MINIMUM VARIANCE FOR MANY-BODY WAVE FUNCTIONS

by

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B.S., New Mexico State University, 1986

A MASTER'S THESIS

submitted in partial fulfillment of the
requirements for the degree

MASTER OF SCIENCE
Department of Physics

KANSAS STATE UNIVERSITY

Manhattan, Kansas

1988

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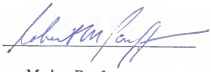


Major Professor

Table of Contents

List of Figures ii

List of Tables iii

Acknowledgements iv

1.0 Introduction 1

2.0 Principles Involved 2

3.0 Methods for Testing the 'Extended Principle' 5

3.1 The VMC Scheme 5

3.2 The VMC Scheme vs. the 'Extended Principle' 8

3.3 The Liquid ^{3}He System 11

3.4 The Computational Codes 16

4.0 Some Computational Considerations 17

5.0 Results and Comparisions 20

6.0 Conclusions and Suggestions 39

References 45

List of Figures

Figure 1: Sample Triplet Correlation Functions 15

Figure 2: Generating Jastrow Correlations 19

Figure 3: Indicated Triplet Correlations 33

Figure 4: A 'Bad' Triplet Correlation 35

Figure 5: E_{vmc} vs. Average Relative Error 36

List of Tables

Table 1: VMC energies for the test triplets 21

Table 2: Standard error for different Jastrow functions 22

Table 3a: Standard errors for one set of configurations 25

Table 3b: Relative errors for same configurations 25

Table 4: Ranked standard errors for another set of configurations 27

Table 5: Ranked relative errors for same configurations 28

Table 6: Ranked average relative errors for the twelve triplets 31

Table 7: Ranked average relative errors, fewer configurations 40

Acknowledgements

I would like to express my sincere graditude to Dr. Robert M. Panoff for his patience, guidance, and suggestions throughout the course of this work. I also wish to thank my committee members Dr. Larry Weaver and Dr. Christopher Sorensen for their input and assistance during this work. This work was supported in part by the Applied Mathematical Sciences subprogram of the Office of Energy Research, U. S. Department of Energy, under contract number DE-AC02 76ER03077.

On a more personal note, a very special thanks goes out to my wife and best friend, Julia, for her seemingly infinite patience and understanding during this work, and my entire academic career.

Finally, I would like to thank my parents, Robert and Nancy Lee, for giving me the opportunity to study Physics, and earn a graduate degree.

1.0 Introduction

Monte Carlo techniques have become widely used for the simulation of quantum many-body systems. Ever since McMillan [1.1] observed that trial wave functions chosen as products of correlation factors could be integrated via Monte Carlo methods, the use of these methods in conjunction with the variational principle has become widespread. Since then, various thermodynamic properties, as well as ground-state wave functions for systems, have been successfully numerically calculated using these techniques. The improvement of these techniques, both in terms of efficiency and results, is a natural desired development.

The accurate calculation of various thermodynamic properties is closely related to the accurate calculation of the ground-state energy for a given system. Furthermore, the accurate calculation of the ground-state energy is naturally dependent on the form for the wave function that is chosen as the *best* to represent the system and the estimated ground-state energy . For optimum results, one obviously needs to begin with the best, or *optimal*, *trial* wave function. In particular, one can use the variational method to improve the ground-state wave functions of various systems, and use the Monte Carlo method of Metropolis, *et. al.* [1.2], to carry out the integrations. That is, one can use the variational principle to improve estimates for the ground-state wave function for some system, by minimizing the *variational energy* with respect to the ground-state wave function. The Monte Carlo method mentioned above is used in this process to calculate the variational energy. Variational energies calculated in this manner are compared by examining

their value and their statistical error. The minimum variational energy would be that energy that has the lowest value, and the smallest error. If numerical techniques are to be employed, one *must* know the error in the calculation to compare numerical values of the energy. For a particular choice of the trial wave function, if the variational energy is minimized (usually with respect to parameters in the trial wave function), other thermodynamic properties of the system at hand are then believed to be reasonably close, as obtained by the trial wave function. If it were possible to examine a large family of wave functions quickly and efficiently, and decide which of the family best represents the system at hand using this method, it would be an invaluable addition to the theoretical description of any applicable system.

It is the intention of this paper to discuss the extent to which this is possible.

2.0 Principles Involved

At the center of any such discussion is the variational principle. The variational principle states that for any trial wave function, $\Psi_T(\mathbf{R})$, the variational energy, E_v, is given by

$$E_v = \frac{\int d\mathbf{R}\Psi_t^*(\mathbf{R})H(\mathbf{R})\Psi_t(\mathbf{R})}{\int d\mathbf{R}|\Psi_T(\mathbf{R})|^2} \tag{2.1}$$

and will be a minimum when the trial wave function is the ground-state eigenfunction of the Schroedinger equation. Thus, the variational energy constitutes a rigorous upper bound to the ground-state energy, *viz*,

$$E_v \geq E_{g.s.}$$

The variational method usually consists of parameterizing some chosen form of a wave function, as in $\Psi_T(\mathbf{R}, a, b, c, \cdots)$, then calculating the variational energy in (2.1) for a chosen family of parameters. The idea is, of course, to determine that set of parameters that minimizes † the variational energy, E_v. Then, the wave function represented by this parameter set will be a good† approximation to the ground-state wave function.

The fact that the variational energy is a rigorous upper bound to the ground-state energy means that a variational calculation involving the true ground-state eigenfunction will yield the ground-state energy with zero error in the calculation. As this is a central point, it is shown below.

Consider the expectation value of the Hamiltonian, $\langle H \rangle$

$$\langle H \rangle = \frac{\langle \Psi | H | \Psi \rangle}{\langle \Psi | \Psi \rangle} \tag{2.2}$$

This is exactly equal to the ground-state energy if $|\Psi\rangle$ is the ground-state eigenfunction of the Hamiltonian. The variance about the mean is of course

$$\sigma^2 = \langle H^2 \rangle - \langle H \rangle^2 \tag{2.3}$$

where

$$\langle H^2 \rangle = \frac{\langle \Psi | H^2 | \Psi \rangle}{\langle \Psi | \Psi \rangle} = \frac{\langle \Psi | H \cdot H | \Psi \rangle}{\langle \Psi | \Psi \rangle} \tag{2.4}$$

† Clearly, a global minimum in the energy is required.

So, if $|\Psi\rangle$ is an eigenstate, then (2.3) becomes

$$\begin{aligned}\sigma^2 &= \frac{\langle\Psi|H\cdot H|\Psi\rangle}{\langle\Psi|\Psi\rangle} - \left(\frac{\langle\Psi|H|\Psi\rangle}{\langle\Psi|\Psi\rangle}\right)^2 \\ &= E\frac{\langle\Psi|H|\Psi\rangle}{\langle\Psi|\Psi\rangle} - E^2\left(\frac{\langle\Psi|\Psi\rangle}{\langle\Psi|\Psi\rangle}\right)^2 \\ &= E^2 - E^2 = 0.\end{aligned} \tag{2.5}$$

Thus, we see that if we calculate the expectation value of the Hamiltonian with the *exact* eigenfunction, the result will be the exact ground-state energy with zero variance and hence zero error, as shown by (2.5).

We now wish to take this a step further, and examine to what extent a *lower* variance in a calculation such as this with some assumed form for the wave function implies a better estimate of the 'true' ground-state energy of the system, regardless of the details of the calculation (assuming it is done correctly). As suggested by Umrigar, *et. al.* [2.1], one might be able to , in theory, optimize families of wave functions by minimizing the *variance* in a calculation of the variational energy with respect to the wave function parameters, rather than minimizing the variational energy itself. It is the purpose of this thesis to investigate this. Three basic points will be addressed; (1) To what extent is this 'extended principle' valid? ; (2) How well can it be applied to the improvement of ground-state wave functions? ; (3) What are some of the pitfalls of using it in this manner?.

Thus, the remainder of the thesis is organized as follows. In section 3.0 to 3.2, the VMC and other computational codes are discussed, and usefulness of the extended principle is made clear. In section 3.3, the system that was used to test the validity and usefulness of the extended principle is introduced. In section 4,

some computational considerations are discussed. Section 5 contains the results and discussion from the test system. Section 6 contains conclusions and suggestions for applications of this method to different problems, and improvements that may be explored in the future.

3.0 Methods for Testing the 'Extended Principle'

As stated earlier, the variational method is basically a procedure in which the variational energy is minimized with respect to wave function parameters. Computationally, this means that *each* trial wave function must be put into a variational code which calculates *each* variational energy. In a variational Monte Carlo (VMC) scheme†, this means that each wave function must be put into a VMC code and equilibrated. Depending on the number of particles in the system, satisfactory convergence may be very expensive (computationally speaking), even on a large parallel machine.

In order to understand the possible usefulness of the so-called extended principle, it is necessary to understand the details of a VMC calculation. This will help illustrate the usefulness of the extended principle as a time saving method for finding good candidates for improved variational wave functions.

3.1 The Variational Monte Carlo Scheme

The evalutation of the variational energy is done via the algorithm of Metropolis, et. al. (the $M(RT)^2$ algorithm) [1.2]. This is employed to carry out the

† Here, only Monte Carlo schemes are discussed

multi-dimensional integrations in (2.1). By using the M(RT)^2 algorithm, we avoid having to make any additional approximations, other than the fact that the integrations will be done numerically. To use the M(RT)^2 algorithm, the expression for the variational energy (2.1) is written as

$$E_v = \int \frac{d\mathbf{R}\Psi_T^*\Psi_T}{\int d\mathbf{R}|\Psi_T(\mathbf{R})|^2} \left(\frac{H\Psi_T}{\Psi_T}\right). \tag{3.1}$$

The variational energy is then computed as the average of the local energy,

$$\left(\frac{H\Psi_T(\mathbf{R})}{\Psi_T(\mathbf{R})}\right)$$

evaluated at the particle positions (configurations) drawn from a probability distribution proportional to

$$\frac{|\Psi_T(\mathbf{R})|^2}{\int d\mathbf{R}|\Psi_T(\mathbf{R})|^2} \tag{3.2}$$

The M(RT)^2 algorithm generates points (i.e., the particle positions) with the desired probability distribution (3.2). In general, if $w(\mathbf{X})$ is the probability density (like (3.2)), M(RT)^2 generates a sequence of points $\mathbf{X}_0, \mathbf{X}_1, \ldots$ as those visited by a random walker through $\mathbf{X}$-space. The longer the walk, the closer the points it connects approximate the desired distribution. The basic M(RT)^2 algorithm is illustrated below.

Say we are at a point $\mathbf{X}_n$ in the sequence. We wish to generate $\mathbf{X}_{n+1}$ randomly from the given distribution. This is done as follows:

1. Choose a trial point $\mathbf{X}_t$ — this is a uniformly chosen random number somewhere in a small cube about $\mathbf{X}_n$

2. Calculate

$$r = \frac{w(\mathbf{X}_t)}{w(\mathbf{X}_n)}$$

3. If $r > 1$, accept the move $\Rightarrow$ let $\mathbf{X}_{n+1} = \mathbf{X}_t$. Return to step 1.

If $r < 1$, still accept the move, but with a probability $r \Rightarrow$ compare r with a uniformly distributed random number $(0, 1)$ and reject the move if this number is greater than r.

4. If the trial step was rejected, put $\mathbf{X}_{n+1} = \mathbf{X}_n$ and generate $\mathbf{X}_{n+2}$ from $\mathbf{X}_n$ (by returning to step 1).

The walk can be started from any arbitrary point in position space.

Thus, one uses the $M(RT)^2$ algorithm in the variational method to calculate E_v, given a particular $\Psi_T(\mathbf{R})$. It should be clear from the above discussion that the points in the sequence that the $M(RT)^2$ algorithm generates are highly correlated. It therefore stands to reason that the energies thus calculated will also be statistically dependent. Hence, estimates for the statistical error can no longer be done assuming independent samples (energies, in this case). Since the $M(RT)^2$ algorithm generates a sequence of points with the desired distribution, this problem is easily overcome. The random walk is allowed to progress for a long time, long enough to generate a large number of points with the desired distribution. Then, instead of using each point in this set, only points in the sequence that are separated by fairly large number of *other* points in the sequence are used. These points, that are, say, every 100^{th} or so in the entire sequence, are then used to calculate the integrals and errors. Doing this allows one to reassert the assump-

tion of statistical independence, as points separated by many other points are not nearly as highly correlated as points right next to each other in the sequence, depending on the probability distribution chosen. It is also a good idea to allow the random walker to move for a while before accepting any moves. This removes any "memory" of a starting point in the sequence.

Therefore, we see that although the $M(RT)^2$ algorithm is a convenient way of sampling (3.2), it can be computationally expensive, due to the length of the required random walk. As we shall see, the extended principle avoids much of this.

3.2 The VMC Scheme versus the 'Extended Principle'

If one were to 'optimize' a family of wave functions using the variational principle via the $M(RT)^2$ algorithm discussed above, it seems clear that it may well take a great deal of computer time, due to the length of the walk and the fact that the walk must be repeated for *each* wave function in the chosen family. However, if one had a set of previously generated particle positions (configurations), and one could successfully use this distribution of points to calculate a "minimizeable quantity" for different wave functions, one could very quickly examine a family of wave functions, since the $M(RT)^2$ algorithm need not be repeated. Clearly, if one had the correct eigenfunction, then it would not matter what particle positions were used. The average of the local energy would be the ground-state energy, and the error would be zero, as discussed in section 2.0. This is the basic idea behind using the extended principle, the minimizeable quantity being the *variance* in the

variational, or average of the local, energy [2.1].

The idea is to do one walk through position space to generate the configurations that will be used to average the local energy. A suitable† wave function is chosen for the Metropolis walk, but instead of evaluating the variational energy with the generated configurations, one simply writes out the particle positions at each accepted stage in the walk as a "snapshot" of the system. These are the configurations that are then used to calculate (3.1). It is understood that since the generating wave function (i.e., the wave function that was used in the Metropolis walk to generate the configuration) will not match the trial wave functions, the "variational energy" that is calculated will not be correct, as the probability distribution, (3.2), will not match the trial wave function. However, one calculates the *standard error* in this "variational" energy ($\tilde{E}_v$) defined by

$$e_s = \left[\frac{\dfrac{\sum_{i=1}^{N} (\tilde{E}_{v_i})^2}{N} - \left(\dfrac{\sum_{i=1}^{N} \tilde{E}_{v_i}}{N} \right)^2}{N} \right]^{\frac{1}{2}} \tag{3.3}$$

$$= \sqrt{\frac{\langle \tilde{E}_v^2 \rangle - \langle \tilde{E}_v \rangle^2}{N}}$$

where the summations naturally run over all of the stored particle positions, N, that is, the i indexes are the snapshots of the system. Thus, as our extended

† Suitability arguments will follow in forthcoming sections

principle states, this error will be the minimized quantity. Note that (3.3) is the *standard error*, and is related to (2.3) by a factor of one over the square root of the number of configurations. Therefore, the standard error will not just be a function of the wave function, but of the configuration sets as well. This equation, (3.3), can be very quickly calculated for sets of wave functions, much quicker than any useful VMC run for each wave function. The utility of the extended principle should now be clear; since we are not really concerned with the energy in the extended principle, only the variance, we need not be concerned with a correctly weighted evaluation of (3.1), and can thus skip the expensive walk through configuration space for each wave function. This proposed algorithm using the extended principle is summarized below:

1. Given a set of previously generated configurations, calculate (3.1) and (3.3) for all wave functions desired.

2. Examine the errors in an appropriate way to determine the 'best' wave function(s) from the family tested. As shall be seen later, this means comparing the standard errors via the relative error.

3. Calculate the true VMC energy using the set(s) of wave functions from step **2** and see if the resulting errors and energies are lower than previous estimates, thereby signaling a good candidate for a better trial wave function.

Clearly then, the method proposed may depend on the nature of the configurations generated. Naturally, for (3.3) to be valid, estimates of E_v must be independent, and hence so must the configurations used, as mentioned earlier.

However, there may be more subtle considerations for the generation of the configurations, such as the extent of position space visited during the walk by the M(RT)^2 algorithm, and how close particles are allowed to come to one another. These possibilities, and others, must be carefully evaluated.

3.3 The Liquid ^{3}He System

To explore the various aspects of the proposed algorithm, the liquid ^{3}He system was chosen. This system was chosen primarily for two reasons. First, the computation of macroscopic bulk properties of ^{3}He is seen as a proving ground for many-fermion theories and methods. In fact, this system continues to receive much scrutiny by condensed matter theorists [3.1]. Second, and naturally related to the above, the description of the liquid ^{3}He system constitutes a complex problem. Most of the interesting many-body systems consist of a finite number of fermions, and are difficult to model. Hence, the liquid ^{3}He system is complex enough to support a faster method of finding a better trial ground-state wave function.

Since ^{3}He particles are fermions, the chosen wave function must be antisymmetric. For fermi liquids such as ^{3}He , a wave function of the form [3.2]

$$\Psi_T = D(\mathbf{R}) \times e^{\left(-\frac{1}{2}\sum_{i<j} u(r_{ij})\right)} \tag{3.4}$$

$$= \prod_{i<j} e^{-\frac{1}{2}u(r_{ij})} \times D(\mathbf{R})$$

can be used. Here, $D(\mathbf{R})$ is a Slater determinant of plane wave orbitals, and

$u(r_{ij})$ is the pseudopotential. While (3.4) takes care of the symmetry requirements (due to the Slater determinant), it unfortunately complicates the random walk in the Metropolis algorithm as it introduces the requirement of computing the ratio of two determinants, in addition to the pseudopotential, at each step of the walk to evaluate the transition probability [3.3] (see section 3.1). Again, this is a complication that warrants a faster approach to finding better forms for a wave function.

The pseudopotential, $u(r_{ij})$, in (3.4) that was chosen for this system is of that used by McMillan [3.4]

$$u(r) = \left(\frac{b}{r}\right)^5 .$$

This form is really due to the WKB solution of the Schroedinger equation using the Lennard-Jones potential

$$v(r) = 4\epsilon \left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6} \right].$$

A pseudopotential was also chosen (more "optimally") by a Fermi-hypernetted-chain theory (FHNC/C) [3.5] calculation of $u(r_{ij})$. The details of this calculation are found in reference [3.5].

These two approaches to the pseudopotentials were undertaken to expand the 'optimization' process into choosing the best two-body plus more-body correlated wave function. By choosing different parameters in the pseudopotential, comparisons can be made at the two-body level *alone*, in addition to the higher order correlations. These correlations are discussed in more detail below.

It is assumed that the ^{3}He liquid can be represented by a few particles in a periodic box. That is, this simple model assumes that a VMC calculation on a few particles restricted to a cube of a specific size interacting via appropriate n-body potentials with periodic boundary conditions applied at the sides of the cube will accurately represent the ^{3}He liquid system. This model has proved to be successful in representing this system [3.1], [3.2].

In addition to the two particle correlations, it has been found that three-, and perhaps more-, particle correlations are important in a ground state energy calculation of ^{3}He [3.3]. In the present study, only three-body correlations ("triplet" correlations) were applied. This simplifies matters and speeds up the codes, as opposed to including higher-order correlations. Explicit three-body correlations may be incorporated into the total wave function as follows [3.4]:

$$\Psi_T = D(\mathbf{R}) \times exp\left[-\frac{1}{2}\sum_{i<j}\tilde{u}(\mathbf{r}_{ij}) - \frac{\lambda_t}{4}\sum_{i<j}\sum_{l}\xi(\mathbf{r}_{li})\xi(\mathbf{r}_{lj})\mathbf{r}_{li}\cdot\mathbf{r}_{lj}\right] \tag{3.5}$$

where

$$\tilde{u}(r) = u(r) - \lambda_t\xi^2(r)\cdot r^2 \tag{3.6}$$

The triplet correlation function ξ that was chosen is of the form used by Schmidt, *et. al.* [3.6],[3.7]

$$\xi(r) = e^{-((r-r_t)/w_t)^2} \tag{3.7}$$

In (3.5) λ_t is the triplet (Gaussian-like) strength, and in (3.7), r_t is the center, and w_t is the width. Some triplet correlations are plotted in Figure 1, superimposed on the Jastrow part, in order to illustrate their dependencies. Note that (3.6)

necessarily removes the possibility of counting two-particle correlations more than once, due to the introduction of the triplet term. Thus, the total wave function (3.5) is a product of the two- and three-body correlations, and a Slater determinant of plane wave orbitals. It should be pointed out that this form for the wave function (3.5) is not very close to the true ground-state wave function, but it will suit the purposes of testing the proposed method.

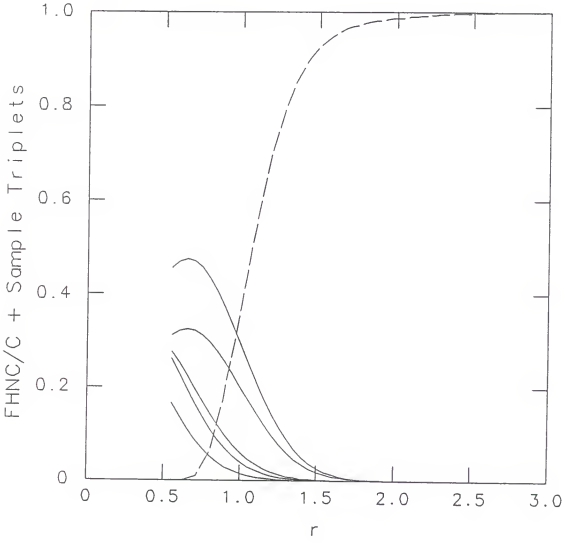
It should be noted that the finite size adaptation induced by the boundary conditions forcing the correlations to vanish at the sides of the box has no real effect on the magnitude of the correlations which minimize the variational energy as these correlations turn out to be relatively short ranged in nature [3.3].

Finally, some remarks about the Hamiltonian for this system are in order. The Hamiltonian chosen for the system was

$$H = \frac{-\hbar^2}{2m} \sum_{i=1}^{N} \nabla_i^2 + \sum_{1 \le i < j \le N} V(r_{ij}) \tag{3.8}$$

The first term is, of course, the kinetic energy of the system, and m is the mass of the neutral ^{3}He atom. The potential, $V(r_{ij})$, that was chosen was the Aziz pair potential [3.8], which is a state-independent atom-atom interaction potential, and which has been shown to be an accurate effective potential [3.3].

Figure 1: The long dashed line is the FHNC/C pseudopotential in the Jastrow part of the wave function. The group of solid lines are the triplet correlation functions for different values of λ_t, r_t, and w_t. Note how different triplet correlations cross the two-body correlation in different regions, and at different angles. These triplets are merely samples to illustrate how they appear and how they interact with the two-body part.



3.4 The Computational Codes

There are two basic codes that were involved in testing the proposed method; a VMC code and an "analysis" code.

The VMC code actually serves two purposes. By implementing the $M(RT)^2$ algorithm, this code is used to not only generate the configurations, but to calculate variational energies as well. Thus, this is the code that *generates* the sets of appropriate configurations that are used to examine large families of wave functions for maxima and minima in the variances. It is also used to "test" an indicated wave function by calculating the "correct" variational energy and the error, to see if this wave function gives rise to an energy and error lower than previous estimates.

The analysis code serves only one purpose. Given any set of particle configurations, and a trial wave function; it evaluates the error in the (incorrect) variational energy. The code has the ability to examine large families of wave functions at one time by reading sets of parameters that appear in the parameterized form of the wave function, discussed above. Thus, each parameter set represents a different wave function, and the error in the "variational energy" is calculated for each parameter set. This code calculates the errors in such a way that the results from other generated configurations can be easily combined, to aid in the investigation of the configuration requirements.

4.0 Some Computational Considerations

As was indicated earlier, the results of using the extended principle in the proposed manner may be subject to subtleties in the generated configurations themselves. Thus, the generation and use of these particle positions must be carefully considered.

We have already seen that the configurations used must be approximately statistically independent (section 3.2). As alluded to in that section, one needs to ensure that, computationally, only independent points in the generated $M(RT)^2$ sequence are used (this means independent particle positions) To serve this end, most of the configurations were generated by using points in the $M(RT)^2$ sequence that were separated by 100 other points. This should be enough to, at least, approximate statistical independence.

We must also carefully consider the wave function that is used to generate these particle positions. In this case, only wave functions with a Jastrow factor were used. The triplet contributions were not included in the wave functions that were used to generate any configurations. The reasoning behind this is that it was assumed from the start that a "less restricted" wave function that samples more of configuration space would produce more useful configurations. The triplet contribution to the wave function would tend to limit the volume of configuration space that the random walk would visit, when used with the Jastrow factor, and is an unnecessary complication at his level. Thus, only Jastrow factors were introduced to the generation of the configurations. The Jastrow values (b) that were used

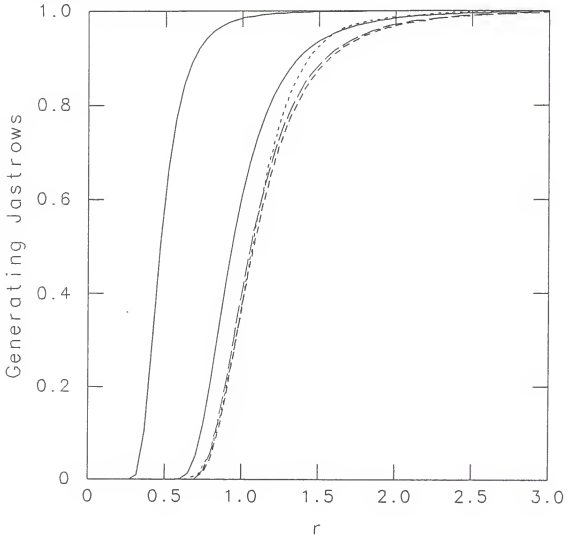
varied, again to examine the effect of this value on the generated configurations and the final results. They ranged from a value of $b = 0.5$, to $b = 1.15$, that is, from a broad wave function to a more narrow one. The FHNC/C pseudopotential was also used in the Jastrow to generate some configurations. In Figure 2, plots of the correlation functions used to generate configurations are shown.

In addition, the effect of starting the Metropolis walk must be considered. If we start from lattice sites, as has been done previously [3.3], we may have to worry about any "bias" this may introduce into the resulting configurations. So, it might be a good idea to allow the $M(RT)^2$ algorithm to walk for a while in position space before accepting any points in the sequence, or writing out any particle positions. This was done here. Typically, the walk was allowed to progress through 20 or so accepted $M(RT)^2$ moves before any variational energies were calculated and before any particle positions were written out.

We must also decide on the number of particle positions that are needed. Here, this problem was somewhat solved by the ability of the analysis code to combine results from different configurations. In the present case, all configurations were generated with 2,000 particle positions in each. The analysis code could then combine any number of these sets into error estimates for the variational energy, as required by our extended principle.

Finally, when we have a set of errors associated with some set of possible wave functions parameters, we must consider the extent to which we can distinguish the errors from one another. This is naturally important when a decision on the

Figure 2: These two-body correlations are those that generated the configurations that were used to analyze the wave functions. The solid line nearest the left vertical axis is the McMillan form with $b = 0.5$. The next line (also solid) to the right of this is for $b = 1.00$. The long dashed line is $b = 1.13$ and the medium dashed line is for $b = 1.15$. The short dashed line is for the FHNC/C pseudopotential.



best wave function from the set must be made. This decision, and its hopeful validity, are the ultimate desired ends to using the extended principle in the proposed manner.

5.0 Results and Comparisons

Since this thesis is concerned with examining the validity and usefulness of the proposed algorithm, a set of parameters for the given form of the wave function must be presented, for which a VMC calculation has determined a numerical estimate of the variational energy, and an error. In Table 1, sets of parameters are shown with their kinetic, potential, and total energies, and the estimated errors for each. In each case, the VMC calculation was done in exactly the same way, to ensure that no 'bias' entered these control results. Note also that the total energy is not simply the sums of columns four and five, since the standard errors of the total energies are too low. If columns four and five were simply added to yield column six, their errors would add as the square root of the sum of the squared individual errors. The total energy was actually calculated as the average of the sum of the kinetic and potential energies per particle. Thus, the errors were calculated accordingly. It is these sets of parameters that will be examined in detail in the remainder of this thesis. These will be used to examine the parameter set(s) that are indicated by the proposed algorithm, to see to what extent a reduced variance implies an improved estimate of the ground-state energy. Since these computations were done equivalently, they naturally required the same amount of

Table 1: Variational Monte Carlo potential, kinetic, and total energies for the test set of parameters. The Jastrow factor uses the FHNC/C pseudopotential. All energies are in Kelvins. The reported errors are the standard errors in the energies.

λ_t	r_t	w_t	P. E.	K. E.	Tot. E.
-1.65	0.70	0.5	-14.643 ±0.042	12.958 ±0.044	-1.685 ±0.014
-1.85	0.65	0.5	-14.768 ±0.035	13.116 ±0.037	-1.652 ±0.012
-1.80	0.65	0.5	-14.728 ±0.032	13.098 ±0.035	-1.631 ±0.011
-1.90	0.65	0.5	-14.673 ±0.036	13.047 ±0.039	-1.626 ±0.012
-0.75	0.75	0.5	-14.540 ±0.039	12.921 ±0.043	-1.619 ±0.015
-1.75	0.65	0.5	-14.757 ±0.029	13.141 ±0.034	-1.616 ±0.012
-1.25	0.65	0.5	-14.708 ±0.036	13.119 ±0.039	-1.589 ±0.012
-0.75	0.65	0.5	-14.544 ±0.036	13.054 ±0.040	-1.490 ±0.017
-1.65	0.55	0.5	-14.674 ±0.039	13.209 ±0.044	-1.465 ±0.013
-1.90	0.55	0.5	-14.733 ±0.035	13.268 ±0.037	-1.465 ±0.011
-1.35	0.80	0.5	-14.484 ±0.036	13.023 ±0.037	-1.461 ±0.017
-1.85	0.35	0.5	-14.573 ±0.035	13.281 ±0.042	-1.292 ±0.019

computing time. This will be exploited later when the main advantage to using this method is pointed out — the savings in computing time. Naturally, validity arguments must proceed this.

At the purely two-body correlations level, the results from the proposed algorithm quite clearly indicate that the FHNC/C version of the pseudopotential (see section 3.3) is the best choice for the two-body interaction over all of the McMillan parameters tested. Table 2 illustrates this by a showing a representative set of wave function parameters along with their standard errors, as calculated via (3.3). By examining this table, it is clear that in each case, the FHNC/C pseudopotential in the Jastrow portion has the lowest standard error independent of the wave function that was used to generate the configurations, and independent

Table 2: Comparison of standard errors (from (3.3)), e_s, for representative parameter sets. These are depicted in groups of three. The first group results were calculated using configurations generated from a wave function with $b = 1.13$ (set A), the second with $b = 1.00$ (set B), the third with the wave function utilizing the FHNC/C pseudopotential (set C). The M below denotes the McMillan form of the pseudopotential was used in the Jastrow portion of the wave function, and the number following the 'M' is the value of b that was used. The FHNC/C denotes the FHNC/C pseudopotential was used in the Jastrow of the trial wave function. The E_{vmc} below is the VMC calculated total energy, for the first group only. The standard error in the VMC energies are also reported. The VMC results are included to illustrate that the FHNC/C pseudopotential gives the *best* variational result from this group.

Set	Jastrow	λ_t	r_t	w_t	e_s	E_{vmc}
	M,1.15	-1.25	0.65	0.5	0.293	-1.486 $\pm$0.017
A	M,1.13	-1.25	0.65	0.5	0.291	-1.448 $\pm$0.018
	M,1.00	-1.25	0.65	0.5	0.764	3.390 $\pm$0.072
	FHNC/C	-1.25	0.65	0.5	0.280	-1.589 $\pm$0.012
	M,1.15	-1.80	0.65	0.5	1.780	
B	M,1.13	-1.80	0.65	0.5	1.183	
	M,1.00	-1.80	0.65	0.5	1.652	
	FHNC/C	-1.80	0.65	0.5	0.619	
	M,1.15	-1.90	0.55	0.5	0.383	
C	M,1.13	-1.90	0.55	0.5	0.338	
	M,1.00	-1.90	0.55	0.5	0.769	
	FHNC/C	-1.90	0.55	0.5	0.276	

of the triplet parameters.

However, nothing has been said about the possible numerical overlap in the standard errors calculated. Thus, perhaps the errors shown are actually numerically indistinguishable. This is resolved by considering the fact that, on the average, *all* of the parameter sets generated illustrated this kind of behavior, *i.e.*, that the FHNC/C pseudopotential gave the lowest standard error. Therefore, according to the 'extended principle' that is being tested, this should have the lowest

variational energy of these parameter sets. Thus, it is assumed that this is the better wave function for this family. This is also shown by examining the VMC variational energies. Note that in Table 2, the energy and error that is shown is lower for the FHNC/C Jastrow than for the others, in the first group. This was also true for all of the parameters that were examined via a VMC calculation.

Having estabilshed that the FHNC/C pseudopotential is best, at the Jastrow level, for this form of the wave function, we may now turn our attention to the three-body interactions level, *i.e.*, the triplet level. As described above, for the Jastrow level, it is assumed that the lower standard error corresponded to the best choice of tested parameters. This was true due to the pattern in the 'average' behavior of the parameter sets. However, at the triplet level, a more sensitive way of distinguishing the standard errors is needed. That is, a 'good' way of examining and comparing the standard errors from different parameter sets is needed (recall that the 'error in the error' is not a calculated quantity).† The fact that a more efficient and sensitive way of comparing the standard errors might needed can best be seen from the following argument.

Suppose that parameter set 1 had the lowest standard error when sampled using configuration set A. However, when configuration set B is used, parameter set 2 is indicated. When configuration set C is used, parameter set 3 is indicated. There are several possible explanations for this: (1) the method is very sensitive to the generation of the configurations; (2) the standard errors for set 1, 2, and

† and if it were, what about the 'error in the error in the error'?

3 overlap, and cannot be distinguished; (3) the standard errors are not being compared properly; (4) none of these parameter sets are very good, meaning, perhaps all three parameter sets are very far from the best one. A quick way to eliminate at least some of this ambiguity is to try and find a different, perhaps better way, of comparing the standard energies to one another. Notice that in calculating the standard error, the 'incorrect energy' is also being calculated. As explained in earlier sections, these numbers correspond to the variational energy from a VMC calculation. Up to this point, these 'energies' have been essentially ignored, and all of the focus has been on the standard error. However, since the standard error is merely the 'spread' in this number, it is conceivable that a small standard error might result from a small 'energy', just because the 'energy' is small.† In other words, the standard error in a big number might be big, while the standard error in a small number may be small†. If this is the case, it may not be wise to simply compare the standard errors alone. It may be better to somehow take the size of the numbers into account, along with their errors. This can be done by calculating the *relative error* for the numbers. With respect to the discussion above, this number is the standard error, divided by the 'energy'. In this manner, the errors are compared *relative* to the number that they are representing. Consider Table 3a. In this table, the parameter sets shown are ranked in terms of increasing standard error. In Table 3b, the same set of parameters are ranked in terms of increasing *relative* error. Note that the order of increasing standard error

† recall that the 'energy' is very far from the correct value

Table 3a: Parameter sets ranked in terms of increasing standard error, e_s as analyzed using configurations drawn from a generating wave function using the FHNC/C pseudopotential. The $\tilde{E}$ represents energies that are are not the correctly weighted variational energies. The e_s values are the standard errors in $\tilde{E}$ calculated from (3.3), as in Table 2. E_{vmc} are the VMC calculated energies. The Jastrow factor that was used in the tested parameter sets was the FHNC/C pseudopotential.

λ_t	r_t	w_t	$\tilde{E}$	e_s	E_{vmc} (K)
-1.90	0.55	0.5	-1.333	0.276	-1.465 ±0.011
-1.65	0.55	0.5	-1.316	0.276	-1.465 ±0.013
-0.75	0.65	0.5	-1.316	0.278	-1.490 ±0.017
-1.25	0.65	0.5	-1.402	0.281	-1.589 ±0.012
-1.85	0.35	0.5	-1.264	0.287	-1.292 ±0.019
-0.75	0.75	0.5	-1.447	0.289	-1.619 ±0.015
-1.75	0.65	0.5	-1.528	0.296	-1.616 ±0.012
-1.80	0.65	0.5	-1.543	0.297	-1.631 ±0.011
-1.85	0.65	0.5	-1.559	0.300	-1.652 ±0.012
-1.90	0.65	0.5	-1.574	0.302	-1.626 ±0.012
-1.65	0.70	0.5	-1.722	0.326	-1.685 ±0.014
-1.35	0.80	0.5	-2.278	0.426	-1.461 ±0.017

Table 3b: Parameter sets ranked in terms of increasing relative error, e_{rel}, analyzed as Table 3a. The e_{rel} are just the standard errors, e_s, divided by $\tilde{E}$. $\tilde{E}$ represent energies that are not the correctly weighted variational energies.

λ_t	r_t	w_t	$\tilde{E}$	e_{rel}	E_{vmc} (K)
-1.35	0.80	0.5	-2.278	0.187	-1.461 ±0.017
-1.65	0.70	0.5	-1.722	0.189	-1.685 ±0.014
-1.90	0.65	0.5	-1.574	0.192	-1.626 ±0.012
-1.85	0.65	0.5	-1.559	0.192	-1.652 ±0.012
-1.80	0.65	0.5	-1.543	0.193	-1.631 ±0.011
-1.75	0.65	0.5	-1.528	0.193	-1.616 ±0.012
-0.75	0.75	0.5	-1.447	0.200	-1.619 ±0.015
-1.25	0.65	0.5	-1.402	0.200	-1.589 ±0.012
-1.90	0.55	0.5	-1.333	0.207	-1.465 ±0.011
-1.65	0.55	0.5	-1.316	0.210	-1.465 ±0.013
-0.75	0.65	0.5	-1.316	0.211	-1.490 ±0.017
-1.85	0.35	0.5	-1.264	0.227	-1.292 ±0.019

in Table 3a also displays the behavior that the larger the number, the larger the reported standard error, on the average. In Table 3b, the relative error inverts this to a degree, but at least takes into account the *magnitude* of the 'energy' that corresponds to a given calculated standard error. We see from both of these tables that a much different picture can be deduced depending on how the errors are compared. This is an important point, as the crux of this method requires the comparison of errors of this nature.

Returning to our ambiguities, if in comparing the relative errors, the ranked order (in terms of increasing relative error) of the parameter sets is essentially the same regardless of the configurations used, then we may have found a good, efficient way of comparing the variances (via the relative error). Furthermore, the method itself may not be as sensitive to the configurations used as may have been previously thought. These possibilities will be explored in more detail below.

Again, at the simple level of comparing the standard errors alone, consider Table 4. In this table, the test parameters are ranked in order of increasing standard error. We see that the set $(\lambda_t = -0.75, r_t = 0.75, w_t = 0.5)$ (which shall be denoted $(-0.75, 0.75, .05)$ henceforth) is on top of the list, therefore, is indicated as the 'best' from the rest of the list. However, in Table 3a, the set $(-1.90, 0.55, 0.5)$ is indicated. Here, the Jastrow that generated the configurations was the 'optimal' numerical pseudopotential discussed above, while in Table 4, the generating Jastrow was $b = 1.00$. We also see that *neither* of these parameter sets possesses the lowest energy or error. This pattern (or rather the lack thereof)

Table 4: Results from the proposed algorithm, on the test parameter set, ranked in order of increasing standard error, e_s. The $\bar{E}$ values are the unweighted energies calculated via the proposed method. The e_s are the standard errors in $\bar{E}$. The E_{vmc} are the VMC calculated variational energies. These results were analyzed using 2,000 particle positions generated with a wave function using b=1.00.

λ_t	r_t	w_t	$\bar{E}$	e_s	E_{vmc} (K)
-0.75	0.75	0.5	-2.449	0.606	-1.619 ±0.015
-1.25	0.65	0.5	-3.058	0.614	-1.589 ±0.012
-1.75	0.65	0.5	-3.286	0.617	-1.616 ±0.012
-1.80	0.65	0.5	-3.317	0.619	-1.631 ±0.011
-1.85	0.65	0.5	-3.349	0.620	-1.652 ±0.012
-1.90	0.65	0.5	-3.383	0.623	-1.626 ±0.012
-1.90	0.55	0.5	-3.389	0.628	-1.465 ±0.011
-1.65	0.70	0.5	-3.126	0.630	-1.685 ±0.014
-1.65	0.55	0.5	-3.323	0.633	-1.465 ±0.013
-0.75	0.65	0.5	-2.977	0.634	-1.490 ±0.017
-1.85	0.35	0.5	-3.231	0.684	-1.292 ±0.019
-1.35	0.80	0.5	-2.445	0.688	-1.461 ±0.017

is indicative of the fact that the standard errors alone cannot be compared this simply with confidence, and that different configurations *do* give different results when the wave function is *not* the eigenstate.

Instead of using the standard errors alone, let us examine ranked lists of relative errors over the same configurations. In Table 3b, we see that $(-1.35, 0.80, 0.5)$ is on top, and we see that the energy for this set is quite poor. However, notice that right below this parameter set, we see $(-1.65, 0.70, 0.5)$, then $(-1.80, 0.65, 0.5)$, whose energies are among the *lowest*. Now examine Table 5. Here, the set nearest the top of the list are again those that have low energies. However, there are still some parameter sets that are not high on the list, but have low energies as well,

Table 5: Results from the proposed algorithm, on the test parameter set, ranked in order of increasing relative error, e_{rel}. The $\tilde{E}$ values are the unweighted energies calculated via the proposed method. The E_{vmc} are the VMC calculated variational energies. These results were analyzed using 2,000 particle positions generated with a wave function using b=1.00.

λ_t	r_t	w_t	$\tilde{E}$	e_{rel}	E_{vmc} (K)
-1.90	0.65	0.5	-3.383	0.184	-1.626 ±0.012
-1.90	0.55	0.5	-3.389	0.185	-1.465 ±0.011
-1.85	0.65	0.5	-3.349	0.185	-1.652 ±0.012
-1.80	0.65	0.5	-3.317	0.187	-1.631 ±0.011
-1.75	0.65	0.5	-3.286	0.188	-1.616 ±0.012
-1.65	0.55	0.5	-3.323	0.190	-1.465 ±0.013
-1.25	0.65	0.5	-3.058	0.201	-1.589 ±0.012
-1.65	0.70	0.5	-3.126	0.202	-1.685 ±0.014
-1.85	0.35	0.5	-3.231	0.212	-1.292 ±0.019
-0.75	0.65	0.5	-2.977	0.213	-1.490 ±0.017
-0.75	0.75	0.5	-2.450	0.247	-1.619 ±0.015
-1.35	0.80	0.5	-2.445	0.281	-1.461 ±0.017

and should be indicated by our method. This leaves three possibilities. First, and potentially most catastrophic, the method fails to predict the best parameter set from the list. Second, the standard errors are still not being compared as carefully as they should be. Or third, the method is somewhat sensitive to the type of configuration used.

We already know that the method works to some degree, since it pointed out that the FHNC/C pseudopotential was best, at the Jastrow level. So, we really have no reason to believe that it would completely breakdown at the triplets level. It does seems more likely that it would become increasingly difficult to exploit differences in errors to draw conclusions, however. Therefore, a good assumption

is that both the second and third possibilities mentioned in the preceeding paragraph apply here.

It seems reasonable to believe that the wave function that allows the random walker to visit a larger volume of configuration space will lead to a more desirable configuration. After all, the $M(RT)^2$ algorithm samples position space with the given probability distribution, and it seems reasonable that the system is best represented by a sample that is distributed over a larger region of position space. If Figure 2 is re-examined, it is clear that the lower the value of the parameter b, the closer the particles are allowed to come, and thus the more configuration space is 'seen'. Thus, this could mean that a lower value of b is best for generating the configurations used in this algorithm. However, if the particles are allowed to get too close, the energy increases dramatically (due to the strong repulsive core of the potential), and a 'washing-out' effect occurs in the errors. This was the case for the configurations generated with b=0.5. In this case, the resulting 'energies' were so large, as were the errors, that a simple comparison, even through a relative error calculation was futile. So, from this discussion one restriction is placed on the generating wave function: It cannot allow the particles to get too close. However, it still seems advantageous to use configurations that represent a large sample of position space. If this belief is correct, then many of the ambiguities that still linger in the results should be removed.

In each of the tables discussed, the unweighted energies and the standard and relative errors were calculated from 2,000 stored particle positions. As mentioned

in an earlier section, there were five wave functions that were used to generate configurations. Since we have ruled out the use of b=0.5 above, there are four remaining parameters available: b=1.00, b=1.13, b=1.15, and the FHNC/C pseudopotential. If we wish to test the hypothesis of the preceeding paragraph, we want to use those sets that have 'seen' as much of configuration space as possible. In terms of a *single* set, this is b=1.00. We have already seen some of these results in the data presented. Now consider using *all* of these parameter sets. In doing so, we will truly be visiting as much of position space as possible using these sets of configurations. What was actually done here was to analyze the test set of parameters using 2,000 particle positions from *each* set, and calculate the relative error. Then, the *average relative* error was calculated, meaning, the average of the relative errors for each of the parameter sets, from each configuration, was calculated. This was done so that the *average* behavior over all of the sets could be examined. The results of this calculation are shown in Table 6.

In this table, we see that all of the parameter sets near the top of the list have energies at or below -1.61 K. So, we see that the method indeed does appear to work, provided that; (1) The relative errors are used; (2) The configurations that are used are varied enough to see as much of phase space as possible, provided the particles do not come too close; and (3) The average behavior of the relative error is examined, over all of the configurations. The method does work, in the sense that low variance wave functions are better candidates for improved trial wave functions, since they seem to lead to lower estimates of the variational energy.

Table 6: Ranked relative errors in the $\bar{E}$, $\bar{\epsilon}_{rel}$. These relative errors are the averages over all four types of configurations used, *i.e.*, each average relative error is the average of the relative errors for each of the parameter sets over each of the four configuration types that were used. The E_{vmc} are the VMC calculated variational energies.

λ_t	τ_t	w_t	$\bar{\epsilon}_{rel}$	E_{vmc} (K)
-1.90	0.65	0.5	0.191	-1.626 ±0.012
-1.85	0.65	0.5	0.192	-1.652 ±0.012
-1.80	0.65	0.5	0.192	-1.631 ±0.011
-1.75	0.65	0.5	0.193	-1.616 ±0.012
-1.65	0.70	0.5	0.194	-1.685 ±0.014
-1.25	0.65	0.5	0.202	-1.589 ±0.012
-1.90	0.55	0.5	0.204	-1.465 ±0.011
-1.65	0.55	0.5	0.207	-1.465 ±0.013
-1.35	0.80	0.5	0.213	-1.461 ±0.017
-0.75	0.65	0.5	0.214	-1.490 ±0.017
-0.75	0.75	0.5	0.214	-1.619 ±0.015
-1.85	0.35	0.5	0.227	-1.292 ±0.019

Now, we also see that the parameter set with the lowest energy, namely, $(1.65, 0.70, 0.5)$ does *not* have the lowest error. The $(-1.80, 0.65, 0.5)$ set has the lowest error. Compare

$$E_{vmc} = -1.685 \pm 0.014K$$

with

$$E_{vmc} = -1.631 \pm 0.011K.$$

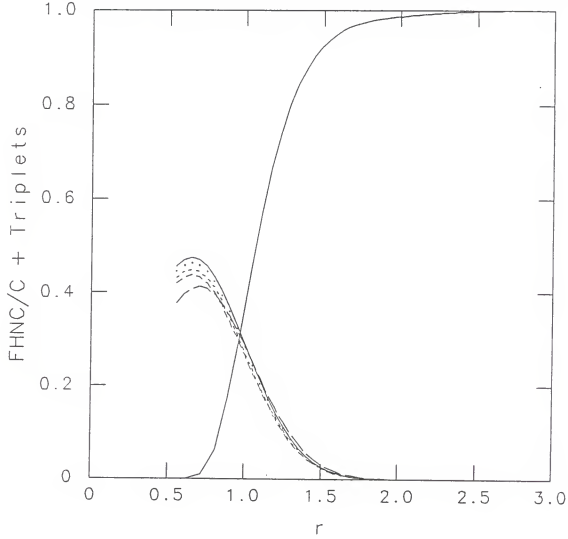
Note also that the kinetic energy of the $(-1.65, 0.70, 0.5)$ set is lower than the others, although it does slightly overlap that of the $(-1.80, 0.65, 0.5)$ set, as an examination of their errors reveal. Just because the $(-1.65, 0.70, 0.5)$ parameter set has the lowest energy, this does not necessarily mean that this is *the* best set

of those available. Although it does have the lowest calculated energy, it also has a relatively large error compared with its counterparts which also have energies in the -1.61K range. The lower error wave function may be the most desirable, particularly if it is to be used as an importance function in, say, Green's function Monte Carlo (GFMC) [3.3], [5.1]. The reason being that since the $(-1.80, 0.65, 0.5)$ set had the lowest error, it may have more *overlap* with the ground-state energy eigenfunction for this Hamiltonian, and its higher energy might be due to a mixing of an excited state in with the variational ground state. Thus, the lowest energy wave function may not be the best one to pick, depending on the intended use of the wave function. This is not the only possibility, however.

To investigate another possibility, examine Figure 3. In this figure, a plot of the first 5 wave functions† from Table 6 appear. Again, all five of these wave functions lead to variational energies below $-1.61K$. From this figure, note that all five triplets appear to be quite similar to one another, as they all cross the Jastrow in the same region. This is particularly striking in the case of the upper four triplets, *i.e.*, the solid line, the points, the short-dashed line, and the medium-dashed line. Here, the triplets look very similar in shape and strength, and they in fact are similar. The long-dashed line is the $(-1.65, 0.70, 0.5)$ triplet. This looks the most different from the other 'indicated' triplets. The $(-1.80, 0.65, 0.5)$ triplet had the lowest error, and is the triplet represented by the short dashed line. Notice that it is also in the middle of the other four similar triplets. The fact that this

† 'wave function' is synonymous with 'correlation function' in this context

Figure 3: The first five triplet correlations from Table 6. All of these correlations give rise to wave functions that lead to VMC energies of $-1.61K$ or less. The solid line spanning the full vertical extent of the graph is the two-body FHNC/C part, as before. The other solid line is the $(-1.90, 0.65, 0.5)$ triplet, the points represent the $(-1.85, 0.65, 0.5)$ triplet, the short dashed line is the $(-1.80, 0.65, 0.5)$ triplet, the medium dashed line is the $(-1.75, 0.65, 0.5)$ triplet, and the long dashed line is the $(-1.65, 0.70, 0.5)$ triplet. Note that all five triplets are similar with respect to the region and manner in which they cross the two-body correlation line.



triplet has the lowest error may, again, imply that it has the most overlap with the true ground-state wave function. The fact that the other similar triplets also lie in the same region, and have low energies, may imply that these upper four triplets are actually indicated due to some 'local minimum' in the relative error. It is clear that the method did eliminate a large number of other parameter sets, and the ones that were indicated all have low energies. On this finer scale, when the triplets are similar to one another, the choice of the trial wave function should be made from the indicated list based on the use for the trial wave function. Perhaps a GFMC study of these wave functions would help eliminate this remaining ambiguity. Again, however, the method does seem to work within this framework. How the results are interpreted and used is more a function of the intended use of the indicated wave function than anything else.

In Figure 4, the $(-1.35, 0.80, 0.5)$ triplet is plotted along with the other five triplets. As can be seen from Table 6, this would be among the worst choices for the trial wave function. Thus, we can conclude from this and from Figure 4 that stronger triplets, that tend to keep the particles apart, are better for the ^{3}He system than are the weaker ones, for triplets of the form used here.

The point is, of course, that this method did eliminate a large set of wave functions. Figure 5 illustrates this fact. Note that the general trend points to the fact that low variance wave functions are good candidates for improved trial wave functions, because they give rise to reduced variational energies. The cluster of five at the lower left of the plot are the wave functions that are exhibiting low-variance

Figure 4: This figure is similar to Figure 3, with the exception of the points. These points represent the (-1.35,.80,.5) triplet. This is a 'bad' triplet, and is not indicated by the proposed algorithm. Notice how this triplet crosses the two-body part compared with the indicated triplets which are indicated by the solid lines). This implies that the stronger triplets are best for liquid ^{3}He. The long dashed line is the FHNC/C pseudopotential in the Jastrow part.

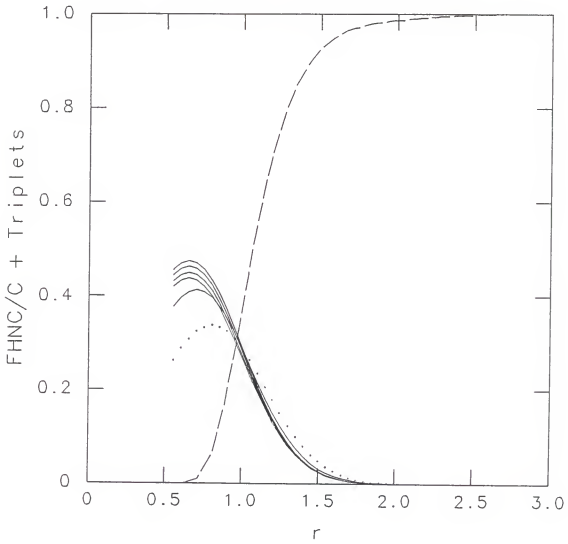
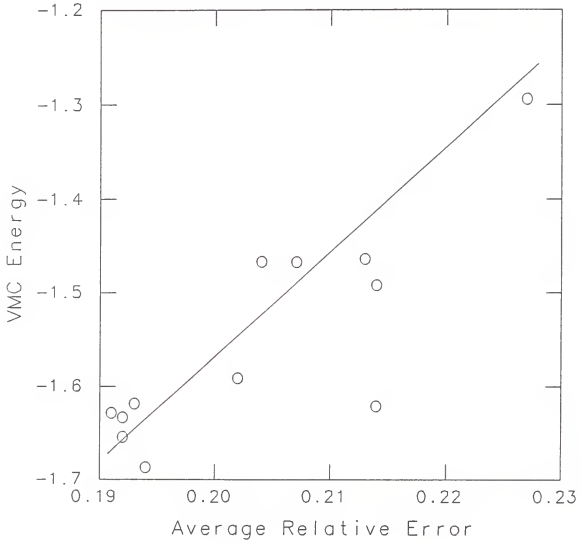


Figure 5: Scatter plot of the VMC energies versus the average relative error. The relative error is averaged over all four types of configurations. The line is present merely to guide the eye. Notice that the trend indicates that low-variance wave functions are good candidates for trial wave functions.



behavior, and are therefore the best candidates from this group for improved trial wave functions. This is the desired end result from this method. Although we are left with essentially five wave functions from which to choose, all of the others have been eliminated from contention. On a much larger grid of parameters, the benefits would be even greater.

Finally, now that the validity of the method has been established, the tremendous savings in time can be illustrated. To calculate just *one* of the variational energies shown in Table 1 took about 72 minutes on a CRAY-XMP. The code that was used was a reasonably optimized version to take advantage of the machine's vectorized structure. Therefore, to calculate all of the variational energies in Table 1 took a grand total of about 864 minutes. To run an analysis using all four of the configurations, each with 2,000 particle positions, for the same set of parameters took a grand total of about 24 minutes. Thus, the proposed method is about 36 times faster in this case than simply doing a VMC for each set of parameters, on the CRAY-XMP. To break this down even farther, it took about 2 minutes to analyze a single set of wave function parameters using the proposed method and all 8,000 particle positions. If the codes were moved to, say a VAX 750, it would take an estimated 14,400 minutes to analyze a single set using VMC, and thus 172,800 minutes (or about 4 months) to analyze this set of twelve parameters. Using the proposed method, it would take about 3 weeks of CPU time. Thus, if a smaller set of parameters were analyzed at a time to eliminate at least some of the really 'bad guesses', it would not be necessary to use a parallel machine until a

larger, and perhaps finer, grid of parameter sets were needed. Naturally, the time estimates for the VAX are just that — estimates.

However, what if one need not use all four configurations to get the same information? By implying earlier that really five parameter sets were indicated by the method since they were at the top of Table 6, and all have low energies, it is also implied that in a 'real' application of this procedure, one should examine all five of these parameter sets in a VMC calculation. Therefore, an 'error bar' has effectively been put on the relative errors that have been calculated. From Table 6, we see that these five parameter sets are within about 2% of the lowest relative error. Thus, in a real application, since one would not have a list such as Table 1 (for if one did, there would be no need to use this method!), all of the parameter sets that are within 2% to 5% of the lowest error should probably be examined with a VMC calculation. Returning to the initial question, what would happen if only two configuration sets were used? It seems reasonable to use the b=1.00 and b=1.15 sets, as these two are far apart in terms of which regions of phase space would be allowed to be seen during the random walk. This is also supported by examining Figure 2. In this figure, we see that the 1.13 curve is actually very similar to the 1.15 curve, and the FHNC/C curve. Thus, eliminating these might not have an adverse affect, since these configurations might not be adding that much 'new information'. Table 7 shows the results from doing this. Notice that the order of the indicated parameter sets is slightly different, however the parameter sets that are within the 2 to 5% 'window' of the lowest relative error

remain the same *five* parameter sets. Therefore, we have effectively extracted the same information and did less work in the process. Here, the method is actually about 72 times faster than a straight VMC calculation of all twelve sets. It cannot be overemphasized that the final choice of the parameter set from the indicated sets is contingent on the intended use of the trial wave function. It may suit the problem at hand fine to simply take the first set that appears on either Table 6 or Table 7, even though this set does not possess the lowest VMC energy. The method at the very least assures that these have *among* the lowest variational energy and error. The general trend is supported by Figure 5, and one can readily state that low-variance wave functions are good candidates for improved trial wave functions.

6.0 Conclusions and Suggestions

Clearly from the results, this method does provide a fast way of finding a near-optimal wave function of a given form. The method is certainly faster than simple VMC calculations of the variational energy for each trial wave function. As Table 1 indicates, the choice of wave function can have a rather large bearing on the physical quantity of interest. In the case of Table 1, note that the kinetic, potential, and total energies are given. These have different values for different wave functions. This serves to underscore the fact that the proper choice of the trial wave function should ultimately be made based on the intended use for the wave function. The point is here that even if this method singles out two, or three,

Table 7: Ranked relative errors, $\bar{\epsilon}_{rel}$. These relative errors are the averages over only two configurations used, *i.e.*, each average relative error is the average of the relative errors for each of the parameter sets over each of the two configuration types that were used. The configurations that were used here are those that were generated with a wave function of $b = 1.00$ and $b = 1.15$. The E_{vmc} are the variational energies calculated via the VMC code.

λ_t	r_t	w_t	$\bar{\epsilon}_{rel}$	E_{vmc} (K)
-1.90	0.65	0.5	0.188	-1.626 ±0.012
-1.85	0.65	0.5	0.189	-1.652 ±0.012
-1.80	0.65	0.5	0.190	-1.631 ±0.011
-1.75	0.65	0.5	0.191	-1.616 ±0.012
-1.65	0.70	0.5	0.195	-1.685 ±0.014
-1.90	0.55	0.5	0.197	-1.465 ±0.011
-1.25	0.65	0.5	0.201	-1.589 ±0.012
-1.65	0.55	0.5	0.201	-1.465 ±0.013
-0.75	0.65	0.5	0.213	-1.490 ±0.017
-1.85	0.35	0.5	0.221	-1.292 ±0.019
-0.75	0.75	0.5	0.224	-1.619 ±0.015
-1.35	0.80	0.5	0.234	-1.461 ±0.017

or five possibilities, it is *still* computationally cheaper to do this, and then test the definite possibilities with a more extensive computational method if necessary.

It also seems clear that the method is indeed dependent on the details of the generation of the configurations. The two obvious requirements discussed thus far are fairly simple to adhere to. First, the configurations that are used cannot have particles that are too close together. In this case, this was dictated by the b value in the McMillan pseudopotential. Second, the configurations used should be very well distributed throughout position space. We thus see that a balance must actually be struck here, between the amount of position space that the configurations represent, and how close the particles are allowed to come. Some

additional tests were also run on some configurations that were not generated with a wave function that was similar to the form of the trial wave function at all. These results indicated that it was possible to obtain a set of configurations that would sample the *trial* wave function where it was very small, thus leading to a large value of the local energy, and thus increase the estimate of the error. This tends to place an additional restriction on the configurations used, or at least point out a possible problem. If possible, the configurations should be generated with wave functions that are *similar* to the family of trial wave functions that are being tested. This would help reduce the chances of this problem occuring at all. It should still be possible to, say, use modified numerical noise. It would have to be modified to remove the close particle pairs, be properly scaled, *and* be filtered such that it would not sample the trial wave function where it was very small. This latter requirement, which constitutes a 'new' restriction on the configurations, can be easily taken care of in another way, which will be discussed below when improvements are suggested. Again, if the *correct* eigenstate is used, it would not matter what particle positions were used — the variance, and hence the standard and relative errors would be zero. In the present case, the configuration space requirement was met by averaging the relative error over a variety of the configurations, and the careful sampling of the trial wave function was handled by generating the configurations with wave functions that were of the same form as the trial wave functions.

Another possible 'pitfall' in this method is the manner by which the standard

errors are compared. As we have seen, it is not necessarily sufficient to simply pick the lowest standard error. In using this method, it does seem to be necessary to *not* throw away any information. Although the 'energies' calculated are not the correctly weighted variational energies, we have seen that they actually provided a valuable bit of information that provided for a more sharp indication of the best wave function parameters from the group. The relative error served very well here. There is at least one improvement that will be discussed below that should sharpen the indication even farther, and might even allow the use of fewer configurations.

The indicated parameter sets indicated that the stronger triplets were, in general, best for liquid ^{3}He. In fact, the method indicated that the variational energy was more sensitive to changes in the r_t parameter than the strength, to a degree. Note that the w_t parameter remained constant for the test set. There is no real reason for this, other than convenience. It should be pointed out here that due to the speed of the method, a rather large number of parameter sets were actually evaluated, including a few in which w_t was varied. The 'chosen twelve' were simply representative choices from the set. The wave function for this system might be improved by introducing higher order correlations, such as four-particle correlations, or state-dependent correlations, such as 'backflow' correlations [3.3]. In fact, as was mentioned in section 3.3, the assumed form for the trial wave function (3.5) is very far from the true ground state wave function, and the method will work better on a form that is closer to the correct ground-state wave function. This is a subject for future study [3.3], [6.1].

Another improvement that could be made has to do with the way that the 'energies' are calculated themselves by the proposed method. Consider doing the following. At the time that the particle positions are written out, write out the value of the generating wave function at that point, $\Psi_{gen}(\mathbf{R})$. Then, rather than averaging the local energy,

$$\left(\sum \frac{H\Psi_T(\mathbf{R})}{\Psi_T(\mathbf{R})} \right),$$

average

$$\left(\frac{\sum \left(\frac{|\Psi_T(\mathbf{R})|}{|\Psi_{gen}(\mathbf{R})|} \right)^2 \left(\frac{H\Psi_T(\mathbf{R})}{\Psi_T(\mathbf{R})} \right)}{\sum \left(\frac{|\Psi_T(\mathbf{R})|}{|\Psi_{gen}(\mathbf{R})|} \right)^2} \right).$$

The summations naturally run over all of the particle positions generated with $\Psi_{gen}(\mathbf{R})$. This 're-weighting' of the variational energy has been suggested before [6.1], and while this is still not the 'correct' variational energy, it is an improvement over simply averaging the local energy alone. By re-weighting the local energy in this manner, the generating wave function's effect on the results is taken into account, at least to first order. This improved estimate of the variational energy, combined with the estimate of the variance, may allow one to get by with using very few configurations to extract the best wave function parameters from a group of parameters. Thus, this improvement could speed up the method even more. Furthermore, this would also tend to negate the problem that might occur if the configurations used sample the wave function where it is small. If this were to happen, the large value for the local energy would be re-weighted with a small number, and thus contribute negligibly to the final outcome.

Finally, while it is certainly true that a zero-variance calculation of the local energy implies an eigenstate of the Hamiltonian, one is usually faced with comparing different approximate wave functions, none of which are eigenstates. Furthermore, as we have seen, a non-zero local minimum in the variance (or relative errors, as were used here) does not necessarily indicate a more optimized wave function, that is, an improved energy *and* a lower error than previous estimates. The method did point to a group of wave functions, all of which possessed low energies and relatively low errors, but the lowest energy wave function did not have the lowest error. The determining factor in a final decision on the trial wave function must be made based on this method and the *use* of the trial wave function. The wave function with the lowest energy may not be the best choice. If the wave functions are to be used as both generating and importance functions for GFMC, the lower variance wave functions are of more interest than the lowest energy ones. This method, if it is done carefully and correctly, assures one of a wave function that possesses either a lower energy, or a lower error, or both, and thus points to good candidates for improved trial wave functions.

References

[1.1] W.L. McMillan, Phys. Rev. **A 138**, 442 (1965).

[1.2] N. Metropolis, A.W. Rosenbluth, M.N. Rosenbluth, A.H. Teller, and E. Teller, J. Chem. Phys. **21**, 1087 (1979).

[2.1] C.J. Umrigar, K.G. Wilson, and K.E. Schmidt, "Optimized Trial Wavefunctions for Quantum Monte Carlo", abstract, Bulletin of the American Physical Society, **32** (1987).

[3.1] See "Condensed Matter Theories", vol. 1 , F. Malik, ed. (Plenum Press, New York, 1986).

[3.2] Due to Dingle, Jastrow, and Mott. See "MC Methods in Statistical Physics", K. Binder ed, M.H. Kalos, D.M. Ceperley, Chapter 4 (Springer-Verlag, Berlin, Heidelberg, 1979). The expansion from Ψ_{fermi} to $\Psi_{boson} \times D(\mathbf{R})$ was done by Wu and Feenberg, F.Y. Wu, E. Feenberg, Phys. Rev. **128**, 943 (1962).

[3.3] R.M. Panoff, in "Condensed Matter Theories", vol. 2, ed. by P. Vashista, R. Kalia, and R. Bishop (Plenum Press, New York, 1987).

[3.4] R.M. Panoff, J.W. Clark, Phys. Rev. **B 36**, 5527 (1987).

[3.5] E. Krotscheck, R.A. Smith, J.W. Clark, and R.M. Panoff, Phys. Rev. **B 24**, 6383 (1981).

[3.6] K.E. Schmidt, M.H. Kalos, M.A. Lee, and G.V. Chester, Phys. Rev. Lett. **45**, 573 (1980).

[3.7] K.E. Schmidt, M.A. Lee, M.H. Kalos, and G.V. Chester, Phys. Rev. Lett. **47**, 807 (1981).

[3.8] R.A. Aziz, V.P.S. Nain, J.S. Carley, W.L. Taylor, and G.T. McConville, J. Chem. Phys., **70**, 4330 (1979).

[5.1] M.A. Lee, K.E. Schmidt, M.H. Kalos, and G.V. Chester, Phys. Rev. Lett. **46**, 728 (1981).

[6.1] D. Ceperley, G.V. Chester, and M.H. Kalos, Phys, Rev. **B 16**, 3081 (1977).

MINIMUM VARIANCE FOR MANY-BODY WAVE FUNCTIONS

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B.S., New Mexico State University, 1986

AN ABSTRACT OF A THESIS

submitted in partial fulfillment of the
requirements for the degree

MASTER OF SCIENCE

Department of Physics

KANSAS STATE UNIVERSITY

Manhattan, Kansas

1988

Abstract

The Rayleigh-Ritz variational principle may be used to optimize a many-body wave function by minimizing the variational energy, a true upper bound to the ground-state energy expectation value for a given Hamiltonian. This minimization is usually attempted by evaluating, for each trial wave function, the multi-dimensional integrals entering into the energy expectation value. This procedure for a truly many-body problem, such as the description of the ground state of liquid helium, may be both difficult and expensive to implement, even with the accurate and relatively efficient evaluation of these integrals by Monte Carlo methods.

The variational energy of an eigenstate of the Hamiltonian, calculated as the average of the local energy evaluated at particle coordinates chosen with a probability proportional to the square of the trial wave function, is stationary, that is, it has zero variance. In this thesis, the variance in the expectation value of an energy estimator for different variational wave functions averaged over a fixed set of particle coordinates, is studied as a means of improving the optimization procedure. For those trial wave functions which minimize or nearly minimize the variance or relative error, the actual variational energies, calculated via the full variational Monte Carlo procedure, are examined to study the extent to which a wave function with a low relative error in the energy estimator implies a low variational energy.

The system used for such a test was liquid ^{3}He. This liquid is modeled as 54

particles in a periodic box interacting via phenomenological potentials. Two and three body correlations are included in the trial wave function. For a wide range of parameters entering the correlations, wave functions which have the lowest overall relative errors for several independent sets of particle coordinates are found to have the lowest variational energies. Furthermore, wave functions which exhibit low-variance behavior nearly minimize the variational energy. Analyzing wave functions in this manner is typically 35 to 70 times faster than simple evaluation and comparison of variational energies alone. Consequently, good candidates for improved variational wave functions may be accurately and efficiently identified by this variance minimization procedure.