observables that each is a linear combination of the old ones. This new set of uncorrelated observables, $\{Q_z\}$, can then be defined from the eigenvectors of $C$ as

$$B_z = \sum_k R_{zk}Q_k,$$

$$\sum_k C_{zk}R_{kz} = \lambda_z R_{zz},$$

$$C = R\Lambda R^T.$$ (15)

Here $R_{kz}$ is the $z$th eigenvector of $C$, while $\Lambda \equiv \text{diag}(\lambda_1, ..., \lambda_{2n^2})$. The new (independent) observables satisfy the condition

$$\text{cov}(Q_kQ_z) = \delta_{kz}\lambda_z,$$ (16)

i.e. their covariance vanishes and their variance is equal to the eigenvalues of $C$. The error associated with the new observables is their standard deviation, which according to the above equation can be found as

$$\left(\Delta Q_k\right)^2 = \frac{\lambda_k}{N-1},$$ (17)

with $N$ denoting the number of samples taken for the observable. This way equation (10) can be written as

$$\Delta E = \frac{1}{C_kN_{kn}C_n} \sqrt{\sum_k \left( \sum_{ij} C_{i}(R_{H,i,k} - ER_{N,i,k})C_{j} \right)^2 \left(\Delta Q_k\right)^2},$$ (18)

where the errors corresponding to the independent set of observables, $\{Q_k\}$, can be added in quadrature.

3. Variational Monte Carlo and Error Estimate

The generalised eigenvalue problem of equation (7) requires the computation of the Hamiltonian and overlap matrix elements which in general are complicated integrals and one may wish to choose Monte Carlo sampling to perform the integration. The matrix elements of equations (5) and (6) can be written as

$$\mathcal{H}_{kn} = \int dx \ w(x) \left( \frac{f_k(x)H(x)f_n(x)}{w(x)} \right),$$ (19)

$$\mathcal{N}_{kn} = \int dx \ w(x) \left( \frac{f_k(x)f_n(x)}{w(x)} \right).$$ (20)
where \( w(x) \) plays the role of the probability density function provided that is definite positive and shares the same symmetries as the full wave function. The eigenvalue problem leads to

\[
\sum_n C_n \int dx \, w(x) H_{kn}(x) = E \sum_n C_n \int dx \, w(x) N_{kn}(x),
\]

\[
\sum_n (H_{kn}) C_n = E \sum_n (N_{kn}) C_n, \tag{21}
\]

which can be viewed as the expectation value of two distinct arbitrary functions of a random variable \((H_{kn} \text{ and } N_{kn})\) taken from the same probability distribution.

Because of the parametrization of the wavefunction in terms of the unknown coefficients \( C_n \) a single probability distribution function appropriate for each individual matrix element cannot be extracted. Although in principle is possible to sample each matrix element based on its own distribution leading to \( n^2 \) distinct Monte Carlo algorithms (or \( \frac{n(n+1)}{2} \) for a symmetric matrix), time requirements make such a calculation impractical. A way around this difficulty is to sample all of the matrix elements based on a single probability distribution. Although this approach reduces the number of required simulations, it can lead to a large variance for individual matrix elements and special care is required.

### 3.1. Statistical sampling

In Monte Carlo methods, \( \langle H_{kn} \rangle \) or \( \langle N_{kn} \rangle \) are estimated using a large but finite set of values for \( x \) (a finite set of configurations \( \{x_i\} \) for the multi-dimensional case) distributed according to \( w \). In order to avoid referring to individual matrix elements we consider the expectation value of a general operator \( O \) which is denoted by \( \langle O \rangle \).

One well-known method of obtaining the required distribution is the Metropolis algorithm and this is the one we shall use. In order to generate values of the variable \( x \) having the required distribution the Metropolis algorithm makes use of a random walk: An initial point (set of coordinates), \( x_0 \), is chosen and subsequent points are generated in steps by moving in a random direction, but each time within a prescribed radius from each individual coordinate. Not all points, however, are kept but an ‘accept or reject’ method is used. This means that every point \( x_l \) in the random walk belonging to the \( l_{th} \) step, is weighted against the previous point, \( x_{l-1} \), and is either chosen or rejected. The decision process is given by the Metropolis algorithm which generates a Markov chain. In order to fulfil the criteria for a Markov chain it is essential for each step that the decision process governing the evolution of the random walk should not have any dependence on configurations belonging to previous steps. This means that the decision of keeping or rejecting point \( x_l \) should only depend on the value of the point \( x_{l-1} \) and not on any previous points. An equivalent statement would be to say that the set of values, \( \{O(x_i)\} \), chosen to form the average should be uncorrelated with each other.

The random walk provides us with a statistical average that is different from the exact expectation value, but can be used as an approximation. The expectation value \( \langle O \rangle \) corresponds to the average of the quantity \( O \) over an infinite ensemble of statistically independent trials. This average can in principle be obtained exactly if integrals similar to
(19) and (20) can be evaluated analytically. The random walk that is actually performed in simulations provides an average over a finite sequence of measurements. This sample average or mean will be denoted by \( \bar{O} \). In the case of \( N \) samples taken from a distribution, the expectation value is approximated as
\[
\langle O \rangle \approx \bar{O},
\]
\[
= \frac{1}{N} \sum_{i=1}^{N} O(x_i),
\]
(22)
where the \( x_i \) represents the set of appropriate coordinates that are distributed according to a probability density \( w(x) \).

3.2. Error estimate and correlations

Provided we have a statistical average composed of \( N \) uncorrelated samples taken from an arbitrary probability distribution, the central limit theorem states that in the limit of large \( N \), the above average follows a normal distribution with mean \( \langle O \rangle \) and variance
\[
\sigma^2 = \frac{1}{N} \sigma^2_0,
\]
(23)
with
\[
\sigma^2_0 = \langle O^2 \rangle - \langle O \rangle^2.
\]
(24)

However, in a Monte Carlo sampling we are limited to a finite sample average \( \bar{O} \) and we would like to know how to estimate the error of such an average which is the deviation from \( \langle O \rangle \) (the limiting case provided by the central limit theorem). The theoretical value of this error can be obtained by considering an ensemble of independent random walks, where we can introduce the notion of the expected value of a sample average, \( \langle \bar{O} \rangle \), as well as that of the expected value of any single measurement \( O_i = O(x_i) \) corresponding to a particular step \( i \) of the random walks, denoted by \( \langle O_i \rangle \). The demand that the individual measurements belong to a Markov chain and must in principle satisfy
\[
\langle O_i \rangle = \langle O_j \rangle = \langle \bar{O} \rangle = \langle O \rangle,
\]
(25)
meaning that all samples or measurements in the random walk are independent of their position relative to the others. The fact that there is a correlation between individual measurements corresponds to the case where
\[
\langle O_i O_j \rangle \neq \langle O_i \rangle \langle O_j \rangle
\]
(26)
When the above is taken into consideration the variance of the mean becomes
\[
\sigma^2(\bar{O}) = \langle (\bar{O} - \langle O \rangle)^2 \rangle
\]
\[
= \langle (\bar{O} - \langle \bar{O} \rangle)^2 \rangle
\]
\[
= \langle \bar{O}^2 \rangle - \langle O \rangle^2,
\]
\[
= \frac{1}{N^2} \sum_{ij} \langle O_i O_j \rangle - \langle O_i \rangle \langle O_j \rangle.
\]
(27)
This describes the deviation of the calculated mean from the theoretical expectation value.

However, in practise it is impossible to have an algorithm which can generate samples that are completely uncorrelated. This is indeed the case of the Metropolis algorithm which is used to generate the Markov chain. By the nature of the algorithm used the individual measurements are not statistically independent. Such correlations between statistical measurements have in general two effects. First, they reduce the number of independent measurements from the total number of performed measurements, hence the calculation converges more slowly. Second, the estimation for the statistical error will have to incorporate the effect of such correlations otherwise any error estimate will be an underestimate. As for any numerical method a correct error estimate is of crucial importance for the validity of the results. The rest of this section is devoted to the analysis of the error estimates for correlated data. Most of the results are taken from 13 and 14.

In case that (26) does not hold the equation for the variance of $\bar{O}$ reduces to that of equation (23). However, when (26) holds the true variance for the mean can be written as

$$\sigma^2(\bar{O}) = \frac{1}{N} \left[ \sigma_0 + 2 \sum_{t=1}^{N-1} \left( 1 - \frac{t}{N} \right) \rho_t \right], \quad (28)$$

where

$$\rho_t \equiv \langle O_i O_j \rangle - \langle O_i \rangle \langle O_j \rangle \quad t = |i - j|,$$

$$\rho_t = \langle O_i O_{i+t} \rangle - \langle O_i \rangle \langle O_{i+t} \rangle. \quad (29)$$

Furthermore, the presence of correlations also influences the value of the covariance between the means of two different quantities, $O$ and $O'$, since

$$\text{cov}(\bar{O}\bar{O}') = \langle O O' \rangle - \langle O \rangle \langle O' \rangle$$

$$= \frac{1}{N^2} \sum_{ij} \left( \langle O_i O'_j \rangle - \langle O_i \rangle \langle O'_j \rangle \right)$$

$$= \frac{1}{N} \left[ \gamma_0 + 2 \sum_{t=1}^{N-1} \left( 1 - \frac{t}{N} \right) \gamma_t \right], \quad (30)$$

where similarly to equation (29) we define

$$\gamma_t \equiv \langle O_i O'_j \rangle - \langle O_i \rangle \langle O'_j \rangle \quad t = |i - j|.$$  

(31)

An essential assumption for both $\rho_t$ and $\gamma_t$ is the invariance under 'time translations’, meaning that only the separation between the measurements is of importance and not their place in the random walk (something also included in (25)), i.e.

$$\langle O_i O_j \rangle = \langle O_j O_i \rangle,$$

$$\langle O'_i O'_j \rangle = \langle O'_j O'_i \rangle. \quad (32)$$

As we have seen earlier a reliable error estimate requires two quantities. Firstly, an estimate of the error for each individual matrix element, something provided by the variance
of the mean for the particular matrix element. Secondly, an estimate for the covariance between different matrix elements, so that a set of uncorrelated observables can be obtained. In theory both of these objects are provided by $\rho_t$ and $\gamma_t$. However, in a practical simulation only approximate measurements can be made.

### 3.3. Estimation of variance and covariance

An estimate for $\rho_t$ and $\gamma_t$ can be obtained through the auto- and cross-correlation coefficients. The auto-correlation coefficient, $C_t$ is defined in the case of $N$ samples as

$$ C_t(O) = \frac{1}{N-1} \sum_{i=1}^{N-t} (O_i - \bar{O})(O_{i+t} - \bar{O}), \quad (33) $$

while the cross-correlation coefficient as

$$ C_t(O, O') = \frac{1}{N-1} \sum_{i=1}^{N-t} (O_i - \bar{O})(O'_{i+t} - \bar{O}'). \quad (34) $$

The variable $t$ will be refereed to as the correlation time. These two coefficients provide biased estimators for $\rho_t$ and $\gamma_t$, in the sense that they underestimate the actual values. This is expressed as

$$ \langle C_t(O) \rangle = \rho_t - \sigma^2(O) + \Delta_t, \quad (35) $$
$$ \langle C_t(O, O') \rangle = \gamma_t - \sigma^2(O) + \Delta'_t, \quad (36) $$

where the terms $\Delta_t$ and $\Delta'_t$ are given as

$$ \Delta_t = 2 \left( \sigma^2(\bar{O}) - \frac{1}{N(N-t)} \sum_{i=1}^{N-t} \sum_{j=1}^{N} \gamma_{ij} \right), \quad (37) $$
$$ \Delta'_t = 2 \left( \text{cov}(\bar{O}, \bar{O}') - \frac{1}{N(N-t)} \sum_{i=1}^{N-t} \sum_{j=1}^{N} \gamma'_{ij} \right), \quad (38) $$

with

$$ \gamma_{ij} = \langle O_i O_j \rangle - \langle O_i \rangle \langle O_j \rangle, $$
$$ \gamma'_{ij} = \langle O_i O'_j \rangle - \langle O_i \rangle \langle O'_j \rangle. $$

However, in most applications the largest correlation time in $\rho_t$ and $\gamma_t$ is finite, meaning that equations (28) and (30) can be approximated by

$$ \sigma^2(\bar{O}) \approx \frac{1}{N} \left[ \sigma_0^2 + 2 \sum_{t=1}^{T} \left( 1 - \frac{t}{N} \right) \rho_t \right], \quad (39) $$
$$ \text{cov}(\bar{O}, \bar{O}') \approx \frac{1}{N} \left[ \text{cov}(O, O') + 2 \sum_{t=1}^{T} 2 \left( 1 - \frac{t}{N} \right) \gamma_t \right]. \quad (40) $$
The meaning of the above approximation for a random walk is that the correlation between different samples is of finite range in the sense that \( \langle O_i O_j \rangle - \langle O_i \rangle \langle O_j \rangle \) and \( \langle O_i O'_j \rangle - \langle O_i \rangle \langle O'_j \rangle \) become zero for large enough correlation time \( t = |i - j| \). The parameter \( T \) in the above equations represents a cutoff parameter and is the maximum correlation time that will be taken into account. The significance of a finite correlation time is that the biases \( \Delta t \) and \( \Delta'_t \) in equations (35) and (36) will become arbitrarily small for sufficiently large number of samples \( n \).

Provided that \( \frac{T}{N} \) is sufficiently small, the variance and covariance can be approximated by

\[
\sigma^2(0) \approx \frac{\sigma^2_0 + 2 \sum_{t=1}^{T} C_t}{N} = \left( 1 + 2 \sum \frac{C_t}{\sigma^2_0} \right) \frac{\sigma^2_0}{N} 
\]

(41)

\[
\text{cov}(O, O') \approx \frac{C_0 + 2 \sum_{t=1}^{T} C_t}{N} = \left( 1 + 2 \sum \frac{C_t}{C_0} \right) \frac{C_0^2}{N} 
\]

(42)

The above equations provide as with a way of measuring the strength of correlations in a particular simulation through the ‘normalised’ correlation coefficients, \( C_t / \sigma^2_0 \) and \( C_t / C_0 \). These can be obtained for a particular simulation as a function of the correlation time \( t \).

3.4. Application and results

In order to examine the accuracy of the variance estimate provided by equation (41) a simple one dimensional problem was considered. A hamiltonian of the form

\[
H(x) = -\frac{1}{2} \frac{\partial^2}{\partial x^2} - \frac{1}{\cosh^2 x} 
\]

(43)

was used, where the exact value of the lowest eigenvalue is known and is equal to \(-\frac{1}{2}\). We can approximate this value through a variational problem in terms of the eigenvalue equation (7). A Gaussian non-orthogonal expansion of the form

\[
f_n = e^{-\mu_n x^2} 
\]

(44)

was used to approximate the wave function with the \( \{ \mu_n \} \) belonging to a geometric series. Since a numerically exact result can obtained for this approximation, we can also use Monte Carlo sampling in order to verify the error estimate. The probability density function was taken to be the square of the first Gaussian. Since we can obtain the numerically exact values for \( H_{kn} \) and \( N_{kn} \), we can use this to construct an unbiased estimator for the variance and thus to obtain an uncorrelated estimate for the variance of each matrix element. For
The variance for the Hamiltonian matrix elements is given as

$$\frac{\sigma^2(H_{kn})}{N} = \langle (H_{kn} - E_{kn})^2 \rangle \approx \sum_{i=1}^{n} (\bar{H}_{kn}^i - E_{kn})^2,$$

(45)

where $E_{kn}$ corresponds to the exact value while the summation is over a number of distinct random walks with $\bar{H}_{kn}^i$ denoting the distinct average obtained in the $i$th walk consisting of $N$ samples. The approximation symbol becomes an equality in the limit of large $n$. For our simple one-dimensional model the convergence is relatively fast and the results obtained can be referred to as statistically exact. Simultaneously we can obtain the value of the variance through the biased estimator of (41) for any one of the performed averages.

Fig. 1. The (biased) variance estimate for different matrix elements of the Hamiltonian matrix as a function of the correlation time $t$, for a simple one-dimensional model. The fact that the biased estimate approaches a constant value with respect to $t$ indicates that there is a cutoff in the correlation coefficients (as shown previously). The dotted lines represent the value for the variance obtained through an unbiased measurement. The statistically exact value of the variance and that of the biased estimator depending on the correlation time are shown in figure 1, which is a demonstration for the accuracy of the variance estimate. Provided that the correlation time is large enough, the value for the variance obtained from equation (41) agrees with that of the statistically exact value of (45). Although the statistically exact value cannot be obtained directly for practical calculations (it requires the analytical results), the biased estimator (41) becomes statistically exact for large $t$, provided there is a cutoff in the correlation.

When the maximum correlation time is relatively small an unbiased error estimate can be obtained without having to consider the correlation coefficient. This is done by rejecting
a number of the samples taken and only considering those which are adequately separated in simulation time and thus uncorrelated. Since the samples are consecutively obtained from each other their separation in simulation time is exactly equivalent to the correlation time. If we call the maximum correlation time $T$, then each sample is correlated with samples separated from it by at most $T$ steps. Therefore, if from the total number of samples obtained only the ones separated by at least $T$ steps (or random walk moves) are considered, this new set of samples will be uncorrelated. In the literature these intermediate moves are usually referred to as ‘thermalisations’\(^1\), where is expected that a relatively small number is adequate. However, for more complicated models, the maximum correlation time might be too large for either completely removing the correlations or estimating the effect of the correlation coefficient without any intermediate moves.

In order to get an idea about the correlation coefficient for the many-body problem we can consider the linearised approximation of the many-body wavefunction in terms of correlations operators acting on a starting function\(^{15,16}\). This provides a translationally invariant description of the many-body problem and was applied to a number of closed-shell systems in terms of an alpha-cluster model\(^{17}\). We firstly consider the ground-state of the alpha-particle. The many body Hamiltonian is of the form

$$H = \sum_{i=1}^{4} \frac{\hbar^2}{2m_i} \nabla_i^2 + \sum_{1 \leq i < j}^{4} V(ij), \quad (46)$$

where $V(ij)$ is a realistic nucleon-nucleon interaction that is composed of a sum of Gaussian functions:

$$V(ij) = \sum_k c_k \exp(b_k r_{ij}^2), \quad (47)$$

with $r_{ij}$ being the distance between the the $i$th and $j$th particles. The wavefunction $\Psi$ is given as

$$\Psi = \hat{F}\Phi_0, \quad (48)$$

where $\Phi_0$ represents the wavefunction for the uncorrelated four-particle system that we take to be the product of harmonic oscillator wavefunctions. $\hat{F}$ is a correlation operator that is approximated by a linear expansion of the form

$$\hat{F} = \sum_{i=1}^{N} \hat{F}_i \Phi_0 = \left( \sum_{i=1}^{N} a_i \sum_{i<j} f(ij) \right) \prod_{i<j} g(ij), \quad (49)$$

$$f(ij) = \exp(d_k r_{ij}^2), \quad g(ij) = k_1 \exp(-\lambda_1 r_{ij}^2) + k_2 \exp(-\lambda_2 r_{ij}^2). \quad (50)$$

This type of wavefunction (referred to as the J-TICI(2) scheme) has been extensively used for the alpha-particle\(^{18,19,20,21}\) where it was shown to provide an adequate description for the ground-state properties. The probability density function $w$ was taken to be the square of one of the components in the expansion of the wavefunction i.e

$$w = (\hat{F}_0 \Phi_0)^2. \quad (51)$$
Fig. 2. The variance (lower part) and the normalised auto- and cross-correlation coefficients (upper part) as a function of correlation time. These results are for the matrix elements of the hamiltonian and overlap matrices of the alpha-particle calculation. The variance graphs start from a value belonging to the unbiased estimator and increase as the estimator becomes biased by including the effects of the correlation coefficient.
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This is a natural choice for the pdf since the wavefunction can always be written as the product of $w$ and a function $\Psi'$.

The variance of equation (41) and the normalised auto and cross-correlation coefficients of (33) and (34) were sampled as functions of correlation-time. This was done for the matrix elements of both the hamiltonian and overlap matrices. The result is shown in figure 2. We can see in the lower part of the figure that the variance strongly depends on the correlation coefficient, starting from a minimum (unbiased estimator) and finally converging. According to the previous analysis this indicates that despite the fact that the variance depends on the correlation time, there is a cutoff in the correlation coefficient, which implies that the dependence on the correlation coefficient will be over a restricted range of the correlation time (approximately about the cutoff). This is backed up by sampling the correlation coefficient (upper graphs of figure 2), where we can see that the value of the normalised correlation coefficient decays rapidly as the correlation time increases. According to the figure we can safely assume 50 samples as the value of the cutoff, something that can be compensated by taking 50 intermediate moves in the random walk.

The alpha-particle wavefunction is spherically symmetric and depends on 12 variables ($4 \times 3$ cartesian coordinates). It is an easy numerical calculation both in terms of computation time and complexity. We can go one step further by introducing one or two additional nucleons, corresponding to the cases of $^5$He and $^6$He. We shall do so by considering scalar interactions that do not mix the spatial and spin-isospin terms. The inclusion of additional nucleons leads to two complexities. On one hand the wavefunction must be antisymmetrized, something that does not imply a straight forward choice for the pdf $w$ and on the other hand the nuclear potential is composed of several parts including spin, isospin and spin-isospin exchange terms. The wavefunction has the form

$$
\Psi = \hat{F}A\{\Phi_0\chi_{\sigma\tau}\},
\Psi = \sum_i c_i A\{\Phi_i\chi_{\sigma\tau}\},
$$

(52)

where the correlation operator has been approximated as before, while $\chi_{\sigma\tau}$ is the tensor product of the individual spin and isospin terms. $A$ represents an antisymmetrization operator. The linear correlation operator is invariant under permutation of particle labels and can be taken outside the antisymmetrizer. Special attention is required for the antisymmetrization operator, otherwise the number of terms entering the wavefunction will be too many for any practical calculation. For simplicity we do not discuss the quantum numbers corresponding to angular momentum, total spin and total isospin, having in mind that the wavefunction must be an eigenstate of good quantum numbers. The function $\Phi_0$ is not the uncorrelated harmonic oscillator but is modified to include the motion of the additional nucleon(s) relative to the alpha-particle. In general the function $\Phi_0$ depends on a number of non-linear variational parameters that are related to the average separation between the individual clusters.
The norm of the wavefunction can be written as
\[ \Psi = |A\Phi|, \]
\[ = k|\sum_i c_i A_{\text{eff}} \Phi_i|, \]
\[ = k \sum_{ij} c_i c_j (A_{\text{eff}} \Phi_i)(A_{\text{eff}} \Phi_j), \]  
(53)

where \( k \) is a constant and \( A_{\text{eff}} \) is an ‘effective antisymmetrizer’ that is only composed of a much smaller number of permutations than \( A \). This provides a relatively simple pdf \( w \), for example
\[ w = |A_{\text{eff}} \Phi_0|. \]  
(54)

This is not the natural choice as in the case of the alpha-particle (or any totally symmetric wavefunction) but is rather artificial. We made use of this type of pdf for going beyond the alpha-particle. Figure 3 illustrates the variance estimation for the \(^6\text{He}\) calculation. In the case of the hamiltonian matrix the correlation coefficient decays rather rapidly and we get a similar result to the alpha-particle i.e. the estimation of the variance converges within a relatively small correlation time, something that can be compensated by taking a number of intermediate moves. However, in the case of the overlap matrix we see that the correlation coefficient has a very slow decay so that the variance estimate does not converge with a reasonable correlation time that can be compensated with intermediate moves alone. Furthermore, if we go beyond the \(^6\text{He}\) into heavier systems such as \(^8\text{Be}\) we observe the same behaviour for the Hamiltonian matrix elements.

Therefore, in order to obtain a converging estimate for the variance it might be more convenient to make use of both intermediate moves and the unbiased estimator of (41). For example by introducing a small number of intermediate moves we can force a cutoff to the correlation coefficient and thus obtain a converging variance through equation (41). This is illustrated in figure 4 for the correlation coefficient of the \(^6\text{He}\) overlap matrix: without any intermediate moves the correlation coefficient decays rather slowly, while after taking a number of intermediate moves a reasonably small cutoff is obtained.

It must be noted that the more samples are discarded or the largest the correlation time is, the more time consuming the simulation becomes. Therefore, in general the most efficient approach that can guarantee a correct variance estimate is to make use both of intermediate moves and the correlation coefficient.

4. Variance Reduction

Although correlations can be taken into account or even removed from the sampling of a particular observable, this can only provide an algorithm with a reliable error estimate. In order to get an adequate error a large number of samples are required, the number depending on the particular observable. The so called ‘zero-variance principle’ is a way of increasing the efficiency of a Monte Carlo algorithm by reducing the variance. In general the principle is to replace each observable to be computed by an improved estimator which has the same mean but a different variance. The method is described in \(^{22}\) where
Fig. 3. The variance (lower part) and the normalised auto- and cross-correlation coefficients (upper part) as a function of correlation time. These results are for the matrix elements of the Hamiltonian and overlap matrices of the $^6$He calculation. The variance graphs start from a value belonging to the unbiased estimator and increase as the estimator becomes biased by including the effects of the correlation coefficient.

Fig. 4. The correlation coefficient before and after taking intermediate moves (indicated by the arrow). The presence of intermediate moves introduce a reasonably small cutoff.
applications of the zero-variance principle were shown to be very powerful. This variance reduction technique is examined in order to establish its usefulness for the case of many-body cluster models.

4.1. Method
We consider the expectation value of an observable $O_{kn}$ given as

$$\langle O_{kn} \rangle = \int w(x) O_{kn}(x) dx,$$

where as usual $w(x)$ represents a normalised probability density function (pdf). In our case $\langle O_{kn} \rangle$ corresponds to a particular matrix element of either the Hamiltonian or overlap matrices, where for practical purposes all expectation values are over the same single pdf. This implies that we can optimise $w(x)$ for at most one of the matrix elements.

We introduce the ‘renormalized’ observable $\tilde{O}_{kn}$ where

$$\tilde{O}_{kn} = O_{kn} + \frac{\hat{h}\psi_{kn}}{\sqrt{w}},$$

with $\hat{h}$ and $\psi_{kn}$ representing a trial operator and a trial function appropriate for the expectation of each individual matrix element. In order for the expectation value of $\tilde{O}_{kn}$ to be the same as that of the original observable the operator $\hat{h}$ must satisfy the condition

$$\hat{h}\sqrt{w} = 0$$

This leads to the equation

$$\hat{h}\psi_{kn} = (\langle O_{kn} \rangle - O_{kn})\sqrt{w},$$

which has the consequence that the error of the calculation, $\sigma(\tilde{O}_{kn})$, vanishes. Although in principle equation (58) should be satisfied, in practise an approximate solution can be searched that minimises the variance of the calculation. The variance for the expectation value of the new operator of equation (56) now becomes

$$\sigma^2(\tilde{O}_{kn}) = \sigma^2(O_{kn}) + \sigma^2(\tilde{O}_{kn}) + 2(\langle O_{kn}\tilde{O}_{kn} \rangle - \langle O_{kn} \rangle \langle \tilde{O}_{kn} \rangle).$$

A possible way to approximate the function $\psi_{kn}$ would be to consider a finite expansion linear in some coefficients like in the case of the wavefunction $\Psi$ (equation (2)). This means that $\psi_{kn}$ can be given as

$$\psi_{kn} = \sum_i A_i^{kn} g_i,$$

where the functions $\{g_i\}$ are taken to be common for all matrix elements, while the coefficients $\{A_i^{kn}\}$ are determined by minimising the variance of a particular matrix element, in this case the observables $\langle \tilde{O}_{kn} \rangle$. The condition that the variance is minimised can be
imposed by demanding that upon variation of the coefficients $A_{kn}^i$ the value of the variance reaches a minimum:

$$\delta \sigma^2(\tilde{O}_{kn}) = 0$$

$$\Rightarrow \frac{\partial \tilde{O}_{kn}}{\partial A_{kn}^i} = 0, \quad \forall A_{kn}^i.$$  \hspace{1cm} (61)

This leads for each matrix element to an equation of the form

$$\sum_j A_{kn}^j \Delta_{ij} + K_{kn}^i = 0,$$  \hspace{1cm} (63)

where

$$\Delta_{ij} = \left\langle \frac{\hat{h}g_i\hat{h}g_j}{\sqrt{w}} \right\rangle - \left\langle \frac{\hat{h}g_i}{\sqrt{w}} \right\rangle \left\langle \frac{\hat{h}g_j}{\sqrt{w}} \right\rangle,$$  \hspace{1cm} (64)

$$K_{kn}^i = \left\langle O_{kn} \frac{\hat{h}g_i}{\sqrt{w}} \right\rangle - \left\langle O_{kn} \right\rangle \left\langle \frac{\hat{h}g_i}{\sqrt{w}} \right\rangle.$$  \hspace{1cm} (65)

Therefore, for a particular set of functions $\{g_i\}$, the coefficients $\{A_{kn}^i\}$ can then be obtained as

$$A_{kn}^i = -\sum_j (\Delta)_{ji}^{-1} K_{kn}^i.$$  \hspace{1cm} (66)

One difficulty that might arise is when one or more of the eigenvalues of $\Delta$ is near zero (especially when it is zero within the numerical accuracy of the inversion procedure), in which case solving equations (63) by inverting $\Delta$ will lead to numerical instabilities. Diagonalising $\Delta$ is equivalent to obtaining linear superpositions of the functions $\{g_i\}$ that are uncorrelated with respect to the operator $\frac{\hat{h}}{\sqrt{w}}$. However, this might not be possible for the entire set $\{g_i\}$. This problem can be bypassed by solving (63) with singular value decomposition, which is equivalent to considering a reduced set of functions $\{g_i\}$.

By substituting the coefficients back to equation (59) the variance of each particular matrix element becomes

$$\sigma^2(\tilde{O}_{kn}) = \sigma^2(O_{kn}) + \sum_{ij} K_{kn}^i A_{kn}^i,$$

$$= \sigma^2(O_{kn}) - \sum_{ij} A_{kn}^i \Delta_{ij} A_{kn}^j,$$  \hspace{1cm} (67)

which is always bound to be less than $\sigma^2(O_{kn})$, whatever the choice for the $g_i$’s due to the fact that the eigenvalues of $\Delta$ are always positive.

An efficient method of obtaining an appropriate set of functions $g_i$ is to run a number of short Monte Carlo algorithms until a set that reduces the variance of the calculation efficiently is found. The set of coefficients $\{A_i\}$ can be obtained from a short sampling and used as input for a larger computation.
Note: The error for the zero variance calculation can also be obtained from a set of uncorrelated errors giving an equation similar to (18). The only difference is in the covariance matrix to be calculated. The new matrix elements are

\[
C_{ij} = \text{cov}(\tilde{B}_i, \tilde{B}_j),
\]

\[
= \text{cov}([B_i + \bar{B}_i][B_j + \bar{B}_j]),
\]

\[
= \text{cov}(B_iB_j) + \sum_n A_n^i K_n^j + \sum_n A_n^j K_n^i + \sum_{nm} A_n^i A_m^j \Delta_{nm},
\]

(68)

where \(i\) is a collective index representing a particular matrix element of either the Hamiltonian or overlap matrix (\(\{O_{nm}, N_{nm}\} \equiv \{B_i\}\)), while \(\Delta\) and \(K\) are defined in equations (64) and (65).

4.2. Application and results

Although the variance reduction technique can in principle reduce the variance of an observable, for practical calculations we are confined to the linear approximation of equation (60). For a complicated many-body problem the choice of the functions \(\{g_i\}\) entering (60) is not at all obvious. For our calculations we shall use the same set as the one used for the linear eigenvalue problem. This is the simplest available choice. We can examine the applicability of this approach through the same one-dimensional problem as before before going to the many-body case. In this case the integrals of equation (67) can be solved in a numerically exact manner without having to make use of Monte Carlo sampling. The numerically exact results for the variance of the one-body problem are shown in figure (5). In this case the variance reduction greatly reduces the variance of the matrix elements and can lead to a zero variance (within the numerical accuracy of the machine used).

We can then proceed and apply the same method to the case of the alpha-particle in the J-TICI(2) approximation, this time using Monte Carlo sampling. Figure 6 is the variance of a few of the Hamiltonian matrix elements as functions of the number of linear components used in equation (60). Although there is a substantial reduction in the variance, the effect is not as strong as in the one-dimensional case (not a zero-variance principle any more).

Although there is a substantial reduction in the variance of the alpha-particle calculation (about 90%), this is not a reduction that can be of practical help. Having in mind that the error is given by the standard deviation (that is the square root of the variance) we have that its value changes with the number of samples as \(\frac{1}{\sqrt{N}}\). A 90% reduction is (approximately) equivalent to an error dependence of the form \(\frac{1}{3\sqrt{N}}\). This is not much of an error reduction, particularly when compare with the simple one-dimensional case. For the ‘zero variance’ principle to be valuable we require a radical variance reduction. Therefore, the variance reduction for the alpha particle is not sufficient for aiding the numerical calculation. A similar situation was also observed in the case of the more complicated systems of \(^5\)He and \(^6\)He. Although a variance reduction was possible it was not of a substantial contribution to the simulation. Furthermore, the amount of reduction was considerably lower than that for the alpha-particle. This is not unexpected since the wavefunction is more complicated and
Fig. 5. The variance of some matrix elements of the hamiltonian matrix for the one-dimensional problem as a result of applying the zero variance principle. The variance was plotted against the number of components used to approximate the trial function.

Fig. 6. The variance of some matrix elements of the hamiltonian matrix for the alpha-particle in the J-TICI(2) approximation as a result of applying the ‘zero-variance’ principle. The variance is plotted against the number of components used to approximate the trial function.
the issue of antisymmetrization is also present.

It seems that the complicated structure of the many-body wavefunction requires a different kind of approximation of (58) than the simple linear one, for any effective reduction of the variance.

5. Summary and Conclusions

The variational Monte Carlo method is an important ingredient for cluster-like models since it allows us to investigate different structures in the cluster model without having to worry about the analytical solution of many-body integrals. This requires the numerical method to be both accurate and precise in the error estimate. Furthermore, it is a starting point for more sophisticated methods such as GMC.

In our cluster model the VMC is applied to the generalised eigenvalue problem, where the total error requires to decorrelate the individual matrix elements of the Hamiltonian and overlap matrices. This requires knowledge of the covariance matrix, where the diagonal elements coincide with the variances. This is a straightforward task that does not impose any difficulty for the many-body calculations.

We have illustrated that the knowledge of the correlation coefficient is crucial for a correct estimate of the variance (or covariance), particularly for complicated systems i.e. the simulation variance is different from the analytical one due to the presence of correlations. This requires to make use of a biased variance estimator, where the bias becomes arbitrarily small as the number of samples increases. For such an estimator to be practical we require that the correlation coefficient has a reasonable cutoff, i.e. that a particular sample in the random walk is only correlated up to a finite number of previous samples. In the case where the cutoff is relatively large it can be reduced by discarding a number of samples between the values taken. The most efficient approach that can guarantee a correct variance estimate is to make use both of intermediate moves and the correlation coefficient.

We also examined a variance reduction technique that can be used to improve the efficiency of a calculation, the so-called ‘zero variance principle’. This was taken from 22. The principle is in general complicated to apply and we only considered a linear approximation. This sufficiently decreased the variance of the alpha particle calculation. For more complicated systems a different kind of approach is required. In principle we could have looked for a more complicated approximation than the one at hand, but this is beyond our purpose. It seems that variance minimisation for the many-body problem is not a straightforward matter, particularly when antisymmetrization is involved.

In general we have analysed the application of the VMC method for the nuclear many-body problem, and in particular for the case of the generalised eigenvalue problem. We discussed and analysed the required steps for a reliable error estimate.

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