
#### Abstract

One of the recent discoveres in nuclear Physics is the existance of Halo nuclei .

Therefore, halo nuclei are very weakly-bound exotic states of nuclear matter in which the outer one or two valence nucleons (usually neutrons), and a nuclear core with normal nuclear density is surrounded by a region of dulite nuclear matter, referred to as the neutron halo. Such nuclei occur from light to heavy masses and have been the subject of a alarge number of theoretical studies to try and understand them. A number of theoretical models have been proposed over the years.

In this thesis the structure of light halo nuclei is examind through a fully microscopic variational model, where the Pauli exclusion princple explicity satisfied and semi-realistic nucleon-nucleon interactions are used. The model is an extension of previous work of closed shell nuclei. The wavefunction is obtained from a starting or reference state, which includes the required symmetries nd provides a translationally invariant description of the system in terms off several uncorrelated clusters. Medium to long-rang linear and short-range non-linear corrlation operators are then applied to obtained a good wavefunction, these models are important to solve the Shrodenger equation.

The model developed is then used to examine the nuclei ${ }^{5} \mathrm{He},{ }^{6} \mathrm{He}$, ${ }^{8} \mathrm{Be}$ and ${ }^{9} \mathrm{Be}$. By making use of one-and two-body density distributions a qualitative picure of the matter distribution in the nucleus is obtained.

The analysis provided indicates for a bound state one requires spin-orbit force, something that we don't include. Nevertheless working in the L-S coupling scheme have shown that our model is capable of producing bound states for open-shell sysytems by artificially altering the central term of the semi-realistic interactions in use. And to find the relashonshipe between the energy and the width of shell, and find the


behavioer of nuclei from throught the relation between energy and distance to the center of mass of alpha partical, 5 He and 8 Be are known halo nuclei. The general behaviour obtained was that the energy approached a minimum, as the separation between the several constituents increased. This could be monitored by observing the spherically averaged one-and two-body density distributions. We could clearly see that the energy was minimized as the one-body distribution broadened with the center shifting a way from the origin. The two-body density distribution separated into two parts: a main body similar to the alpha-particle and a small tale effect. We used algorithmic scaling in order to distinguish the two parts.

Despite the fact our interaction is not adequate for the light halo nuclei of 6 He and 9 Be we demonstrated that our model can produce bound state for such open-shell systems by modifying the inter-nucleon force.in this thesis used programes in Fortran (77).

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## Certification

We certify that this thesis was prepared under our supervising at the College of Science of Al-Nahrain University in partial fulfillment of the requirements for the degree of Ph.D. of Science in Physics.

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In view of the recommendations, we present this thesis for debate by the examination committee.

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Date: / /2008

## 5-1 introduction

In previous chapters we discussed the structure of cluster like model as well as the technical requirements such as the inclusion of $\operatorname{SU(4)}$ symmetry and the evaluation of expectation values by Monte Carlo sampling. In this chapter we apply the cluster model in the simplest cases where halo phenomena observed.

Hansen and Jonson[Han87] have proposed a "neutron halo" model of 11Li to account for these observations. In the case of 6 He the two neutrons are more tightly bound and the structure is called "neutron skin"

The structure of nuclei far from stability and close to the particle drip lines is very rich. In neutron-rich nuclei, in particular, exotic phenomena include the weak binding of the outer most neutron, pronounced effects of the coupling between bound states and the particle continuum, regions of nuclei with very diffuse neutron densities and the formation of neutron skin and halo structures.

Weekly bound systems provide a sensitive test of the nuclear force, and the neighborhood of the drip lines provides a unique proving ground for the development of our understanding of these interactions which are of fundamental importance.

It can be shown how the three-body system changes. On the bound side of the drip line lies a variety of rather intriguing substructures. Amongst them there are the Borromean nuclei which possess the property that none of the two-particle subsystems are bound, and it requires three-body correlations to bind the system. An example of such a nucleus would $6 \mathrm{He}(4 \mathrm{He}+\mathrm{n}+\mathrm{n})$.

Equally, it is possible to have three-body systems in which only two of the constituents are bound, but the $4 \mathrm{He}+\mathrm{n}(5 \mathrm{He})$ subsystems are not.

The comparison between these nuclei and Borromean systems allows a detailed understanding of the three-body correlations to be achieved.

As we have illustrated in the case of alpha-particle the role of state-dependent correlations is to lower the binding structure but does not seem to effect any of the structure of the system. One important issue in the model is the absence of the spinorbit component from the nucleon force. For this reason a preliminary of experimental results is provided for the cases of interest.

## 5-2 Experimental results for ${ }^{5} \mathrm{He},{ }^{6} \mathrm{He},{ }^{8} \mathrm{Be}$ and ${ }^{9} \mathrm{Be}$

As an example are ${ }^{5} \mathrm{He},{ }^{6} \mathrm{He},{ }^{8} \mathrm{Be}$ and ${ }^{9} \mathrm{Be}$. Therefore, it is useful to include some of the experimental results for these nuclei focusing at the ground state properties. These are summarized in table (5-1) and are taken from [Tun, Nat] and show table (52).

The nucleus of ${ }^{4} \mathrm{He}$ is bound by about -28 MeV with a difference of a bout 20 MeV between the $0^{+}$ground and first excited state $0^{+} .{ }^{5} \mathrm{He}$ is unbound by -0.798 MeV and is observed as a $J^{\pi}=\frac{3^{-}}{2}, T=\frac{1}{2} \quad$ resonance. There is also a $\frac{1^{-}}{2}$ resonance that lies 1.27 MeV . In this illustrates that spin-orbit coupling for single particle is required in order to produce the observed resonance, since both can result from the coupling of an $S=1 / 2$ with an $L=1$ state giving a valence neutron in the $0 p 1 / 2$ and $0 p 3 / 2$. The next resonance state for ${ }^{5} \mathrm{He}$ is a $\frac{3^{-}}{2}$ and occurs at 16.84 MeV .In the case of ${ }^{6} \mathrm{He}$ we have a Borromean structure as a result of the fact that ${ }^{5} \mathrm{He}$ is unbound, while the ${ }^{6} \mathrm{He}$ ground state is a stable $0^{+}$bound state.
Table 5-1: Some simple ground state properties of the nuclei ${ }^{5} \mathrm{He},{ }^{6} \mathrm{He},{ }^{8} \mathrm{Be}$ and ${ }^{9} \mathrm{Be}$. We indicate the ground or resonance states in the $\left(J^{\boldsymbol{\pi}}\right)$ form. For the lowest lying resonances give the difference in MeV from threshold, while in the cases where the nucleus is unbound the decay channel is indicated.

| Nucleus | Ground state $\mathbf{J}^{\boldsymbol{\pi}}$ | Lowest <br> resonances | Isospin ( $\boldsymbol{T})$ | Decay channel |
| :---: | :---: | :---: | :---: | :---: |
| ${ }^{5} \mathrm{He}$ | $3 / 2(-0.798 \mathrm{MeV})$ | $1^{-} / 2(1.27 \mathrm{MeV})$ | $1 / 2$ | ${ }^{4} \mathrm{He}+\mathrm{n}$ |
| ${ }^{6} \mathrm{He}$ | $0^{+}$ | $2^{+}(1.797 \mathrm{MeV})$ | 1 | bound <br> ${ }^{8} \mathrm{Be}$ |
| ${ }^{9} \mathbf{B e}$ | $0^{+}(0.09 \mathrm{MeV})$ | $2^{+}(3.06 \mathrm{MeV})$ | 0 | ${ }^{4} \mathrm{He}+{ }^{4} \mathrm{He}$ |
|  | $3 / 2$ | $1^{-} / 2(1.68 \mathrm{MeV})$ | $1 / 2$ | bound |

Table(5-2) Cluster decomposition of nuclei

| Nucleus | Configuration | Cluster Model | Isospin (T) | $\mathbf{Z}$ |
| :---: | :---: | :---: | :---: | :---: |

for decay into an alpha-particle and two neutrons ${ }^{4} \mathrm{He}+2 n$ and thus ${ }^{6} \mathrm{He}$ is weakly bound. The first resonance of ${ }^{6} \mathrm{He} J^{\pi}=2^{+}$lie 1.797 MeV above the ground state and has a strongly decay to the ${ }^{4} \mathrm{He}+n$ channel. The next resonance state for ${ }^{6} \mathrm{He}$ occur at 5.6 MeV and has uncertain spin assignment $2^{+}, l^{-}, 0^{+}$. Therefore it seems reasonable to consider ${ }^{6} \mathrm{He}$ as a weakly bound three-body system where a $0^{+}$alpha-particale ground state is accompanied by two weakly bound neutrons. Then the total spin of the two valance neutrons has only two possible values $S=0,1$ and thus the total orbital momentum is confined to the positive parity states $L=0$ and $L=1$, both with positive parity.

The nucleus ${ }^{8} \mathrm{Be}$ is also unbounded and is observed as a resonance in the scattering of two alpha-particles, just 0.09 MeV above the ${ }^{4} \mathrm{He}^{+4} \mathrm{He}$ threshold. There is another low-lying resonance that occurs at $3.06 \mathrm{MeV}, J^{\pi}=2^{+}$, and is part of the deformed band., so that we find positive parity. We analyze this later on within the frame work of our cluster model.
${ }^{9} B e$ is another interesting nucleus with a stable $\frac{3^{-}}{2}$ ground state and with orbital
isospin $T=\frac{1}{2}$. Since ${ }^{8} B e$ and ${ }^{5} \mathrm{He}$ are unbound ${ }^{9} \mathrm{Be}$ is again a Borroman nucleus, made from two alpha-particles and a neutron. There is a number of known resonance states, the lowest of which is a $\frac{1-}{2}$ at 1.68 MeV and lies just above the ${ }^{8} B e+n$ threshold by a few KeV . The next resonances are $\frac{5^{-}}{2}(2.429 \mathrm{MeV}), \frac{1^{-}}{2}(2.8 \mathrm{MeV})$ and $\frac{1^{-}}{2}(3.05 \mathrm{MeV})$.These resonance decay to the ${ }^{8} B e+n$ configuration, which indicates that the ${ }^{9} B e$ ground state is not far from the three-body picture $\alpha+\alpha+n$ with $S=1 / 2$ The ground state orbital momentum is then $L=1$ assigned to the neutron relative to the two alpha-particles, which explains the negative parity.

The experimental results provide strong evidence for the importance of spin-orbit coupling in binding the light halo nuclei of ${ }^{6} \mathrm{He}$ and ${ }^{9} \mathrm{Be}$. For example the splitting of the $L=1$ level into $\frac{3}{2}$ and $\frac{1}{2}$ occurs both in ${ }^{5} H e$ and ${ }^{9} B e$. However, we will need (and do) to justify the implications of the absence of a spin-orbit force.

## 5-3- Application and discussion of results

One major characteristic of nuclear halo nuclei is the weak binding energy of the halo nucleon.

The model is then used to examine the nuclei ${ }^{5} \mathrm{He},{ }^{6} \mathrm{He},{ }^{8} \mathrm{Be}$ and ${ }^{9} \mathrm{Be}$. By making use of one-and two-body density distributions a qualitative picure of the matter distribution in the nucleus is obtained. The analysis provided indicates for a bound state one requires spin-orbit force, something that we don't include. Nevertheless working in the L-S coupling scheme have shown that our model is capable of producing bound states for open-shell sysytems by artificially altering the central term of the semi-realistic interactions in use.

## 5-3-1 ${ }^{5} \mathrm{He}$

Although experimentally ${ }^{5} \mathrm{He}$ is not a bound system we can use it as a starting point to test our cluster model. In the $\mathrm{J}-\mathrm{TICI}(2)$ method the wavefunction is given by
equation (3-36);

$$
\Psi=\sum_{i}\left|\begin{array}{l}
{[4,1] i}  \tag{5-1}\\
L, M_{L}
\end{array}\right\rangle\left|\begin{array}{c}
{\left[2,1^{3}\right] i} \\
S=\frac{1}{2} M_{s}, T=\frac{1}{2} M_{T}
\end{array}\right\rangle
$$

where the two necessary ingredients are the reference state and the correlation operator entering the wavefunction that will take the form:

$$
\left|\begin{array}{l}
{[4,1] i}  \tag{5-2}\\
L, M_{L}
\end{array}\right\rangle=\hat{F} Y_{i}^{[4,1]} \Phi_{L, M_{L}}^{\text {ref }}
$$

Where $\Phi_{L, M_{L}}^{\text {ref }}$ is the reference function, while $Y_{i}^{[4,1]}$ is an operator projecting it to the ith basis state of the $\mathrm{Y}^{[4,1]}$ irrepresentation. of $S_{5}$. while the correlation operator has the same form as in the case of alpha-particle.

The choice we make for the reference state, $\Phi_{\alpha}$, of the alpha-particle by adding a part representing the weakly bound neutron. One way to do this that preserves translational invariance to assign coordinates to the extra particle relative to the alpha-particle center-of mass. Therefore, the reference state for ${ }^{5} \mathrm{He}$ look like
where

$$
\begin{align*}
& r_{\alpha 5}=\frac{1}{4}\left(r_{1} \rightarrow+r_{2}+r_{3} \rightarrow+r_{4}\right)-r_{5} \\
& r_{\alpha 5}=\left|r_{\alpha 5}\right| . \tag{5-5}
\end{align*}
$$

The purpose of the function $f\left(r_{\alpha 5}\right)$ is to localize the additional neutron with respect to the alpha-particle center-of-mass, while $y_{M}^{L}\left(r_{\alpha 5}\right)$

$$
\begin{equation*}
y_{M}^{L}\left(r_{\alpha 5}\right)=R\left(r_{\alpha 5}^{L}\right) Y_{M}^{L}(\theta, \Phi) . . \tag{5-6}
\end{equation*}
$$

that assigns angular wavefunction (spherical harmonic) dependence to the same neutron with respect to the alpha-particle center-of-mass. And $R\left(r_{\alpha 5}^{L}\right)$ radial wavefunction.

A possible choice for $f\left(r_{\alpha 5}\right)$ is in terms of spherical shells

$$
f\left(r_{\alpha 5}, d, \omega\right)=\exp \left(-\alpha^{2} \frac{\left(r_{\alpha 5}-d\right)^{2}}{\omega^{2}}\right) . .
$$

where $\alpha$ is the Harmonic oscillator parameter appearing in the reference state of the alpha-particle. The parameter d represent the "distance" of the shell from the center-of-mass of the alpha-particle, while $\omega$ stands for the "width" of the shell. This is a structure that has been used before in [Gua01]. The parameters $d, \omega$ and the set of parameters entering the Jastraw factor of the correlation operator are variational parameters. The correlation operator is given as in the case of the alpha-particle, where the linear coefficients used for the expansion are minimized by a linear eigenvalue problem.

The value of the energy was obtained for variations of $d$ and $\omega$ for the $L=1$ state. In the case of the spin and isospin quantum numbers there is there is only the possibility of ( $S=1 / 2, T=1 / 2$ ). It can be clearly seen that for a particular value of the "distance" parameter $d$, there is no variational stationary point but as the "width" $\omega$ and despite the value of $d$ the energy approaches the same value, i.e., the driving parameter is the "width" $\omega$. when we move from $L=1$ to some other value of $L$ there is no change in the overall behaviour of the ground state energy and the same asymptotic behaviour is observed for large $\omega$ as is illustrated in figure $5-1$. The only difference between the different values of $L$ is for relatively small values of the parameters $d$ and $\omega$.


Figure (5.1): The ground state energy for the state-independent $\mathbf{J}-\mathbf{T I C I}(2)$ calculation of ${ }^{5} \mathrm{He}$ for different values of $L$ using the $S 3$ interaction. The broken line corresponds to the alphaparticle ground -state energy for the same type of calculation. The value of $\omega$ is in relative units (i.e scaled fm) since is multiplied by the harmonic oscillator parameter $\alpha$.

The fact there is no variational minimum that no bound, state exits for ${ }^{5} \mathrm{He}$ within our approximation. For this purpose, we can make use of the spherically averaged one and two-body density distribution introduced for the alpha-particle (equations $(2-55)$ and (2-56)). The results obtained for the density matrices with the $S 3$ are shown in figures (5-2) and (5-3).

We expect that the parameters $d$ and $\omega$ will be associated with the separation of the additional neutron from the alpha-particle. Intuitively the value of $\omega$ is associated with the "freedom" that we assign to the additional neutron in the model state, that is
centered at $d$, when this is acted upon by the correlation operator the resulting picture can be different. The spherically averaged one body density distribution $\rho_{1}(r)$ measures the probability of finding a nucleon at a distance $r$ from the center-of-mass. We expect that when the additional neutron is moved away from the center (in terms of $d$ and $\omega$ ), that the overall one-body probability distribution will be effected.

The effect of changing $d$ and $\omega$ is displayed one the right hand graph of figures (52 ) and (5-3), respectively.


Figure (5.2) The one - bodyand two - body density distribution for ${ }^{5} \mathbf{H e}$ (using the S 3 interaction) for a number of values of the width parameter $w$.

Figure (5-3) shows the increasing value of $w$ broadens the distribution from the origin. A similar behavior is illustrated in figure (5-4) for the case of the parameter $d$ but the influence of $d$ on the one-body density distribution is less strong than that of $\omega$.


Figure (5.3) The tail of the two - body density distribution for ${ }^{5} \mathrm{He}$ (using the S 3 interaction) for a number of values of the width parameter $w$ and the entire graph plotted on a logarithmic scale.

Figure (5-4) also illustrated the effect of adding orbital momentum to the additional nucleon relative to the alpha-particle, where by adding orbital momentum we get less distribution close to the center-of- mass.

The effect of the variational parameters on the two-body density distribution is more subtle. The separation of the additional neutron from the alpha-particle on the two-body density appears as a small change in the behaviour of the tail


Figure (5.4) The one-body spherically averaged density distribution for ${ }^{5} \mathrm{He}$ (using the $\mathbf{S 3}$ interaction) for a number of values of the distance parameter $d$ and orbital momentum $L$. The value of $w$ was kept constant

In the $\mathrm{J}-\mathrm{TICI}(2)$ formalism the wavefunction of equation (5-2) has the property that the correlation operator $\hat{F}$ is invariant under the exchange of particles. Thus the antisymmetrized reference function is the same for all the required integrals of the Hamiltonian and overlap matrix elements. This can be an advantage over the RGMlike method where the reference function is approximated by a linear expansion and each matrix element requires it own-antisymmetrization, particularly when a numerical method like Monte-Carlo integration is used. The results obtained for $S 3$ interaction are equivalent to the ones obtained for the $\mathrm{J}-\mathrm{TICI}(2)$ method. However, we shall a band on this method since carrying out the antisymmetrization for every matrix element is an unnecessary complexity that can reduce the efficiency of our numerical algorithm.

Despite the fact that ${ }^{5} \mathrm{He}$ provides a non bound structure the calculation has
provided as with the important lesson that the variation of the energy with respect to the variational parameters and $L$ is different between a reference function.

### 5.3.2 ${ }^{6} \mathrm{He}$

Contrary to the case of ${ }^{5} \mathrm{He}$, where there is only a single choice for the permutation symmetry, We study the $6 \mathrm{He}(4 \mathrm{He}+\mathrm{n}+\mathrm{n})$ under an inert core assumption for 4 He .6 He represent (based ) on core $+\mathrm{n}+\mathrm{n}$ microscopic three-body cluster modek, which is a typical Borromean system.[Kiy01]
${ }^{6} \mathrm{He}$ has two options for the wavefunction of equa. (3-36) resulting in two distinct spin-isospin configurations with $T=1$. The two wavefunctions can be represented as:

$$
\left.\begin{array}{c}
\Psi^{(0,1)}=\sum_{i}\left|\begin{array}{l}
{[4,2] i} \\
L, M_{L}
\end{array}\right\rangle\left|\begin{array}{c}
{\left[2^{2}, 1^{2}\right] i} \\
S=0, T=1 M_{L}
\end{array}\right\rangle
\end{array}\right) . \begin{gathered}
{\left[3,1^{3}\right] i} \\
\Psi^{(1,1)}=\sum_{i}\left|\begin{array}{l}
{\left[4,1^{2}\right] i} \\
L, M_{L}
\end{array}\right\rangle\left|\begin{array}{c}
{\left[\begin{array}{l}
M_{S}
\end{array}\right) T=1 M_{t}}
\end{array}\right\rangle \tag{5-9}
\end{gathered}
$$

The above wavefunctions can be assigned several values for the total orbital momentum $L$.

We can construct a reference state for ${ }^{6} \mathrm{He}$ similar to that of ${ }^{5} \mathrm{He}$, that looks like
where

$$
\begin{align*}
& r_{\alpha 5}=\frac{1}{4}\left(r_{1} \rightarrow r_{2}^{\rightarrow}+r_{3}^{\rightarrow}+r_{4}^{\rightarrow}\right)-r_{5} .  \tag{5-11}\\
& r_{\alpha 6}=\frac{1}{4}\left(r_{1} \rightarrow+r_{2}^{\rightarrow}+r_{3}+r_{4}\right)-r_{6} . \tag{5-12}
\end{align*}
$$

The purpose of the functions $f\left(r_{\alpha 5}\right)$ and $f\left(r_{\alpha_{6}}\right)$ is to localized the additional neutrons with respect to the alpha-particle center-of-mass. $y_{M}^{L}\left(r_{56}\right)$ as a angular wavefunction (spherical harmonic)

$$
y_{M}^{L}\left(r_{56} \rightarrow\right)=\sum_{l_{1} l_{2}} a_{l_{2} l_{2}}^{L}\left(\sum_{m_{1}, m_{2}} C_{l_{1} m_{1}, l_{2} m_{2}}^{L_{o}} y_{m_{1}}^{l_{1}}\left(r_{\alpha 5}^{\rightarrow}\right) y_{l_{2}}^{m_{2}}\left(r_{\alpha 6}^{\rightarrow}\right)\right) \ldots \ldots \ldots .(5-13)
$$

Where $C_{l_{1} m_{1}, l_{2} m_{2}}^{L_{0}}$ are the Clebsh-Gordan coefficients, while the $a_{l_{1}, l_{2}}^{L}$ are linear
variational coefficients. The function $f\left(r_{56}\right)$ describes the relative motion of the two neutrons with respect to each other.

As in the case of ${ }^{5} \mathrm{He}$ a possible choice for the $f\left(r_{\alpha_{5}}\right)$ and $f\left(r_{\alpha_{6}}\right)$ is in terms of spherical shells:

$$
\begin{align*}
& f\left(r_{\alpha 5}, d_{1}, \omega_{2}\right)=\exp \left(-\alpha^{2} \frac{\left(r_{\alpha 5}-d_{1}\right)^{2}}{\omega_{1}^{2}}\right) . .  \tag{5-14}\\
& f\left(r_{\alpha 6}, d_{2}, \omega_{2}\right)=\exp \left(-\alpha^{2} \frac{\left(r_{\alpha 5}-d_{2}\right)^{2}}{\omega_{2}^{2}}\right) \ldots  \tag{5-15}\\
& r_{56}=\left|r_{\alpha 5}^{\vec{s}}-r_{\alpha 6}^{\overrightarrow{6}}\right| . . \tag{5-16}
\end{align*}
$$

where $\alpha$ is the Harmonic oscillator parameter appearing in the reference state of the alpha-particle. The "distance" parameters $d_{1}, d_{2}$ and the "width" parameters $\omega_{1}$ and $\omega_{2}$ localized each particle individually. In the case of $f\left(r_{56}\right)$ we choose the similar parametrization:

$$
\begin{equation*}
f\left(r_{56}, d_{3}, \omega_{3}\right)=\exp \left(-\alpha^{2} \frac{\left(r_{56}-d_{3}\right)^{2}}{\omega_{3}^{2}}\right) \ldots \tag{5-17}
\end{equation*}
$$

The intuitive picture of the structure provided by the reference function is relatively straight forward as is illustrated in figure (5-5).


Fig. 5-5: Artists impression of ${ }^{6} \mathrm{He}$

When compared with ${ }^{5} \mathrm{He}$ the calculation for ${ }^{6} \mathrm{He}$ is substantially more complicated. The variational non-linear parameters entering the reference function increase from just $d$ and $\omega$ to $\left\{d_{1}, d_{2}, d_{3}\right\}$ and $\left\{\omega_{1}, \omega_{2}, \omega_{3}\right\}$. Furthermore, the linear expansion used to approximate the correlation operator becomes bilinear in order to accommodate the coefficients $a_{l_{1}, l_{2}}^{L}$ that superimpose different coupled configurations of orbital
momenta $\left(l_{1}, l_{2}\right)$ into a total $L$. The behavior of the energy with respect to the number of coefficients $a_{l_{1}, l_{2}}^{L}$ is displayed in figure (5-6), for a restricted number of the variational parameters.


Figure (5.6) The dependencce of the ground-state energy of ${ }^{6} \mathrm{He}$ with respect to the number of linear coefficients $a_{l_{1}, l_{2}}^{L}$. The results were taken using the $\mathbf{S 3}$ interaction.

We carried out the calculation for ${ }^{6} \mathrm{He}$ with state-independent correlations for various sets of quantum numbers $L, \mathrm{~S}$ and $T$. Although there exits a dependence of the energy on the various configurations, this happens at a small values of the width parameters $\omega_{1}$ and $\omega_{2}$ and $\omega_{3}$ where the value for the energy is well above that of the alpha-particle without passing through a stationary point or going below the alphaparticle limit.

Instead of using reference function of equation (5-10) we can use a related form that corresponds to an alpha-particles correlated with a di-neutron structure:

$$
\Phi_{L}^{r e l}=\Phi_{\alpha} f\left(r_{\alpha 6}, d_{1}, \omega_{1}\right) f\left(r_{56}, d_{2}, \omega_{2}\right) y_{M}^{L}\left(r_{56}^{\rightarrow}\right) . .
$$

$$
\begin{equation*}
r_{56}=r^{\rightarrow}-\frac{1}{2}\left(r_{5} \rightarrow+r_{6}\right) . \tag{5-19}
\end{equation*}
$$

where the function $f\left(r_{56}\right) y_{M}^{L}\left(r_{6}\right)$ can be through of as the $d i-$ neutron. The functions $f\left(r_{\alpha_{56}}\right)$ and $f\left(r_{56}\right)$ have the same structure as before, but instead of correlating each individual.

Neutron with the alpha-particle independently we correlate the $d i$-neutron with the alpha-particle. This description of the model state is compatible with all the spin/isospin configurations as long as the required permutation symmetry is included in the $d i$-neutron part,

We use the above structure to illustrate the behavior of ${ }^{6} \mathrm{He}$ since it provides a restricted configuration, where the key variational parameters are $d_{1}, d_{2}$ and $\omega_{1}, \omega_{2}$. The results for the ground state energy for the $S=0, T=1$ and $L=0$ configuration using the $S 3$ interaction are shown in figure (5-7).


Figure(5.7) The ground-state energy of ${ }^{6} \mathrm{He}$ for the reference function of equa. (5.18). the S3interaction was used, while $S=0, T=1$ and $L=0$. The parameter $d 1$ is related to the separation of the di-neutron from the alpha-particle, while $d 2$ is the separation between the two neutrons of the di-neutron. The width parameter $w$ is in relative units since is multiplied by the harmonic oscillator parameter.

Figure (5-7) indicates that the system becomes less localized. This is valid both when the $d i$-neutron is moved away from the alpha-particle while keeping the two neutron at a fixed distance from each other, and in the opposite situation where the $d i-$ neutron is kept at a fixed distance from the alpha-particle, but the two-neutrons are separated from each other. In figure (5-8) we display the results from the ( $S=0, T=1$ ) spinisospin configuration and for $L=0$, using the $S 3$ interaction. The choice made for the distance and width parameters is that where $d_{l}=d_{2}$, while $d_{3}$ and $\omega=\omega_{1}=\omega_{2}=\omega_{3}$ are valid.


Figure(5.8) The ground - state energy for the state-independent J-TICI(2) calculation of ${ }^{6} \mathrm{He}$ as function of $w$ for $L=0, S=0, T=1$ using the $S 3$ interaction. $d 1$ and $d 2$ correspond to the value of the 'distance' parameter for each of the two weakly bound neutrons (corresponding to the instance between them and the alpha-particle). d3 corresponds to the 'distance' parameter describing the separation between the two weakly-bound neutrons. In this configuration $d 1=d 2$ and a single 'width' parameter is used for each point. The broken line corresponds to the alpha-particle ground-state energy for the same type of calculation. This can lead to a $0+$ state when spin - orbit coupling is used.

Furthermore, when we move to the $(S=1, T=1)$ spin-isospin configuration a very similar behaviour is observed as illustrated in figure (5-9). The set of quantum numbers $(S=0, T=1)$ and $(S=1, T=1)$ are the only ones in our approximation that correspond to two-neutrons (or two-proton because of charge independence) added to an alpha-particle.


Figure (5.9) The ground-state energy for the state-independent J-TICI(2) calculation of ${ }^{6} \mathrm{He}$ as function of $w$ for $L=1$; ( $11=12$ ), $S=1, T=1$ using the $S 3$ interaction. $d 1$ and $d 2$ correspond to the value of the 'distance' parameter for each of the two weakly bound neutrons (corresponding to the instance between them and the alpha-particale). d3 corresponds to the 'distance' parameter describing the separation between the two weakly-bound neutrons. In this configuration d1=d2 and a single 'width' parameter is used for each point. This can lead to a 0 - state when spin-orbit coupling is used, rather than to a $0+$.

We can again refer to the spherically averaged one-and two-body density distributions to get an idea of the structure provided by the wavefunction. These are displayed in figures (5-10) and (5-11)


Figure (5.10) The one - body density distribution for ${ }^{6} \mathrm{He}$. The wavefunction was obtained for the $S 3$ interaction, while $S=0, T=1$ and $L=0$. The parameter $d 1$ and $d 2$ are the ones of equation (5.21) d1 is related to the distance of the di - neutron from the alpha- particle, while d2 to distance between the two neutrons. $W$ is the width parameter.

In the case of the two-body density, the logarithmic graphs of figure (5-11) clearly demonstrate the tail effect on the alpha-particle probability distribution.


Figure(5.11) The two -body density distribution for ${ }^{6} \mathrm{He}$. The wavefunction was obtained for the S3interaction, while $S=0, T=1$ and $L=0$. The configuration is the same as that of figure (5.10)

### 5.3.3 ${ }^{8}$ Be

Within our approximation the case of two alpha-particles, corresponds to the nucleus of ${ }^{8} \mathrm{Be}$. Although, ${ }^{8} \mathrm{Be}$ is not a bound system we wish to examine it since by adding one more neutron we have ${ }^{9} B e$ that is a bound halo nucleus. This will be examined later on. The choice we make for the reference state of ${ }^{8} B e$ is to add together two translationally invariant alpha-particle wavefunctions correlated by a function depending on the relative distance between the two alpha-particles centers-of mass. The reference function can have the form :

$$
\Phi_{L}^{\text {ref }}=\Phi_{\alpha_{1}} \Phi_{\alpha_{2}} f\left(r_{\alpha 12}\right) y_{L}^{M}\left(r_{\alpha 12}\right) .
$$

where

$$
\begin{align*}
& r_{\alpha_{1}}=\frac{1}{4}\left(r_{1} \rightarrow+r_{2}+r_{3}+r_{4}\right) \\
& r_{\alpha_{2}}^{\overrightarrow{2}}=\frac{1}{4}\left(r_{5} \vec{~}+r_{6}+r_{7} \vec{~}+r_{8}\right) .  \tag{5-22}\\
& r_{\alpha_{12}}=\left|r_{\alpha_{1}}-r_{\alpha_{2}}\right| . \tag{5-23}
\end{align*}
$$

The purpose of the function $f\left(r_{\alpha_{12}}\right)$ is to correlate the two alpha with each other while $y_{L}^{M}\left(r_{\alpha 12}^{\rightarrow}\right)$ is a angular wavefunction(spherical harmonic),

$$
\begin{equation*}
y_{M}^{L}\left(r_{\alpha_{12}}^{\rightarrow}\right)=r_{\alpha_{12}}^{L} Y_{M}^{L}(\theta, \Phi) . \tag{5-24}
\end{equation*}
$$

The assigns angular dependence to one alpha-particle with respect to the other. Thus the reference function for ${ }^{8} B e$ is the same as that of ${ }^{5} \mathrm{He}$ with the only difference that $\mathrm{r}_{5}$ is replaced by $r_{\alpha_{2}}$. The choice we make for $f\left(r_{\alpha 5}\right)$ is again in terms of spherical shells, where

$$
\begin{equation*}
f\left(r_{\alpha_{12}}, d, \omega\right)=\exp \left(-\alpha^{2} \frac{\left(r_{\alpha_{12}}-d\right)^{2}}{\omega^{2}}\right) . \tag{3-25}
\end{equation*}
$$

A selection of the results that can be obtained for the ground stale energy as a function of $d$ and $w$ are displayed in figure (5-12). Two different values for the orbital momentum were used $(\mathrm{L}=0)$. Again we made use of the S 3 interaction. The pattern appearing is similar to that of 5 He . For small values of the width $\omega$ the energy depends on the values of d and L . however, as $\omega$ becomes large enough the dependence on the other parameters vanishes. Furthermore, there is not a stationary
value but the energy approaches the limit corresponding two non-interacting alphaparticles. Therefore, we can conclude that in the J-TICI(2) approximation 8 Be is not a bound system.


Figure (5.12) The ground-state energy for the state-independent J-TICI(2)calculation of ${ }^{8} B e$ for $\mathbf{L}=\mathbf{0}$ using the S 3 interaction. The broken line corresponds to twice the alpha-particle ground-state energy for the same type of calculation. The value of $w$ is in relative units (i.e. scaled fm) since is multiplied by the harmonic oscillator parameter

Again we can make use of one-and two-body density distribution to get an idea of the structure provided by the different variational parameters. The results for the spherically averaged one-and two-body density distributions are displayed in figures (5-13) and (5-14), for orbital momentum values of $L=0$, the density distributions were taken for a fixed value of the distance parameter $d$. although $d$ does effect the density distributions, as in the case of the energy the width $\omega$ is the driving parameter.

This is an indication that the two alpha-particles prefer to be separated from each other. When orbital momentum is present the one-body density distribution becomes broader, something that further indicates the breaking of the ${ }^{8} B e$ nucleus into two alpha particles. This is not unexpected since the presence of the orbital momentum provides a distribution around the axis of symmetry and thus reducing the probability of finding a nucleon at the center-of-mass.


Figure (5.13) the one-body spherically-averaged density distribution of ${ }^{8} B e$. The wavefunction was obtained using the $S 3$ interaction for the $L=0$ state. The density distributions were obtained for the several values of $w$ for a fixed valued of $d$. The arrow indicates increasing values of $w$.

In the case of the two-body distribution we get a more pronounced tail effect than the previous cases of ${ }^{5} \mathrm{He}$ and ${ }^{6} \mathrm{He}$. This is indicated in figure (5-14) furthermore, the presence of orbital momentum provides secondary maxima to the distribution indication that the system tend to break into distinct structures, as is illustrated in the figure (5-14).


Figure (5.14) the logarithmic spherically averaged two-body density distribution of ${ }^{8} \mathrm{Be}$
For the $\mathbf{L}=\mathbf{0}$ states. The wavefunction was obtained for the $\mathbf{S 3}$ interaction.

### 5.3.4 ${ }^{9} \mathrm{Be}$

We can obtain the nucleus of ${ }^{9} \mathrm{Be}$ by adding one neutron to the configuration of ${ }^{9} \mathrm{Be}$. When we add one more nucleon e.g, 9 Be then one possibility for $\Phi_{L, S, T}^{\text {rel }}$ is:

$$
\begin{equation*}
\Phi_{L S, T}^{r e l}=\Phi^{L}\left(r_{9}^{\rightarrow}\right) R_{1}\left(r_{\alpha_{1} \alpha_{2}}\right) R_{2}\left(r_{\alpha 19}, r_{\alpha 29}\right) . \tag{3-26}
\end{equation*}
$$

Where $r_{9}$ is coordinate of the additional nucleon with respect to the system center of mass, while ${ }^{r_{\alpha 19}}$ and ${ }^{r_{\alpha 29}}$ are it's coordinates with respect to the two alpha-particles. Increasing the number of weakly bound neutrons greatly complicates the structure of $\Phi_{L, S, T}^{\text {rel }}$ as well as the required coupling. However, we will only deal with three cluster systems where the number of weakly bound neutrons is restricted to two. Furthermore, working with an alpha particle not confined in the scalar $0+$ state would involve further implications.

This case is very similar to that of ${ }^{6} \mathrm{He}$ where instead of an alpha-particle and two neutrons, we have two alpha-particles and one neutron. The reference function can be composed from that of equa. (5-20) for ${ }^{8} B e$ by adding a term correlating the additional neutron with the two alpha-particles:

$$
\begin{equation*}
\Phi_{L}^{\text {ref }}=\left(\Phi_{\alpha_{1}} \Phi_{\alpha_{2}} f_{1}\left(r_{\alpha 12}\right)\right) f_{2}\left(r_{\alpha 19}\right) f_{3}\left(r_{\alpha 29}\right) y_{L}^{M}\left(r_{\alpha 12}, \overrightarrow{r_{\alpha 2}}, r_{9}^{\rightarrow}\right) \ldots \tag{5-27}
\end{equation*}
$$

where

$$
\begin{array}{r}
r_{\alpha 19}=r_{\alpha 1}-r_{9} . \ldots . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . ~ \tag{5-28}
\end{array} .
$$

The functions $f_{1}, f_{2}$ and $f_{3}$ are of identical from and like before are given in terms of spherical shells, each characterized by a different set of variational parameters. $f_{2}$ and $f_{3}$ adjust the position of the weakly bound neutron with respect to each of the alpha-particles, while $f_{1}$ adjusts the separation between the two alpha-particles. The inclusion of orbital momentum is more complicated than before. The function describes the angular momentum dependence of the wavefunction and in general depends on the coordinates of the two-alpha-particles and that of the additional neutron in a translationally invariant way.

There are two possible schemes for the inclusion of angular dependence corresponding to two distinct physical situations. One possibility is where we have the orbital momentum of the additional neutron with respect to the center-of-mass of the ${ }^{8} B e$ subsystem $\left({ }^{9} B e \approx^{8} B e+n\right)$. In this case

$$
\begin{equation*}
y_{L}^{M}\left(r_{\alpha 12}, r_{\alpha 2}, r_{9}\right)=y_{M}^{L}\left(r_{p}\right) . \tag{5-29}
\end{equation*}
$$

$$
\begin{equation*}
r_{9} \overrightarrow{ }=r_{9} \overrightarrow{-1} 2\left(r_{\alpha 1}+r_{\alpha 2}\right) \ldots \tag{5-30}
\end{equation*}
$$

There is no restriction as a rest of permutation symmetry in the possible values of $L$ arising from this coupling.

On the other hand we can have the orbital momentum of the additional neutron with respect to one of the alpha-particles and then couple this to the orbital momentum of the other alpha-particle , i.e.,

$$
\begin{align*}
y_{L}^{M}\left(r_{\alpha 1}, r_{\alpha 2} \overrightarrow{ }, r_{9}\right) & =\left[y_{m 1}^{l 1}\left(r_{\alpha 19}\right) \otimes y_{m 2}^{l 2}\left(r_{\alpha 2}\right)\right]_{M}^{L}  \tag{5-31}\\
& =r_{\alpha 2}=r_{\alpha 2}-\frac{1}{9} \sum_{i=1}^{9} r_{i}
\end{align*}
$$

In general the orbital momentum is a linear expansion over different combinations of $l_{1}$ and $l_{2}$ that can be coupled to $L$. this coupling must be symmetric with respect to the two alpha-particles.

In figures (5-15) and (5-16) we illustrate the results from the ground state energy and the spherically averaged density distributions respectively. Again we made a selection for the variation parameters that is conclusive for the behavior we used the variation parameters the $S 3$ interaction and set $L=0$.


Figure(5.15) The ground-state energy of ${ }^{9} \mathrm{Be}$ using the S 3 interaction for $\mathrm{L}=0$. The parameters d 1 and d2 are related to the separation of the additional neutron from each of the two alpha-particle, while d3 is the separation between the two alpha-particles. The width parameter $w$ is in relative units since is multiplied by the harmonic oscillator parameter.


Figure(5.16) The one - and two- body spherically-averaged density distribution of ${ }^{9} \mathrm{Be}$. The waefunction was obtained using the $\mathbf{S 3}$ interaction for the $\mathrm{L}=0$ the density distributions were obtained for several values of $w$.

As in the case of ${ }^{5} \mathrm{He}$ the calculation indicates that ${ }^{9} \mathrm{Be}$ by two correlated alphaparticles is not a bound structure, at least within our approximating

### 5.4 Three-body correlations

As we have seen the trail form of our wavefunction was not adequate to bind the nuclei of ${ }^{6} \mathrm{He}$ and ${ }^{9} \mathrm{Be}$, unless we artificially changed the potential function. We expect that the major reason for this is the absence of spin-isopin coupling in our Hamiltonian. However, there exist further improvements in the correlation mechanism and the reference state, that might also influence the results. The reference function is confined to include an alpha-particle $0^{+}$state in our calculation and it would be interesting to examine the effect of improving the correlation mechanism.

The linear TICI(2) part of the correlation operator consists of pair correlation between all particles, while the non-linear Jastrow part consists of products of pair correlation functions. We can enrich the correlation mechanism by adding linear three-body correlations.

As discussed in chapter 2 the J-TICI(2) method is sufficient for the alphaparticle. Nevertheless we examine the inclusion in our cluster-like model since it can provide further evidence of what might be necessary for a successful calculation. The purpose is to examine whether the inclusion of linear three body terms can radically change the results obtained for the $\mathrm{J}-\mathrm{TICI}(2)$ method.

Figure (5-17) illustrates through some selected configuration the effect that three body correlations have on the variational behavior of the calculation. We can clearly see that the overall behaviour is not changed, despite some local changes in the binding energy .


Figure(5.17) The ${ }^{6} \mathrm{He}$ grround-state energy in the J -TTIIICI(2) calculation and the J-TICI(2) with added three-body correlations (JJ-TICI (2)+J-TICI(3)), for different values of the width parameter w . The results were obtained for the S3 interaction.

We can see that although the three body correlations contribute to the total result, this is only by a very small amount. Both figures (5-17) and (5-18) demonstrate that the contribution of linear three body correlation will not radically change the results, i.e., produce a bound wavefunction.


Figure(5.18) The ground-state energy for the $\mathrm{J}-\mathrm{TICI}(2)+\mathrm{J}-\mathrm{TICI}(3)$ calculation of ${ }^{6} \mathrm{He}$ as a result of the total number of linear components used. The first four components (left-hand side of the vertical broken line) include only two-body correlations while the remaining components (right-hand side of the broken line) include the added three-body correlation. The results were obtained for the S3 interaction.

We extended the variation method discussed in chapter 3 beyond the alphaparticle. Although the number of variation parameters is in some case considerably large, we could restrict the calculation into selected sets of these parameters. Despite the restrictions the results we obtained are conclusive. Furthermore, we could make use of the one and two body density distributions to get a qualitative picture of the wavefunction.

The general approximation scheme can be summarized as follows:
$i$ - One major approximation in the model is the alpha-particle that is kept in the $0^{+}$ state. In terms of the many body trail wavefunction it implies that a restricted
configuration is available. This can be illustrated in terms of the Young tableau.
The reference state should in general be a superposition of several of the above structures. Our approximation for the alpha-particle restricts the calculation to a single structure. Inclusion of a multi reference can be examined in the future.
ii- We have restricted the calculation to include only local scalar semi-realistic interactions. It is possible that a more realistic type of interaction will alter the results. However, inclusion of the further types of interactions in the results is not a problem at all, since it only involves a small change in the numerical algorithms.
iii- We examined two body and a naive three body correlation mechanism. There is still the possibility of improving the correlation mechanism. We avoided using statedependent correlations, a part from the case of ${ }^{5} \mathrm{He}$, where the effect is shown in figure (5-19), where we can see that dependence does not effect the nature of the results.


Figure(5.19) The ground state energy of ${ }^{5} \mathrm{He}$ using the S 3 interaction for state-dependent and stateindependent correlations. The width parameter $w$ is in relative units since is multiplied by the harmonic oscillator parameter

Although state-dependent correlations lower the binding energy they do not provide a
linear correlation mechanism beyond that of pair correlations but rather improve the choice for such terms. It is likely that inclusion of state-dependence in the correlation mechanism will not provide a variational stationary point. The reason for avoiding state-dependence is due to the efficiency of the numerical algorithm when these are present. Furthermore, it is not difficult to write a computer program that can lead with the state-dependence. Never the less no conclusive statement can be made for the correlation mechanism and it can be one of the reasons contributing to the failure of our approximation.

## 1-1 Introduction

Although nuclear physics has a long tradition the exact theory of nuclear forces is not yet knows and thus a number of different phenomenological models are in use. At low energies $(\sim 1 \mathrm{MeV})$ the nucleus behaves like a quantum object and has been the subject of theoretical studies since the birth of quantum mechanics.

Recent advancements in experimental techniques have probed extreme types of nuclear structures not previously known, termed "exotic nuclei" Amongst such structures are the "halo" nuclei and occur all over the periodic table, ranging from light to heavy nuclei, This research is restricted to the case of light nuclei.

The lightest nuclei can be treated by calculating the full many-particle wavefunction with a Hamiltonian where interaction fits the nucleon-nucleon interaction [Ber04].

Before studying the approximation method, discussing the nuclear Hamiltonian and the difficulties involved in determining its eigeinstates In Ref.[Car90] found the traditional description of the nucleus as a system of non-relativistic nucleons interacting.

In a microscopic methods are based on basic principles of quantum mechanics, such as the treatment of all nucleons, with exact antisymmetrization of the wavefunctions. [Des04]

The Hamiltonian of an A- nucleon system is

$$
\begin{equation*}
H=\sum_{i}^{A} T_{i}+\sum_{i<j}^{A} V_{i j}+\sum_{i<j<k} V_{i j k}+\ldots . \tag{1-1}
\end{equation*}
$$

Where $\mathrm{T}_{\mathrm{i}}$ is the kinetic energy of nucleon i and $V_{i j}$ is an effective nucleon-nucleon interaction.[Des01]

The solutions of the schroedinger equation [Car90]

$$
H|\Psi>=E| \Psi>\ldots \ldots . .(1-2)
$$

## 1-2 Methods of the Nuclear Many-Body Problem

As result of the complexity of the many-body problem it is usually only approximately solved but these may not always be easy to interpret in physical terms [Alm04].

There are a large number of methods available for attacking the many-body problem and it is beyond our scope to give a general description of such methods

In general these are methods that can be used to solve the many-body schrodinger equation in a non-relativistic approximation [Car90].

## 1-2-1 The Resonating - Group Method

The resonating-group method allows treating reactions in a fully microscopic.
In a fully microscopic description of nuclear reactions the physics must in principle be entirely derived from a many body Hamiltonian involving the nucleons of the system.

However, since the corresponding schrodinger equation cannot be solved exactly models [Hes02]. In the RGM, the many-nucleon wavefunction is taken to be totally antisymmetric and describes the motion of nucleons grouped into clusters [Tan01]. The resonating-group method (RGM) provides an accurate microscopic description of collisions between light nuclei [Hes02].

Two important subjects in the field of the microscopic RGM. These subjects are (1) the study of reaction mechanisms in nuclear systems, and (2) the study of exchange effects in nuclear reactions [Yos94]. The RGM is devised to provide approximate wavefunctions of a many-body problem involving a microscopic Hamiltonian $H$ depending on the coordinates, moment a and spins of nucleons [Hes02]. This Hamiltonian contains the kinetic energies of all nucleons and potentials (usually effective potentials) acting between them.

The scattering of two nuclei is described in partial wave by the RGM wavefunction

$$
\Psi_{\mathrm{fm}}=\mathrm{N} \Phi_{1} \Phi_{2}{y_{1}}^{\mathrm{m}}(\Omega) \mathrm{r}^{-1} \mathrm{y}(\mathrm{r}) \quad(1-3)
$$

Where N is an anti symmetrization operator. The internal wave functions $\Phi 1_{(i=1,2)}$ of the colliding nuclei (also named clusters). The vector $\mathrm{r}=(\Omega . \mathrm{r})$ is relative coordinate between the cluster centers of mass. The relative function $U(r)$ is unknown

When the trail function in equa.(1-3) is introduced in a variational calculation, obtains the RGM equation.

$$
H_{l} u_{l}=E N_{l} u_{l}(1-4)
$$

With the condition $u_{l(0)}=0$ the Hamiltonian operator $H_{l}$ is defined by

$$
H_{l} u_{l}=r\left(\Phi_{1} \Phi_{2} \mathrm{y}_{1}^{\mathrm{m}}|H| \Psi_{l m}\right)
$$

And the overlap kernel $N_{l}$ by

$$
N_{l} u_{l}=r\left(\Phi_{1} \Phi_{2} \mathrm{y}_{1}^{\mathrm{m}} \Psi_{l m}\right)
$$

[Hes02]

## 1-2-2 The Generation- Coordinate Method

A numerical procedure is introduced which allows us to extract a collective Hamiltonian. The starting point is a microscopic many-body approach, namely the GCM. [Ga181]

For an A-particle system, a trial wave function is constructed of the form $\Psi\left(\times_{1}, \ldots \times_{n}\right)=\int \Phi\left(\times_{1}, \ldots, \times_{n} ; a\right) f(a) d a$.The preliminary nucleonic wavefunction, $\phi$, solves the probme in a "construction potential". This potential depends upon a "generator coordinate", a. the collective wave function, $\mathrm{f}(\mathrm{a})$, or "generator function", is folded into $\phi$ to produced a system wavefunction that depends only upon the coordinates, xi, of the particles.

In typical cases when the generator function contains one or more nodes, it generates nodes in the system wavefunction $\Psi$ of the kind that describe collective kinetic energy. The energy of the system is extreme with respect to choice of the generator function. $f(a)$ no Hamiltonian ever appears except the A-particle Hamiltonian.

All nucleons are treated on the same basis whether in or above closed shells. The appropriate variational calculation leads to an integral equation or "generator wave equation" for $\mathrm{f}(\mathrm{a})$ [Jam57].

$$
\int d a^{\prime}\left(\times_{1}, \ldots, x_{n} ; a\right) H^{\wedge} \Phi\left(\times_{1}, \ldots, x_{n} ; a^{\prime}\right)=E \int d a^{\prime} \Phi\left(\times_{1}, \ldots, x_{n} ; a\right) \Phi^{*}\left(\times_{1}, \ldots, \times_{n}\right) f\left(a^{\prime}\right) \ldots \ldots . . . . . . .(1-5)
$$

That is known as the "Hill-wheeler equation", if the collective wavefunction occurring in the Griffin -Hill -Wheeler integral equation is slowly varying, the equation can be transformed into a schrodinger equation [Ban72]. The numerical treatment of the Griffn -Hill-wheeler equation is studied in a solvable model.[Gal78]

The properties of the subspace of the many-body Hilbert space, which are associated with the use of the generator coordinate method in connection with one-parameter and with two conjugate parameter families of generator states [Jam57]. The RGM and GCM are exactly equivalent [Hes02].

The GCM equation is an integral transform of the RGM one. Differences only appear in the difficultly of derivation of the integral kernels of both methods and in the techniques of numerical resolution. The derivation of the GCM kernals is much simpler because if can be based on well-known properties of slater determinants [Hes02]

## 1-2-3 No Core Shell Models

The no-core shell model (NCSM) is an ab initio configuration interaction (CI) approach based on effective interactions derived from realistic two- and three-nucleon interactions [Rod06,Dea ].

The no-core shell model is abased on a new variation of the well known shell model for nuclei. Historically shell - model calculations have been made assuming a closed inert core of nucleons with only a few active valence nucleons. The interaction of these valence nucleons with the core and with other valence nucleons could not be described by microscopic interactions, as they have been developed for few-nucleon systems, until 1990 with the development of the NSCM, which treats all nucleons in the nucleus as active particles. One starts with the relative Hamiltonian for all a nucleons and add the Harmonic - Oscillator (Ho) centor-of-mass potential

$$
\begin{gathered}
H_{c m}^{H o}=\widehat{T}_{r e l}+V \ldots \ldots \ldots .(1-6) \\
H_{c m}^{H o}=\frac{\hat{P}^{2}}{2 m}+\sum_{i<i} V_{N N}^{\Omega}(i j)
\end{gathered}
$$

Where $-V_{N N}^{\Omega}$ can be any realistic nucleon - nucleon potential.
Where
$\Omega$-Harmonic Oscillator frequency
P-momentum
M - mass of nucleons
The modified Hamiltonian facilitates the use of the convenient HO basis. The strong correlations of the bare nucleon-nucleon interaction, however, lead to slowly converging results in the HO basis. This problem can be solved by deriving an effective A-body Hamiltonian, $H_{\text {eff }}$ in a truncated (model) space from the full HO space. The model space and the excluded space are such that ${ }^{H_{\text {eff }}}$ does not have any matrix elements between the two. For practical purposes $H_{\text {eff }}$ must be further approximated.

In general the no-core shell model is a microscopic approach for a calculating nuclear property [Nar00, Bar03]

## 1-2-4 Correlation Basis Function Theory

The correlated basis function (CBF) theory is one of the most promising many-body tools currently under development to attack the problem of dealing with the complicate structure (short range repulsion and strong state dependence) of the nuclear interaction. The CBF has a long record of applications in condensed matter physics. In nuclear physics the most extensive use of CBF has been done in infinite nuclear and neutron matter [Fab00].

We solve the many-body schrodinger equation by using the variational principle [Fab00].

$$
\begin{equation*}
S E[\Psi]=S \frac{\langle\Psi| H|\Psi\rangle}{\langle\Psi \mid \Psi\rangle}=0 \tag{1-7}
\end{equation*}
$$

 body correlation operator, $\mathrm{F}(1,2, \ldots \mathrm{~A})$, to the model basis functions, $\bar{\phi}_{(1,2, \ldots \mathrm{~A})}$ [ Fab01, Ari96, Fab97]

$$
\Psi(1,2, \ldots A)=F(1,2, \ldots A) \Phi(1,2, \ldots A)(1-8)
$$

Where the operator F is intended to take care of the dynamical correlations, where as the model wavefunctions, ${ }^{\Phi}$, include anti symmetrization effects [Fab99, Bis07]

A correlated wavefunction having spin-isopspin dependent, central and tensor correlations has been used within the correlated basis functions (CBF) theory.

Furthermore, the CBF. With state dependent correlations was used to investigated the ground-state properties of the closed shell nuclei 16 O and 40 Ca using realistic nucleonnucleon interaction including tensor components. [Fab97, Ale03]

## 1-2-5 Greens Function Monte Carlo

Monte Carlo methods are procedures used to investigate the sampling distributions of various statistics and to determine the effects of violating underlying assumptions. The Monte Carlo method can be used to closely approximate the solutions to many probability problems [Dav ].

Monte Carlo methods as applied to few and many-body quantum systems, and in particular to few-body problems in nucleon physics [Car90].

The first application of Monte Carlo Methods to nuclei interacting with realistic potentials was a Variational Monte Carlo (VMC) calculation. We describe this method in some detail in chapter four [Bar03].

The first step to model a nucleus is a VMC calculation to obtain an approximate solution of the many-body schrodinger equation. The basis of the variational approximation is the fact that the real ground-state wavefunction of a Hamiltonian has the lowest energy $E_{\odot}$ of all possible wavefunctions and thus a normalized trail function $\Psi_{V}$ has an energy

$$
\begin{equation*}
\mathrm{E}_{\mathrm{v}}=\frac{\left\langle\Psi_{V}\right| H\left|\Psi_{V}\right\rangle}{\langle\Psi \mid \Psi\rangle} \geq E_{o} \tag{1-9}
\end{equation*}
$$

Variation of the expansion coefficient Ck of a trail function $\Psi_{V}=\Sigma_{k} C k \mid K$ of states $|K\rangle$. with specific spin and isospin in to minimize the expectation value of the Hamiltonian from the nuclear model, leads to the approximate solution. This is the n used as the starting point for the GFMC calculations, which are based on the propagation of the wavefunction under the Hamiltonian, that means [Rod06].

GFMC takes the VMC trial state and evolves it in imaginary time[Car06].
The evaluation of $\exp \left[-\left(H^{\wedge}-E_{o}\right) \tau\right]$ is made by introducing small time step, $\Delta \tau=\tau / n$ and n is the total number of integrated steps. In limit n .,$\Psi_{\text {ois the ground state wavefunction }}$ with exact eigen energy Eo.

$$
\Psi(\tau)\left\{\exp \left[-\left(H^{\wedge}-E_{o}\right) \Delta \tau\right]\right\}^{n} \Psi_{v}=G^{n} \Psi_{v} \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots . .(1-11)
$$

Where G is the short-time green's function.
In general , Monte Carol methods is applied in the nuclear physic and particular for the evaluation of realistic interactions but at the being are restricted to light nuclei due to the complexity of the many-body problem.

## 1-3 Halo Nuclei and Neutron Dripline

A many the isotopes of the lightest elements in the nuclide chart, halo nuclei are the most exotic ones. These halo nuclei consist of a compact core nucleus consistent to the classical picture plus one or several weakly bound nucleons orbiting the inner core with relatively large distances [Gep].

Therefore, halo nuclei are very weakly-bound exotic states of nuclear matter in which the outer one or two valence nucleons (usually neutrons). [Kha ].Several nuclei near the drip lines have been found to have properties which are strikingly different from those of their stable counter parts. These nuclei have a halo structure in their ground states in which loosely bound valence nucleons have a large spatial extension with respect to the respective core [Raj].

Nuclei are composed of two types of interacting fermions, giving rise to a specific degree of freedom, isospin. Therefore, there are magic numbers for both neutrons and protons. [Bec06] Here describe the neutron halo.

Most of the halo nuclei are located close to the neutron drip line and are considered as a core plus a pain of external neutrons [Des01].The neutron halos have been observed in nuclei near the neutron drip line by reaction measurements with intermediate and highenergy radioactive nuclear beams [Tan96].

Therefore the neutron drip line is a concept in particle and nuclear physics. An unstable atomic nucleus beyond the neutron drip line will leak free neutrons. In other words, the neutron drip line is the line on the Z N plane (represent the diagonal).

In general halo structures are characterized by a very low ( $<1 \mathrm{MeV}$ ) Separation energy of the last neutron, and are therefore candidates for halo nuclei. [21] A schematic of the lightest nuclei with halo structures is shown in fig (1-1) [Oza01]


Figure (1-1):The lightest known halo nuclei

Studies of resonances are indispensable for understanding the unique properties of dripline nuclei. Although it is easy to solve resonances of two-body systems, resonances of three-body systems such as the so-called Borromean systems are not simple, because
various kinds of open channel structures appear. For example $6 \mathrm{He}=4 \mathrm{He}+\mathrm{n}+\mathrm{n}$ which is a typical Borromean system, the 9Li $+\mathrm{n}+\mathrm{n}$ model in the first stage presents a serious problem of the binding energy of 11 Li , since such a subsystem 5 He is not bound.

6 He and 11 Li can be described by a model involving the effect of at least three interactions, namely the interaction of each of the two weakly-bound neutrons with the alpha-particle and the interaction between the two neutrons, [Kiy01]. In this thesis we used a cluster model of studying light nuclei, where our main objective is its application to light Borromean system.

## 1-4 Existing Models For Halo Nuclei

Different kinds of theoretical models are currently being used to investigate the halo structure. One of the early works on halo nuclei was an intermediate between shell model calculations and fully microscopic ones, is the so called "cluster-orbital shell model" [Suz98, Suz90, Yos90]. This model employs a wave function of the alpha-cluster form but uses a Hamiltonian which is not fully microscopic.

Over the past few years, a number of review articles covering the field of halo nuclei, from both experimental and theoretical [Kha ].

The field of halo nuclei study of nuclear structure almost twenty years after their discovery. But the field actually begin in 1985 with the Berkeley experiments carried out by Tanihata and his group in which they measured the interaction cross sections of 9 He and 11 Li isotopes and found much larger values for the rms matter radii than would be predicated by the normal A1/3 dependence [Kha ]

The empirical evidence suggests that neutron pairing plays an important role for the stability of nuclei near the neutron drip line by Hansen and Jonsen in 1987 [Han87]
T. Otsuka et al., [Ots93], proposed a variational shell model in order to describe the structure of such nuclei. The model was applied to 11 Be , where by using a Skyrme interaction the observed ground state of this nucleus was reproduced correctly. In general mean field approximations proved to be restricted validity because of the weak binding of the halo neutrons. It was realized that a more realistic approach to the halo structure would rely on microscopic many-body models. After about 1991 a large amount of theoretical
research treating halo structure in such a manner has been going on. An account of all of the current research is impossible, but an outline of main type of models used is described in the rest of this section.

The approximate three-body approach is used to explore the structure of 11Li. This "Borromean" system is discussed with reference to the similar system 6 He for which information on the binary subsystems is more complete in 1992 by M.V. Zhukov, D.V. Fedorov. In 1995 the P. Descouvemont study the 14Be nucleus is investigated in the three cluster generator coordinate method, involving several $12 \mathrm{Be}+\mathrm{n}+\mathrm{n}$ configuration.

The 12Be core nucleus is described in the Harmonic oscillator mode with all possible configurations in the p shell [Des95], and so P. Descouvemont study in 1998 the 11Be nucleus is investigated in the GCM using $10 \mathrm{Be}+\mathrm{n}$ microscopic wavefunction. The 10 Be wavefunction are defined in the Ho model with all p-shell configurations [Des]

More recent work on ${ }^{6} \mathrm{He}$ involves the improvement of the RGM three-cluster wave function, to an "extended three-cluster model" [Des]. The aim is to improve the description of the alpha-particle core, by assuming that is composed of a three-cluster as state and a single nucleon. This results in the inclusion of a $t-t$ (triton-triton) configuration in the initial $(\alpha+n+n)$ model (pure three cluster model) allowing for a core breakup configuration caused by the halo neutrons. The main conclusion of this paper was that the precise value of the energy as well as other properties of a halo nucleus require a realistic treatment of the core.

This was based upon showing that a $(t-t)$ inclusion affects the tail behavior of the core thus effecting the binding of the halo nucleons. The number of existing many-body methods and models for the few-body problem is too large to summarize in just one chapter. We have mentioned only a few and in particular those related to our problem. The numerical accuracy and sophistication of the various methods and models used is constantly improving.

In chapter Chapter Two we examine the coupled cluster method and its truncation to a linearized version.

This is enhanced by the addition of central Jastrow correlations. We pay attention in the inclusion of state-dependent correlations.

The method is examined by applying it to the alpha-particle, where comparison can be made with other methods.

Chapter three describes the cluster model that we shall make use of. Particular emphasis is given to the inclusion of the correct symmetry properties and in particular permutation symmetry. Some types of semi-realistic nucleon-nucleons interactions are discussed.

Chapter four deals with the numerical method. This is a rather technical chapter. The fact that we are using the VMC. Implies that the error estimate is statistical. We ensure that the statistics are "healthy", in the sense that we get a reliable error estimate. The results of the cluster model for a few light nuclei are given in chapter five, while chapter six contains the conclusion and a discussion for possible extensions of this research.

## 1-5 Motivations for this research

This thesis is aimed to an investigation of the low-energy nuclear many-body problem by making use of a number of quantum many-body techniques.

In this thesis we will develop a cluster model of studying light nuclei, where our main objective is its application to light Borromean system, and study some physical properties of the light nuclei,

## 2-1 Introduction

In this thesis we are concerned with the approximation of the few body Schrödinger equation in terms of a linear variational problem. The most basic ingredient in such an approximation is the construction of the trail wavefunction. One way of doing this is by appropriately approximating some rather complicated, usually non-linear parameterization. One type of such a parameterization is given by the coupled cluster model (CCM).

Cluster-structures are interesting phenomena in nuclear physics. Alpha-clusters have been broven to exist in light to heavy nuclei. In light nuclei, other clusters are also expected to play an important role in nuclear structure [Nak03].

The first part of this chapter gives a brief description of the CCM wavefunction and the ways of performing approximations appropriate to our study.

Another type of non-linear parameterization of the many-body wavefunction that is variational in nature is the Jastrow method [Jas95, Gua79, Gua97]. We also provide a brief discussion of this technique and ways of approximating it.

The effectiveness of the approximation scheme is illustrated by considering the calculation for the ground-state of the alpha-particle. For this purpose we quote results from a number of authors as well as our own, we also examine the calculation of the oneand two-body density distributions that can be used to provide qualitative information about the wavefunction.

## 2-2 Coupled Cluster method

The coupled cluster method (CCM) is a non-perturbative microscopic method for approaching the many-body problem.

Cluster methods are derived for open-shell many-fermion systems, for energies, wavefunctions, expectation values, and effective transition operators [Bra67].

Coupled-cluster theory was first introduced in nuclear physics by Coester and Kummel in the early 1960s. [Dea, Gua97]

Initial nuclear structure applications come in the mide 1970s with several papers from the Bochum group [Dea].

During the last three years the scientist developed a set of powerful theoretical tools for the description of nuclear properties in a many-body frame work known as CC theory[Dea05]

Coupled-cluster theory is size extensive, which means that only linked diagrams enter into a given computation. This is not true in typical shell-model particle-hole truncation schemes. [Dea ]

It is based on describing the correlations in terms of exponentiated independent excitations, which are parameterized as multi-configurationally creation operators with respect to some suitable reference state [Wal03]

## 2-2-1 Reference states

In the case of many-body problems it is often convenient to introduce the idea of reference states. In general a set of reference states, $\left\{\Phi_{i}>; i=0,1, \ldots, D\right\}$ is used, where the orthonormality condition $\left\langle\Phi_{i} \mid \Phi_{j}\right\rangle=\delta_{i j}$ can be assumed to be satisfied (since it can always be imposed). The reference states form the basis of a $D$-dimensional subspace of the full Hilbert space referred to as the "model space".

In the case of the coupled cluster model (CCM) the reasoning behind the introduction of these reference states is that the set $\mid \Phi_{i}>$ can act as starting functions, from which we can construct the full wavefunction by the action of correlation operators. A non-degenerate ground state corresponds to the case of a single reference state $D=0$ and is referred to as the "single-reference" version of the CCM.

The reference state should be constructed to obey the symmetries of the exact groundstate; while the correlation operators of CCM can be scalar operators that do not carry any numbers (this is not necessary but is the simplest case). Furthermore, it is always convenient for such a state to have any analytic description. Since a large part of the CCM will require calculations involving the reference function alone. When
considering a many-fermion system, a non-interacting many-body wavefunction or ground state can often be described by a Slater determinant. Such a state can serve as the reference state. It is well known that in the language of second quantization a Slater determinant can be written as

$$
\left|\Phi_{o}\right\rangle=\prod_{i=1}^{N} a_{v_{i}}^{+} \mid 0>
$$

$\qquad$

Where $N$ is the number of particles and the $a_{v_{i}}^{+}$are fermions creation operators that obey the usual anticommutation relations and are defined by their action on the vacuum state $|0\rangle$.

The occupied single particle states $\left\{\left.\right|_{i}>; i=1,2, \ldots, N\right\}$ are referred to as hole states,

Once a reference state is provided in terms of a Slater determinate with respect to a set of hole states $\left\{\mid v_{i}>\right\}$, a more general determinant that mixes particle and hole states is provided by Thouless theorem, where

$$
\left.\left|\Phi>=e^{S_{1}}\right| \Phi_{o}\right\rangle
$$

$\qquad$ (2-2)

The operator $S_{1}^{\wedge}$ is a one-body operator which acts on $\mid \Phi>$ to produce a oneparticle/one hole ( $1 p-1 h$ ) excitation. In the notation of particle/hole states it has the explicit form

The new reference state $\left|\Phi^{\prime}\right\rangle$ is non-orthogonal to the original state $\left|\Phi_{o}\right\rangle$.

### 2.2.2 The exp (S) expansion

The coupled-cluster method, also called the $\exp (s)$ expansion.
The basic idea of coupled-cluster method is that the correlated many-body wavefunction $\Psi$ may be obtained by application of a correlation operator s, such that

$$
\left|\Psi>=e^{S_{1}}\right| \Phi_{o}>\ldots . . . . . . . . . . . . . . . . . . . . . . . .(2-3) \mid
$$

Where $\mid \phi_{>}$is a reference slater determinant chosen a a convenient starting point [Dea07, Wal 06]

$$
\begin{equation*}
S^{\wedge}=\sum_{n=1}^{N} S_{n}^{\wedge} \tag{2-4}
\end{equation*}
$$

Is the cluster correlation operator, sum of operators of the form

$$
S_{n}=\frac{1}{\left(n_{1}\right)^{2}} \sum_{\rho_{1} \ldots \ldots \rho_{n}}<\rho_{1} \ldots . \rho_{n}|S n| 0, \ldots, 0>a_{\rho_{1}}^{+} \ldots a_{\rho_{n}}^{+} a_{\rho_{o}}^{n}(2-5)
$$

[Gua97]
As a result of the fermionic anticommutation properties

$$
\begin{equation*}
\left\{a_{\rho_{i}}^{+}, a_{v j}^{+}\right\}=\delta_{i j} \delta_{\rho v}, \quad\left\{a_{\rho_{i}}, a_{v_{j}}\right\}=0, \tag{2-6}
\end{equation*}
$$

$\qquad$

The time-dependent Schrödinger equation for the ground state wavefunction $\left|\Psi_{o}\right\rangle$ is $H\left|\Psi_{o}>=E_{o}\right| \Psi_{o}>\ldots \ldots . . . . . . . . . . . . . . . . . . . . .(2-7) ~$
where $H$ is a many-body Hamiltonian. As described in the previous section the exact ground state $\left|\Psi_{o}\right\rangle$ can be expanded in terms of a model state ${\left|\Phi_{o}\right\rangle}$ and states orthogonal to $\left|\Phi_{o}\right\rangle$, resulting from the dynamical correlations induced by $H$. Thouless theorem allows the inclusion of the simplest, correlations in terms of $1 \mathrm{p}-1 \mathrm{~h}$ excitations.

The ground state energy Eo are obtained by solving set of formally exact coupled nonlinear equation

$$
E_{o}=<\Phi_{o}\left|e^{-s^{\wedge}} H^{\wedge} e^{s^{\wedge}}\right| \Phi_{o}>\ldots \ldots . . . . . . . . . . . . . . . . . . . . .(2-8) ~
$$

The exponential character of equation (2.3) is an important characteristic of the CCM. As a result of the commutation of the operators in equa. (2.4) the CCM exponential parameterization obeys size-extensively [Dea07] and a set of coupled non linear equations for the unknown coefficients $S_{I}$

$$
<\Phi_{o}\left|c_{I} e^{-s^{\wedge}} H^{\wedge} e^{s^{\wedge}}\right| \Phi_{o}>=0, \forall I \neq 0 \ldots \ldots \ldots \ldots . . . . . . . . . .(2-9)
$$

A very important property of equations (2.8) and (2.9), arising from the exponential representation employed by the CCM, is that the expansion of the terms with in the expectation value is of finite order. This is a result of the nested commutator expansion for the term $\left(e^{-s^{\wedge}} H^{\wedge} e^{s^{\wedge}}\right)$ which has the form

$$
e^{-\hat{s}} H e^{\hat{s}}=\hat{H}+\left[\hat{H}, \hat{S}_{1}\right]+\left[\hat{H}, \hat{S}_{1}\right]+\frac{1}{2}\left[[\hat{H}, \hat{S}], S_{1}\right]+\frac{1}{2}\left[\left[\hat{H}, \hat{S}_{2}\right], S_{2}\right]+\left[\left[\hat{H}, \hat{S}_{1}\right], \hat{S}_{2}\right]
$$

The above expansion is of finite order due to fact that $\hat{H}$ is finite. Although the equations for the ground state energy are of finite order it is necessary for practical purposes to further approximate due to the complexity of the many body problem. The simplest way of doing this is by performing a $\operatorname{SUB}(\mathrm{n})$ truncation. This implies that all parameters $\left\{S_{I}\right\}$. Which describe correlations of clusters of more than $n$ particles-hole pairs, are set to zero. Thus equation (2.4), would be approximated in the $\operatorname{SUB}(3)$ truncation by

$$
\begin{equation*}
S^{\wedge} \approx S_{1}^{\wedge}+S_{2}^{\wedge}+S_{3}^{\wedge} . \tag{2-10}
\end{equation*}
$$

### 2.2.3 Translational Invariance

A problem that can arise in the CCM formalism when performing a $\operatorname{SUB}(n)$ truncation is due to possible symmetry violations. In general the symmetries obeyed by the exact system should also be present in the approximated system, unless the effect on the calculated quantity is with in same accepted limits.

The CCM wavefunction is described in terms of the action of a cluster operator on some reference function, which takes into account the required symmetry properties of the system under consideration. In the application to finite systems, one faces with the wellknown center of mass motion problem.

The proper treatment of the center of mass in the framework of CCM was initiated at the so-called $\operatorname{SUB}(2)$ leve of approximation. It has been shown in these references that the center of mass is properly removed using appropriate combinations of one and two body
operators, and describing the refrence function in terms of single-particle harmonic oscillator wavefunctions.

In general the single particle HO wavefunction is a product of a radial part and an angular part, which can be represented as

$$
\langle r \mid n l\rangle=U_{n l m}(r) Y_{l m}(\theta, \Phi) .
$$

$\qquad$ (2-11)

In the above equation the function $U_{n l m}(r)$ is given in term of the Laguerre polynomial, while $Y_{l m}(\theta, \Phi)$ is a spherical harmonic.
such reformulation of the CCM is called translationally invariant, coupled-cluster (TICC) method, [Gua97]

The CCM is most naturally formulated in the occupation number representation
with the requirement of both translational and rotational invariance. These are:
i- The $S_{1}$ operator cannot occur on its own, otherwise it would violate translated invariance. This requires the coefficients $\left\{S_{1}\right\}$ and $\left\{S_{2}\right\}$ to be coupled, resulting in the transformation of the cluster operator as

$$
S \approx S_{1}+S_{2} \rightarrow S^{(1,2)} \ldots \ldots \ldots \ldots \ldots \ldots \ldots . . . . . . . . . . . .(2-12)
$$

The terms are easily excluded by the simple device of taking $\exp (1,2)$ operator in normal-ordered form so that the TICC2 ansatz for the wavefunction can be finally written as

The reason for the inclusion of the normal order, is due to the fact higher powers of $S(1,2)$ occurring in the exponential would otherwise excite the CM.

The above formulation based on the $\operatorname{SUB}(2)$ level of approximation can be extended to higher order approximation [Dea07] To solve the schrodinger equation

$$
\begin{equation*}
H|\Psi>=E| \Psi> \tag{2-14}
\end{equation*}
$$

To obtain the equations for the amplitudes is to project directly the shcrodinger equation with the ansatz [Gua97]

$$
H^{\wedge}: e^{S(1,2)^{\wedge}}: \mid \Phi>=E: e^{S(1,2)^{\wedge}}: \Phi>
$$

And the ground state energy [Gua97]

$$
\begin{equation*}
E=<\phi\left|H: e^{s(1,2)}:\right| \phi> \tag{2-16}
\end{equation*}
$$

. The cluster operators used in CCM were originally introduced by using the notation of second quantization. In the case of translational invariance, these cluster operators were shown to have a general representation in coordinate space, depending only on the relative coordinates of the involved particles.

This so-called translationally invariant configuration interaction method was applied in ref [Gua96] to calculate at the $\mathrm{SUB}(2)$ level (or TICI2 approach). The main conclusion of this work is that the TICI2 methodology provides a very resonable starting point for the calculation of the binding energies of light-to-medium nuclei. For interactions and correlations of theV4 form, as displayed in the above equation, the TICI2 results are In suitable agreement with ones provided by other methodologies [Gua96]

$$
\begin{equation*}
<r_{1} r_{2} r_{3} r_{4}\left|S^{(1,2)}\right| \Phi_{o}>=2\left(\sum_{i<j} S_{1,2}\left(r_{i j}\right)\right)<r_{1} r_{2} r_{3} r_{4} \mid \Phi_{o}> \tag{2-17}
\end{equation*}
$$

In the above equation the coordinate dependence of the cluster correlation function $S_{1,2}$ is only on the relative coordinates $r_{i j}$,

Although the functional form of the correlation operators could be derived for this simple case, it is by no means guaranteed that this will be possible for the general case, due to the complexity of the many-body problems. However we can generalize the result obtained as an approximation for the coordinate representation of cluster operators [Bis90, Bis93, Gua98], that will preserve translation invariance.

An alternative was is to go to coordiante representation, where

$$
\begin{equation*}
\Psi\left(r_{1}, \ldots, r_{N}\right)=\left(1+\sum_{i<j} f\left(r_{i j}\right)+\frac{1}{2!} \sum_{i<j} \sum_{k<l}^{l} f\left(r_{i j}\right) f\left(r_{k l}\right)+\ldots\right) \Phi\left(r_{1}, \ldots, r_{N}\right) . . \tag{2-18}
\end{equation*}
$$

This equation preserve the essential features of the TICC by an additional constraint imposed a summation and denoted by a prime, indicating that no repeated indices can occur when multiple summations are required. The $f\left(r_{i j}\right)$ are the coordinate representations
of the system and preserve the overall symmetry of the reference function. The above correlation functions can be viewed as producing independent clusters on coordinate space.

The benefit in using the above formalism is in the freedom it provides for approximately choosing the functional form the correlation operators, a according to the problem in equation. For example in the case of equation (2.18) the easiest method is to approximate the two body correlation function $f\left(r_{i j}\right)$ in terms of Gaussin non-orthogonal functions [Bis93], of the form

$$
f\left(r_{i j}\right)=\sum_{n=1}^{n_{\max }} A_{n} \exp \left(-b_{n} r_{i j}^{2}\right) \ldots \ldots \ldots \ldots \ldots . . .(2-19)
$$

The finite value ${ }^{n_{\text {max }}}$ indicates a truncation, as necessary for practical calculations. The coefficients An can now be determined by a numerical calculation or in the case of a linear approximation as the linear coefficients of a generalized eigenvalue problem. The parameters bn,

Although alternative approach have been carried out in order to obtain an optimal functional representation for the correlation functions [Bis93], the particular choice of a Gaussian expansion has been proven to be the best. The TICI is linearise a translational invariant form of CCM

The TICI a voids the complications of the full cluster expansion and was found to provide a very reasonable staring point for the calculation of binding energies of light-tomedium nuclei [Gue98]. The wavefunction of both TICC and TICI can be used to solve the CCM equations (2.8) and (2.9). A variational approach for the binding energy is also possible, giving an upper bound to the estimated energy.

Therefore, the simplest linear approximation for a many body wave function, is given in the frame work of $\mathrm{TICI}(2)$ by

$$
\begin{equation*}
\left.\Psi\left(r_{1}, \ldots r_{N}\right) \approx\left(1+\sum_{i<j}\left(r_{i j}\right)\right) \Phi_{o}\left(\left\{r_{i j}\right)\right\}\right) \Phi_{o}(R) . . \tag{2-20}
\end{equation*}
$$

Provided that the reference state $\Phi_{o}$ can be factor into the product of intrinsic and center of mass part.

### 2.3 Jastrows method

Jastrows method was desinged for the treatment of quantum mechanical systems for N identical particles.

Jastrow's method, which is essentially a combination of cluster expansion and variational techniques has further been studied by Iwamoto and Yamada, Aviles and others [Ali68]. In order to obtain a variational wavefunction using CCM we have to greatly approximate, the full wavefunction as illustrated in equation (2.20).

One way of significantly improving the structure of a many body wavefunction in the case of extended strongly interacting system is that of Jastrow [Jas95]. The method has been adopted for finite systems and applied to a number of light nuclei [Bis93].

### 2.3.1 The general approach

In a system of finite size the wavefunction localizes the particles around the center-ofmass. If the interaction is strongly repulsive at short distance the wavefunction should be very small or even null when any of the relative particle-particle distances, ${ }^{i j}$, vanishes for any pair (ij). Furthermore, when anyone of the particles moves away from the rest the independent particle motion should be preserved.

In the original Jastrow approach a correlated particle wavefunction is decomposed as
where $\Phi_{o}$ is a starting function that incorporates all of the single particle characteristic. [Wal03]. And $f_{J}\left(r_{i j}\right)$ is the product of a Jastrow correlation factor

The choice for the factors $f_{J}(r i j)$ will depend on the problem in question. The simplest choice is to assume functional form for the $f_{J}$ which depend on several parameters. The optimal choice for these parameters is the one that minimizes the expectation value of the Hamiltonian. However, according to the problem in question the $f_{J}$ can incorporate state dependence in terms of operators. A discussion for the inclusion of state dependence is given in [Gua98].

The most general form for the $f_{J}$ is

$$
\begin{equation*}
f_{J}(i j)=1+\sum_{m, p} a_{m, p} g_{m}\left(r_{i j}\right) O_{p}^{\wedge}(i j) . \tag{2-22}
\end{equation*}
$$

where $g_{m}\left(r_{i j}\right)$ are suitable function of the relative coordinates, while the $O_{\rho}^{\wedge}\left(r_{i j}\right)$ are operators acting on the pair (ij). A very common choice for the $g_{m}$ is in terms of Gaussians

The correlation depth $a_{m, p}$ and $g_{m}$ are to be determined by the variational problem[Gua98].

The operators $O_{p}^{\wedge}(i j)$ are, apart from the identity operator, can be chosen to be the exchange operators of spin, isospin and spin-isospin labels. This choice is suitable for a scalar state-dependent potential, since the same operators can be added, such as tensor operators.

### 2.3.2 Jastrow-TICI variational wavefunction

The physical problem of describing many interacting identical particles from a microscopic point of view can be attacked using a number of techniques. For a nuclear system the Jastrow method describes the wavefunction in terms of the product of two-body correlations between all pairs of nucleons acting upon a suitable reference state [Gua98].

This can be enhanced by combining TICC with a Jastrow variational function. This way short rang correlations are accounted for by the Jastrow factors while the TICC correlation operators take abound of the medium to long range effects. The easiest scheme is that where Jastrow and $\operatorname{TICI}(2)$ are combined [Bue02], referred to as the J-TICI (2) scheme. Such a formalism is similar to that of the correlated operators acting on the wavefunction. In the $\mathrm{J}-\mathrm{TICI}(2)$ formalism the variational trial wavefunction is given by the product of a linear TICI (2) operator (FL) with the non-linear Jastrow factor $\left(F_{J}\right)$ as

$$
\begin{aligned}
& \Psi_{J-T I C I 2}=F_{J} F_{L} \Phi_{o} \text {.......................................................(2 - 24) } \\
& =\prod_{i<j} f_{J}(i j)\left(1+\sum_{i j} f_{T I C I 2}(i j)\right) \Phi_{H O} \cdots \cdots .
\end{aligned}
$$

where the latter equation is the specific form we shall mostly make use of in which a Harmonic oscillator reference function, $\Phi^{\text {но }}$, takes care of translational invariance.

The Jastrow factor depends only on the distance between pair of nucleons [Bue04]

## 2-4 The alpha particle

It is consist of two protons and two neutrons bound together into a particle identical to a helium nucleus it can be written $4 \mathrm{He}[\mathrm{Ale} 08]$. The alpha particle wavefunction is the most important ingredient of the calculation scheme and is important that an adequate structure is provided. The fact that this wavefunction can be obtained in a separate calculation is extremely convenient. One of the main assumptions in our model is that the alpha particle will be described by a spin-isospin saturated state i.e., by a $0+$ ground state.

The alpha particle has been one of the starting points for the discussion and testing of various microscopic methods and in particular the CCM, Jastrow method and J-TICI. In this section a comparison of this methods as applied to the alpha particle is made.

## 2-4-1 TICC and TICI methods

One of the major concerns in the description of light nuclei is the center-of-mass motion. The TICC provides a unique way of dealing with this problem by employing HO reference states that are separable into relative and center of mass parts. The bosonic $0+$ state of ${ }^{4} \mathrm{He}$ was extensively described in [Bis90] in the TICC(2) approximation and its linear version $\operatorname{TICI}(2)$, where the general expression equa. (2-16) for the wavefunction was derived. The calculations were performed in the HO basis in view of what they imply for standard shell-model calculations. A sample of the results is shown in table (2.1).

Table 2.1:This table shows the results taken from [Bis90] for the ground state energy in MeV of ${ }^{4} H e$ in the (TICC (2)) and (TICI (2)) calculation using the $S 3$ (winger part) and MT-V potentials. The correlation functions were expanded in terms of the oscillator basis and nmax is maximum principle oscillator number at which the expansion of the correlation function was truncated.

| $S 3$ |  | MT-V |  |  |
| :---: | :---: | :---: | ---: | ---: |
| nmax | TICI(2) | TICC(2) | TICI(2) | TICC( |
|  | -5.375 | -5.379 | -3.347 | -3.640 |
| 10 | -17.695 | -17.818 | -17.181 | -17.65 |
| 20 | -24.462 | -24.634 | -24.445 | -24.78 |
| 29 | -25.294 | -25.473 | -27.769 | -27.06 |
|  |  |  |  |  |

A remarkable result is that for such a finite system as ${ }^{4} \mathrm{He}$ the relatively simple linear version TICI of CCM can provide good results, even at the lowest level of approximation. Although it was found that the TICC(2) calculation is more efficient than its related shellmodel ones the final conclusion was that pursuing such calculations in the oscillator representation is not efficient due to convergence problems.

The work of Ref.[Bis90] high lighted the fact that in order to make such calculations efficient it is necessary to concentrate on the coordinate representation of the cluster function. In the case of the linear TICI (2) the optimal form of the correlation function equ. (2-12) was obtained via an Euler-Lagrange approach [Bis92], a rather cumbersome process. Instead, by making the simpler choice of expanding the correlation functions in terms of Gaussian functions, identical result can be obtained in much more efficient way and certainly less computationally demanding [Gau91].

Further more the idea of the Gaussian basis can be extended to give a variational TICC calculation beyond $\operatorname{TICI}(2)$ by employing double Gaussian expansion and so on [Gau91] for example the TICC(2) wavefunction has the general form

$$
\begin{align*}
& \Psi_{T I C I(2)}=\left(1+\sum_{i<j} f(i j)+\sum_{i<j} \sum_{k<l} f(i j) f(k l)\right) .  \tag{2-25}\\
& f(i j)=\sum_{v=1}^{v_{\max }} A_{v} \exp \left(-\beta_{v} \tau_{i j}^{2}\right) \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots . . . . . . . . . . . . . . . . . . \tag{2-26}
\end{align*}
$$

In the description of ${ }^{4} \mathrm{He}$ up to now the cluster operator were state independent
For the TICI(2) method [Gue96] where the correlation operator had the form

$$
f(i j)=f_{c}\left(r_{i j}\right)+f_{\sigma}\left(r_{i j}\right)\left(\sigma_{i} \cdot \sigma_{j}^{\vec{j}}\right)+f_{\tau}\left(\tau_{i}^{\rightarrow} \cdot \tau_{j}^{\vec{j}}\right)+f_{\sigma \tau}\left(r_{i j}\right)\left(\sigma_{i} \cdot \sigma_{j}^{\vec{j}}\right)\left(\tau_{i} \cdot \tau_{j}^{\vec{j}}\right) \ldots . \ldots \ldots \ldots \ldots \ldots . . .(2-27)
$$

Where $\sigma$ and $\tau$ are the spin and isospin matrices respectively. The results given by the authors are displayed in table 2.2, where there is a significant increase in the binding energy for the case of S3 and MS3 potentials. This is due to the fact that these potentials contain different spin-isospin terms unlike the B1 and MT-V potentials that contain only purely redial (Wigner) and space-exchange (Majorana) terms.[Gua98]

Table 2-2.: These results for the ground-state energy of ${ }^{4} \mathrm{He}$ nucleus (expressed in MeV ) were taken from [48]. The TICI(2) approximation was used performed both with state independent cluster operator (SI) and state dependent ones (SD)

| Method | Potential |  |  |  |
| :---: | :---: | :---: | :---: | :---: |
|  | B1 | S3 | MS3 | MT-V |
| TICI(2) SI | -37.86 | -25.41 | -25.41 | -29.45 |
| TICI(2) SD | -37.86 | -28.19 | -27.99 | -29.45 |

The inclusion of state dependence on cluster operators can be arbitrarily extended in principle so as include any type of operators including non central ones. However, the calculations become greatly complicated and particular in going beyond a spin-isospin operator was achieved [Gue98],

## 2-4-2 Jastrow-TICI methods

We have seen that the application of cluster operator directly in coordinate representation can be very powerful for the description of ${ }^{4} \mathrm{He}$. There is a close relation between these correlations and the Jastrow factors. If we consider the state independent case where the Jastrow wavefunction $\Psi_{J}$ is parameterized by a single Gaussian, this can be expanded as

$$
\begin{aligned}
& \Psi_{J}= \prod_{i<j}\left(1-a \exp \left(-b r_{i j}^{2}\right)\right) \Phi_{o} \ldots \ldots \ldots . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . ~ \\
& \hline
\end{aligned}(2)
$$

Where the prime indicates that the labels k and $l$ are distinct from i and j .
Despite the restrictions in the coefficients the Jastrow variational wavefunction can achieve better results than the state dependent $\operatorname{TICI}(2)$ or the high order state independent cluster expansions.

This was done in Ref. [Gua98], where an expansion up to two Gaussians was used, examining both state dependent and state independent cases for the ground state of ${ }^{4} \mathrm{He}$. The same spin-isospin operators as in equation (2.25) were used. These results are shown in table (2.3).

Table 2-3: Results from [Gua98] for the ground state energy of ${ }^{4} \mathrm{He}$ using the Jastrow variational wavefunction. The SD stands for state dependent correlations, while the SI for state independent ones.

| Potential | Correlation | Energy (Mev) |
| :---: | :---: | :---: |
| S3 / MS3 | SI | -24.4042 |
| S3 | SD | -25.3539 |
| MS3 | SD | -25.3119 |
| S3 / MS3 | SI | -27.2136 |
| S3 | SD | -29.9378 |
| MS3 | SD | -29.7034 |
| MT-I/ III,MT-V | SI | -29.0604 |
| MT-I /III | SD | -29.3460 |
| MT-I / III,MT-V | SI | -30.8752 |
| MT-I / III | SD | -32.0107 |

Rewrite the correlation factors with a simpler state dependence, the ansatz equa.(2-20) becomes:[Gua98]

$$
\begin{equation*}
f_{J}(i j)=1+\sum_{m=1}^{N_{\beta}} e^{-\beta_{m} r_{i j}^{2}}\left[a_{m, c}+a_{m, \sigma} P_{\sigma}^{\wedge}(i j)\right] . \tag{2-29}
\end{equation*}
$$

With central scalar and spin-exchange constituents only. The state independent study is performed, as usual, by setting

As long as central state-independent correlations are concerned the TICI and Jastrow methods provide similar results. When state dependent is include in either the Jastrow or $\mathrm{TICI}(2)$ methods there is a considerable improvement in the calculation of the binding energy.

The simplest way of doing this is by combining central state- independent Jastrow and the state dependent $\operatorname{TICI}(2)$ methods. The alpha-particle can be used as a model to examine the effectiveness of such an approach. These calculations were performed in [Gue98] using improved and extended the application of this method, using the variational Monte Carlo to calculate the matrix elements

## 2-5The linear eigenvalue Problem

## 2-5-1- Matrix elements

The key ingredient of the J-TICI (2) approximation is the linear dependence on the spin and isospin operators, something that gives a very similar formalism to that of state- independent approximation. For completeness we give a description of the linear eigenvalue problem that arises since it will be used all over this thesis. The description is valid for an arbitrary system and is not confined to shell nuclei. For simplicity we restrict our selves to central scalar correlations and to local scalar interactions (to be discussed in detail later on).

In the linear J-TICI(2) approximation the wavefunction is given as[Bue04]

$$
\Psi=F_{L}^{\wedge} \Phi . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . ~(2 ~-~ 30) ~(~) ~
$$

Where $\Phi$ is the part wavefunction that carries all the required quantum numbers, while $F_{L}^{\wedge}$ is the linear operator of the $\mathrm{TICI}(2)$ approximation. For compactness we have absorbed the state independent Jastrow factor (same as in equa. (2.22) but without the state dependence) in the function $\Phi$, giving

$$
\begin{gathered}
\Phi=F_{J} \Phi_{o} \ldots \ldots . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . ~ \\
\hline
\end{gathered}
$$

$\Phi_{o}$ is the model function which will depend on the system in question. For the alpha particle this is the $0^{+} \mathrm{HO}$ ground state parameterized by a single non-linear parameter $\alpha$.

In order to obtain the g.s. energy compute the mean value of the Hamiltonian [Gua98].

$$
\begin{equation*}
\widehat{H}=\frac{h^{2}}{2 m} \sum_{i=1}^{A} \nabla_{i}^{2}+\sum_{i=1}^{A} \widehat{V}\left(x_{i}, x_{j}\right) \tag{2-33}
\end{equation*}
$$

The potential $\widehat{V}$ is a two-body operator that dependes on the relative spatial coordinate and the spin-isospin degrees of freedom of each pair of nucleons.

The interaction employed here have V4 structures which will be transformed to an exchange-operator basis as in the case of the correlation [Gua98]

$$
V=V_{o}+V \sigma+V_{\tau}+V_{\sigma \tau} \ldots \ldots . . . . . . . . .(2-34)
$$

Apart from $V_{o}$ the potential terms depend $s$ on the spin $\sigma$ and isospin $\tau$ variables. The particular form of an individual term such as $V_{\sigma}$ is:

$$
\begin{equation*}
V_{\sigma}=\sum_{i<j} v_{\sigma}\left(r_{i j}\right) P_{i j}^{\sigma} . \tag{2-35}
\end{equation*}
$$

with $r_{i j}$ representing the radial distance between particles $i$ and $j$, while $P_{i j}^{\sigma}$ is an operator that exchanges the spin labels of particles $i$ and $j$ accordance with the interaction the correlation operator F takes the form:

$$
\begin{equation*}
F_{L}^{\wedge}=F_{o}^{\wedge}+F_{\sigma}^{\wedge}+F_{\tau}^{\wedge}+F_{\sigma \tau}^{\wedge} . \tag{2-36}
\end{equation*}
$$

As a result of the $\mathrm{TICI}(2)$ formalism the individual terms are parameterized as:

$$
F_{k}^{\wedge}=\sum_{i<j} f_{k}\left(r_{i j}\right) P_{i j}^{k} .
$$

$\qquad$
Where $\mathrm{k}=0$ for $F_{o}{ }^{\wedge}$ the identity operator $\mathrm{k}=1$ and 2, F 1 and F 2 represent the spin and isospin operator

The function $f_{k}(r)$ and $g_{J}(r)$ are parameterized as a linear combination of Gaussians,

$$
\begin{align*}
& f(r)=1+\sum_{n=1}^{N} C_{n} e^{-d n r^{2}}  \tag{2-38}\\
& g^{(k)}(r)=\sum_{m=1}^{M} a_{m}^{(k)} e^{-b m r^{2}} \tag{2-39}
\end{align*}
$$

Note that the expectation value of the Hamiltonian is quadratic form in $a_{m}^{(k)}$ and therefore their optimum values can be obtained by solving a generalized elgenvalue
problem. The values of the non-linear parameters, bm are not very relevant as long as one uses a significant number of Gaussians to expand $g(r)$. The parameters of the Jastrow correlation function, $C_{n}$ and $d_{n}$ [Bue02]

The eigenvalue problem can be solved by linear variations of the expectation values on the expansion components with the additional constraint that the wavefunction has a finite form:

$$
\begin{equation*}
\frac{\partial}{\partial c_{n}}\left(\langle\Psi| H^{\wedge}|\Psi\rangle-E_{o}<\Psi|\Psi\rangle\right)=0 \quad \forall n . \tag{2-40}
\end{equation*}
$$

Following [Bue06], the expectation value can be written as

$$
\begin{gathered}
\langle\psi| \hat{H}|\psi\rangle=\int d R \psi^{*} \hat{H} \psi \\
=\sum_{x} \int d R\left\langle\Phi_{o}\right|\left(\hat{F}_{L} \hat{F}_{J}\right)^{+}\left|R \chi_{\sigma \tau}\right\rangle\left\langle R \chi_{\sigma \tau}\right| \hat{H} \hat{F}_{L} \hat{F}_{J}\left|\Phi_{o}\right\rangle
\end{gathered}
$$

Where the $R_{i}$ spatial part $R_{i}=R_{n l m}(r)=R_{n l}(r) Y_{m}(\theta, \Phi)$
And spin-isospin part, $\quad \chi_{\sigma \tau}=\chi_{\sigma} \chi_{\tau}$
In matrix form we have to solve a $4 M \times 4 M$ dimensional generalized eigenvalue problem of the form:

$$
\left[\begin{array}{cccc}
H_{0}^{0} & H_{\sigma}^{0} & H_{\tau}^{0} & H_{\sigma \tau}^{0}  \tag{2-41}\\
H_{0}^{\sigma} & H_{\sigma}^{\sigma} & H_{\tau}^{\sigma} & H_{\sigma \tau}^{\sigma} \\
H_{0}^{\tau} & H_{\sigma}^{\tau} & H_{\tau}^{\tau} & H_{\sigma \tau}^{\tau} \\
H_{0}^{\sigma \tau} & H_{\sigma}^{\sigma \tau} & H_{\tau}^{\sigma \tau} & H_{\sigma \tau}^{\sigma \tau}
\end{array}\right]\left[\begin{array}{c}
C_{0} \\
C_{\sigma} \\
C_{\tau} \\
C_{\sigma \tau}
\end{array}\right]=E_{0}\left[\begin{array}{cccc}
N_{0}^{0} & N_{\sigma}^{0} & N_{\tau}^{0} & N_{\sigma \tau}^{0} \\
N_{0}^{\sigma} & N_{\sigma}^{\sigma} & N_{\tau}^{\sigma} & N_{\sigma \tau}^{\sigma} \\
N_{0}^{\tau} & N_{\sigma}^{\tau} & N_{\tau}^{\tau} & N_{\sigma \tau}^{\tau} \\
N_{0}^{\sigma \tau} & N_{\sigma}^{\sigma \tau} & N_{\tau}^{\sigma \tau} & N_{\sigma \tau}^{\sigma \tau}
\end{array}\right]\left[\begin{array}{c}
C_{0} \\
C_{\sigma} \\
C_{\tau} \\
C_{\sigma \tau}
\end{array}\right]
$$

These will depend on the quantum numbers of the model state and will be discussed in detail in the next chapter

## 2-5-2 The alpha particle

If we only consider the spin-isospin saturated state corresponding to the ${ }^{4} \mathrm{He}$ the calculation greatly simplifies. As a result of the spatial symmetry of the ${ }^{4} \mathrm{He}$ ground state and the anti symmetry of the total wavefunction [Ann05]

The exchange operator for the spatial coordinate can be defined through the relation

$$
P^{r} P^{\sigma} P^{\tau}=-1
$$

Since the wave function has to be antisymmetric under the interchange of all coordinates of particles 1 and 2. $P^{\tau}$ can be rewritten [Ann05]

$$
P^{\tau}=-P^{r} P^{\sigma}
$$

therefore, the nucleon-nucleon interaction has the form:

$$
V=V_{o}+V_{\sigma}
$$

and thus the alpha particle wave function has that similar form:

$$
|\Psi\rangle=\left(F_{o}^{+}+F_{\sigma}^{+}\right)|\Phi>| \chi_{\sigma \tau>}>
$$

$\qquad$
where $\left|\chi_{\sigma \tau}\right\rangle$ is just a Slater determinant of the spin and a isospin variables.
The spin-isospin saturated Slater determinant can be expressed by the action of a normalized anti symmetrization operator on a single state,

$$
\begin{aligned}
&\left|\chi_{\sigma \tau}\right\rangle= A++,+-,-+,->, \ldots . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . ~ \\
&(2-43) \\
&=A|0\rangle
\end{aligned}
$$

where $( \pm, \pm)$ refers to the state of the isospin and spin variables of a particular nucleon (up or down). Both operators $\hat{F}_{0}$ and $\hat{F}_{\sigma \text { commute with A }}$

The expectation values of the spin exchange operators are:

$$
\begin{equation*}
\left\langle\chi_{\sigma \tau}\right| P_{i j}^{\sigma}|0\rangle,\left\langle\chi_{\sigma \tau}\right| P_{i j}^{\sigma} P_{k l}^{\sigma}|0\rangle,\left\langle\chi_{\sigma \tau}\right| P_{i j}^{\sigma} P_{k j}^{\sigma} P_{m n}^{\sigma}|0\rangle, \tag{2-44}
\end{equation*}
$$

The key point in the above expectation values is that the action of the exchange operators on the ket state $|0\rangle$ will give zero unless the resultant ket state is different from $|0\rangle$ only by a permutation in which case the expectation value is the parity of that permutation. A sample of such expectation values is shown in table 2-4.

Although the above way provides a systematic method of obtaining the expectation values for the exchange operators the cost of missing some important simplifications. Furthermore, on has to devise an efficient algorithm to perform such a counting process since the number of terms to be considered will rapidly increase with the number of particles. One major simplification that arises as a result of the saturated spin-isospin structure of the alpha particle is the fact that:

$$
\begin{equation*}
\left\langle\chi_{\sigma \tau}\right| P_{i j}^{\sigma}\left|\chi_{\sigma \tau}\right\rangle=\left\langle\chi_{\sigma \tau}\right| P_{i j}^{\sigma} P_{k l}^{\sigma} P_{m n}^{\sigma}\left|\chi_{\sigma \tau}\right\rangle=0 \tag{2-45}
\end{equation*}
$$

Table 2-4: some of the expectation values for the spin exchange operators of ${ }^{4} \mathrm{He} .<\mathbf{P}>$ denotes $\left\langle\chi_{\sigma \tau}\right| P|0\rangle$, with $|0\rangle=|++,+-,-+,--\rangle$, where for each pair $( \pm, \pm)$ the first symbol denotes the isospin and the second the spin.

| $i j$ | $<P_{i j}{ }^{\sigma}$ | $i j k \ell$ | $<P_{i j}^{\sigma} P_{k l}^{\sigma}>$ | $i j k \ell m n$ | $<\boldsymbol{P}^{\boldsymbol{\sigma}}{ }_{i j} \boldsymbol{P}^{\boldsymbol{\sigma}}{ }_{k l} \boldsymbol{P}^{\boldsymbol{\sigma}}{ }_{m n}>$ |
| :---: | :---: | :---: | :---: | :---: | :---: |
| 12 | -1 | $12 \quad 12$ | 1 | $12 \quad 12 \quad 12$ | -1 |
| 13 | 1 | 1213 | -1 | $12 \quad 12 \quad 13$ | 1 |
| 14 | 0 | 1214 | 0 | $\begin{array}{llll}12 & 12 \quad 14\end{array}$ | 0 |
| 23 | 0 | 1223 | 0 | 122334 | 1 |
| 24 | 1 | 1224 | -1 | 142434 | 1 |
| 34 | -1 | 1234 | 1 | 122434 | 0 |

something not immediately obvious from the solution of equations (2-76). These results will be derived in detail in a later and are of central importance to the extension of this method to more complicated systems where the complexity that can be avoided is of crucial importance. The key concept is the decomposition of the total wavefunction into states of conjugates permutation symmetry and the further decomposition of these states into spin/isospin states belonging to $\mathrm{SU}(2)$ symmetry.

As a result of the mentioned simplification the matrices of the generalized eigenvalue problem reduce to :

$$
\left(\begin{array}{cc}
\left(\hat{K}+V_{0}\right)_{0}^{0} & \left(V_{\sigma}\right)_{0}^{0}  \tag{2-46}\\
\left(V_{\sigma}\right)_{0}^{0} & \left(\hat{K}+V_{0}\right)_{\sigma}^{\sigma}
\end{array}\right)\binom{C_{0}}{C_{\sigma}}=E_{0}\left(\begin{array}{cc}
N_{0}^{0} & 0 \\
0 & N_{\sigma}^{\sigma}
\end{array}\right)\binom{C_{0}}{C_{0}}
$$

Where $K^{\wedge}$ and $V_{k}$ represent kinetic and potential block matrices. We carried out the above calculation using the VMC method for the spatial integrals. The results obtained for the ground state energy is given in table (2-5) for a number of local scalar interactions. The calculation is the same as the one performed by [Bue06]. This is due to the fact that we made use of a better approximation for the Jastrow factor, containing two Gaussian components rather than a single one. Furthermore, we used a different set of variational parameters.

Table 2-5: The J-TICI(2) method was applied for the ground state energy for ${ }^{4} \mathrm{He}$ (in MeV). A central state independent Jastrow factor was used together with a state-dependent TICI(2) part. The variational Monte Carlo Method was used.

| Potential | TICI(2) |  | J - TICI (2) |  |
| :---: | :---: | :---: | :---: | :---: |
|  | SI | SD | SI |  |
|  | SD |  |  |  |
| S3 | $-25.42 \pm 0.02$ | $-28.74 \pm 0.02$ | $-27.20 \pm 0.01$ | $-31.38 \pm 0.01$ |
| MS3 | - | $-28.76 \pm 0.02$ | - | $-31.36 \pm 0.01$ |
| B1 | $-37.93 \pm 0.02$ | - | $-38.400 \pm 0.03$ | - |
| MT - V | $-29.44 \pm 0.05$ | - | $-30.91 \pm 0.03$ | - |
| MT - I/ III | $-29.46 \pm 0.05$ | $-31.10 \pm 0.05$ | $-33.10 \pm 0.02$ | $-33.19 \pm 0.03$ |

In the case of the non-linear coefficients entering the expansion of the linear correlation operator we made the choice of a geometric series i.e.,

$$
\beta_{i}=k \beta_{i-}
$$

$\qquad$ . $2-47$ )
as a result of the convergence properties. The behaviour of the ground state energy with the number of components used to expand the linear correlation function is shown in Figure 2.1 (for the $S 3$ interaction). The same set of coefficients was used both for the state-independent and the state-dependent ones. In both cases the value for the contribution to the ground-state energy converges with a relatively small number of components. However, when the Jastrow correlations are considered the convergence of the calculation becomes smoother. The effect of the Jastrow factor can be viewed as a better reference state for the correlation operator to act on, since there is a difference of about 20 MeV between the result obtained with just a single component (only Jastrow).


Figure 2-1: The behavior of the ground state energy with the total number of components used to expand the correlation function was plotted for the TICI(2) and J-TICI(2) calculations for the S3 interaction. SI corresponds to the state-independent part while SD to the state one. The linear SD components (right part of broken line) were added to the linear SI components (left part of broken line) [Bue06].

## 2-5-3 Density Matrices

The representability problem consists in finding an intrinsic characterization of the range of the map from A-fremion wavefunctions to 2-body reduced density matrices. The problem was originally studied by C.N.Yang in connection with superconductivity [Yan62] and by A.J.Coleman in connection with quantum chemistry[Col63], where it is receiving renewed interest due to the fact that available partial results are beginning to be successfully exploited in numerical computations [Yan62].

If the wavefunction, $\Psi$, is normalized and fulfills the antisymmetry condition appropriate for fermions a series of density matrices of various orders can be defined as:

$$
\begin{gather*}
\gamma\left(x_{1}^{\prime} \mid x_{1}\right)=N \int \Psi^{*}\left(1^{\prime} 23 \ldots N\right) \Psi(123 \ldots . . N) d x_{2} d x_{3} \ldots . . d x_{N} \quad \ldots .(2-48)  \tag{2-48}\\
\Gamma\left(x_{1}^{\prime} x_{2}^{\prime} \mid x_{1} x_{2}\right)=\binom{N}{2} \int \Psi^{*}\left(1^{\prime} 2^{\prime} 3^{\prime} \ldots \ldots N\right) \Psi(123 \ldots \ldots N) d x_{3} d x_{4} \ldots \ldots d x_{N} \\
\ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots . . \\
\Gamma^{(P)}\left(x_{1}^{\prime} x_{1}^{\prime} \ldots x_{p}^{\prime} \mid x_{1} x_{2} \ldots x_{p}\right)=\binom{N}{P} \int \psi^{*}\left(1^{\prime} 2^{\prime} 3^{\prime} \ldots p^{\prime} \ldots N\right) \Psi(123 \ldots P \ldots N) d x_{P+1} d x_{P+2} \ldots d x_{N} \\
\ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots . . \\
\gamma^{(N)}\left(x_{1}^{\prime} x_{2}^{\prime} \ldots . x_{N}^{\prime} \mid x_{1} x_{2} \ldots . x_{N}\right)=\Psi^{*}\left(1^{\prime} 2^{\prime} 3^{\prime} \ldots . . N^{\prime}\right) \Psi(123 \ldots . . N)
\end{gather*}
$$

In the above equations $\chi_{i}$ represents all coordinates assigned to the $i t h$ particle including spatial $\left(r_{i}\right)$, spin $\left(s_{i}\right)$ and isospin $\left(t_{i}\right)$ degrees of freedom, while $d x_{i}$ represents both the volume element for the ith particle and any finite summations. The density matrices are ant symmetric for each pair of indices, thus they are symmetric for each pair of particle labels.It is easy to show from the definition that is compact, selfadjoint, nonnegative, trace class, and has trace $\binom{N}{P}$ (=number of p-tuples in the
system). (The latter comes from the widely but not universally used normalization factor in the definition). [Vol05]

We are only interested in the diagonal elements defined as :

$$
\begin{aligned}
& \Gamma\left(x_{1}, x_{2}\right)=\Gamma\left(x_{1} x_{2} \mid x_{1} x_{2}\right) \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots . . . . . . . . . . . . . .(2-50)
\end{aligned}
$$

These are positive definite and have direct physical interpretations. $\gamma\left(x_{1}\right) d v_{1}=$ number of particles $\times$ the probability for finding a particle within the volume $d v_{1}$ around the point $r_{l}$ having the spin $\left(S_{I}\right)$, etc, when all particles have arbitrary positions and spin. $\Gamma\left(x_{1}, x_{2}\right) d v_{1} d v_{2}=$ number of pairs $\times$ the probability for finding one particle within the volume $d v_{1}$ and another within the volume $d v_{2}$ at positions $x_{1}$ and $x_{2}$ respectively.

From the diagonal second and first order density matrices the pair correlation function as

$$
g\left(x_{1}, x_{2}\right)=\frac{\Gamma\left(x_{1}, x_{2}\right)-\gamma\left(x_{1}\right) \gamma\left(x_{2}\right)}{\gamma\left(x_{1}\right) \gamma\left(x_{2}\right)} .
$$

$g\left(x_{1}, x_{2}\right) d v_{1} d v_{2}$ is the difference between the conditional probability of finding a particle is at $\chi_{1}$ with the probability of the finding the particles at $\chi_{1}$ and $\chi_{2}$ independent of each other. The denominator acts as a weight, This difference can be interpreted as the correlation between the positions of particle pairs.

It would be nice if we could associate a pair of observables with the pair correlation function. In the general case the correlation between two observable $A$ and $B$ is given as:

$$
\begin{equation*}
g(A, B)=\frac{\langle A B\rangle-\langle A\rangle\langle B\rangle}{\langle A\rangle\langle B\rangle} \tag{2-52}
\end{equation*}
$$

In the case of the pair correlation function the operators in the place of A and B are $\delta\left(\bar{r}_{1}-\bar{r}_{1}^{\prime}\right) \delta_{s_{1}} \delta_{s_{1}}^{\prime}$ and $\delta\left(\bar{r}_{2}-\bar{r}_{2}^{\prime}\right) \delta_{s_{2}} \delta_{s_{2}}^{\prime}$ since the diagonal elements of the one and two body density matrices can be given as:
$\Gamma\left(x_{1}, x_{2}\right)=\int \Psi^{*}\left(1^{\prime} 2^{\prime} \ldots N^{\prime}\right) \delta\left(r_{1}^{\rightarrow}-r_{2}^{\rightarrow}\right) \delta_{s_{1} s_{2}} \delta\left(r_{1} \rightarrow-r_{2}^{\rightarrow}\right) \delta_{s_{2} s_{2}} \Psi\left(1^{\prime} 2^{\prime} \ldots N^{\prime}\right) d x_{1}^{\prime} \ldots d x_{N}^{\prime} \ldots$

Therefore, we can make use of related quantities that can be very easily obtained through Monte Carlo sampling. Instead of the pair correlation function we can make use of the spherically averaged one-and two-body densities, normalized to unity, defined for an N -body system as

$$
\begin{align*}
& \left.\rho_{1}(r)=\left\langle\frac{1}{N} \sum_{i=1}^{N} \frac{1}{r^{2}} \delta r-\right| r_{i} \rightarrow R^{\rightarrow}| |\right\rangle, \quad R^{\rightarrow}=\frac{1}{N} \sum_{i=1}^{N} r_{i}^{\rightarrow} . \\
& \rho_{2}(r)=\left\langle\frac { 2 } { N ( N - 1 ) } \sum _ { i < j } \frac { 1 } { r ^ { 2 } } \delta \left( r-\left|r_{i}^{\rightarrow}-r_{j}^{\rightarrow}\right|| \rangle \ldots \ldots . . . . . . . . . . . . .\right.\right.
\end{align*}
$$

Both $\rho_{1}$ and $\rho_{2}$ are translationally invariant quantities that can be used in order to provide quantitative information about a physical system and in general it is not easy to obtain these quantities analytically starting from correlated wavefunctions.

It is known in the HO model that the c.m. of the nucleons makes HO. To remove this motion it is necessary to introduce the intrinsic coordinate $\left(r_{i}-R^{\rightarrow}\right)$ instead of the coordinates $\left(r_{i}\right)$.

Where $R^{\rightarrow}=\frac{1}{N} \sum_{i=1}^{N} r_{i}^{\rightarrow}$ is the c.m. of the nucleons

Figure (2-2) shows the difference in the density distributions between the state-independent $\mathrm{TICI}(2)$ and the $\mathrm{J}-\mathrm{TICI}(2)$ formalism. While figure (2-3) shows the difference between state-dependent and state-independent correlations in both the $\mathrm{J}-\mathrm{TICI}(2)$ and $\mathrm{TICI}(2)$ methods. The presence of the Jastrow factor reduces the probability of finding a pair of particles close to each other by introducing short-range correlations, particularly in the presence of state dependent correlations. In the presence of a Jastrow factor there is not any significant difference between the density distributions both in the state dependent cases. Although the difference in binding energy between the state dependent $\mathrm{J}-\mathrm{TICI}(2)$ and $\operatorname{TICI}(2)$ methods is relatively small there is a significant difference in the short range effects of the two- body density distribution, something that emphasizes the importance of the Jastrow correlation.


Figure 2-2: The alpha-particle spherically averaged one- body and two-body density distribution for the TICI(2) and J-TICI(2) methods. The continuous line is for the one-body distribution while the broken line is the two-body one. The purpose of this graph is to show the difference between having and not having the Jastrow factor[Per55].


Figure 2-3:The alpha- particle spherically averaged one- body and tow- body density distribution for the TICI(2) and J-TICI(2) methods with (SI) and without (SD) state dependence. The continuous and dotted lines are for $\rho_{1}$ and $\rho_{2}$ without state dependence, while the broken and chain lines correspond to the state depended cases. The purpose of this graph is to show the difference between statedependent and state- independent correlations, with or without the Jastrow factor in reference.

The basic principle of the CCM is that the exact wave function can be obtained by correlating a starting reference function. This correlation operator can be given directly in coordinate representation. The translationally invariant coupled cluster method provides a parameterization of the correlation operator in terms of functions depending on the relative distance.

We can obtain several truncated forms for the correlation operator that can be used in a variational calculation. The most general variational. Wavefunction consists of a multilinear expansion of the correlation operator.

We are particularly interested in an economic method in terms of effort that does not lack substantial accuracy. The simplest choice would be to consider a linear form for the correlation operator containing only pair correlations. When compared with higher order approximations this choice is rather poor. However, a further improvement is to enrich the structure of the reference function.

The Jastrow correlation factor is such a choice. Combining the simplest approximation of the CCM , namely the $\operatorname{TICI}(2)$, with the Jastrow correlation factor leads to a variational calculation that is easily accessible both analytically and numerically, termed as the $\mathrm{J}-\mathrm{TICI}(2)$ scheme. The alpha particle has provided a reliable method for testing the accuracy of both the method to be used and the numerical calculation. When compared with the statistically exact GFM and DMC methods the results obtained are in close agreement.

Despite the complexity of such methods both in implementation and computer time, $\mathrm{J}-\mathrm{TICI}(2)$ scheme was relatively easy and straight forward to apply. We managed to slightly improve the previously obtained results at no expense, provided a numerical solution of the equations is performed.

## 3-1 Introduction

The linearized variational wavefunction developed for the alpha-particle can be extended to include a number of additional nucleons, especially neutrons, as well as additional alpha-particles. This involves changing the reference state into one compatible with the system in question. The change should be such that the required permutation symmetry can be imposed. Furthermore, the additional particles should be introduced without violating transitional invariance.

Since there is adequate experimental proof (see chapter 1) that halo nuclei are weakly bound systems we can impose a cluster-like structure without removing any of the microscopic model, but by restricting the wavefunction to a particular subspace of the full many-body Hilbert space.

Clusters are a general phenomenon in nature. The existence of clusters has been observed in subnuclear physics, nuclear physics, atomic and molecular physics. Clusters have a strict determined symmetry and geometrical form, and are created as a result of interactions between parts of clusters. [Bis93]

This can be achieved by assuming specific symmetry configurations for the variational wavefunctions. Furthermore, such an approach is convenient as a starting point, since it follows the previous development for the alpha- particle naturally.

This chapter is composed of a description of the structure of the cluster wavefunction, the type of interactions used and a rather extensive discussion for the symmetry of the states. The inclusion of the right permutation symmetry is of particular importance.

## 3-2 The J-TICI (2) formalism

The alpha-particle wavefunction describing the $0^{+}$ground state can be constructed in a very efficient way by the J-TICI(2) method. We can extend this formalism beyond that of the alpha-particle. [Bis93]. A part from the increase in the number of particles the main difference is in the reference function. In the case of the alpha-particle the reference function for the ground-state is simply a

Harmonic Oscillator ground state, saturated in spin-isospin. the wavefunction was not an eigenstate of total angular momentum $J$ ( $L$ in the case of spin-orbit absence) but was a superposition of several $J$ states. We shall adopt a formalism that preserves the right quantum numbers.

We can firstly consider the case of a single alpha-particle accompanied by a number $K$ of nucleons that could be weakly bound. One possibility is to assign to the particles outside the alpha-particle spatial coordinates relative to the alpha-particle center-of mass. The reference function $\Phi_{J, T}$ in the case of an alphaparticle accompanied by $r$ neutrons can be written as :

$$
\begin{aligned}
& \Phi_{J, T}^{r e l}=\Phi_{J, T}^{r e l}\left(r_{\alpha 1}, \ldots, r_{\alpha k}, r_{12}, \ldots, r_{i j}, \ldots, r_{k-1 k}\right) \ldots \ldots . . . . . . . . . . . . . . . . . . . . . . . . . .(3-2) ~
\end{aligned}
$$

where $\left(\Phi_{J, T}^{r e l}\right)$ is a function that contains about the additional nucleons with $r_{\alpha i}$ referring to the set of coordinates assigned to the ith weakly bound neutron relative to the alpha-particle center-of- mass, while $r_{i j}$ are the relative coordinates between the additional nucleons. A is antisymmetrizer and $\Phi_{\alpha}$ is the four-particle Harmonic oscillator ground state or the alpha-particle wavefunction (that can be obtained from a separate calculation). $J$ and $T$ are the total angular momentum and isospin. Translational invariance is preserved in a rather artificial way, since relative coordinates are explicitly included, rather than obtained through some separation process for the wavefunction $\Phi_{J, T}^{r e l}$ and the choices we are going to make are more intuitive than anything else. As described earlier the total wavefunction is described by a correlation operator acting on a reference state. The correlation operator (state-dependent or not) is a scalar commutes with all symmetry operators of the Hamiltonian. All quantum numbers are carried by the references function and despite the intuitive choice for $\Phi_{J, T}^{r e l}$ we shall explicitly impose the right quantum numbers.

One choice for the wavefunction $\Phi_{J, T}^{\text {rel }}$ could be as follows: the additional nucleon can be assigned a wavefunction relative to the alpha-particle that will in general be the product of a radial and an angular part described by an angular momentum $J_{i}$. In order to preserve rotational invariance we have to couple the angular momenta of the additional nucleons to a total angular momentum $J$. However, the additional nucleons will be correlated with each other, something that can imposed with the presence of a function depending on the relative distances $r_{i j}$. This way $\Phi_{J, T}^{\text {rel }}$ is composed of the angular and radial parts and can have the general form:

The $A_{j_{1}, \ldots, j_{r}}^{J M}$ is a set of coefficients that must be truncated for practical purposes. $R\left(r_{12}, \ldots, r_{i j}, \ldots, r_{k-1, k}\right)$ is the wavefunction that correlates the additional neutrons with each other. The functions $\Phi_{i j}$, which represent the extra neutrons, are composed of a product of angular, radial and spin-isospin parts, for example

$$
\begin{equation*}
\Phi_{j i}\left(r_{a i}\right)=\prod_{i=1}^{k} \phi\left(r_{\alpha i}\right)\left[Y^{i n}\left(\theta_{i}, \phi_{i}\right) \otimes \chi\left(\sigma_{i}\right) \chi_{\tau}\right]_{M_{i}}^{\prime i} . \tag{3-4}
\end{equation*}
$$

The angular brackets:

$$
\begin{equation*}
\left[Y^{h}\left(\theta_{i}, \phi_{i}\right) \otimes \chi(\sigma i)\right]_{M_{i}}^{J_{i}}=\sum_{m_{i} S_{i}} C_{l m_{i}, 1 / 2 m_{s}}^{J m_{s}} Y_{m_{i}}^{l_{i}} \chi_{S_{i}}\left(\sigma_{i}\right) . \tag{3-5}
\end{equation*}
$$

Denote spin-orbit coupling and $C_{l_{i} m_{i}}^{J_{i} M_{i}}{ }^{1} 2 m s_{i}$ are the Clebsh-Gordan coefficients for $\operatorname{SU}(2)$. It must be emphasized that the coordinates $r_{a i}$ as well as the angles $\theta_{\mathrm{i}}$ and $\Phi_{i}$ represent the coordinates and angels of the ith neutron relative to the alpha-particles center-of-mass. The importance of this choice is that we preserve the translational invariance of the reference state, in a relatively simple manner.
where the undetermined coefficients will in general depend on the value of the total angular momentum assigned to the $i$ ith particle. However when the spin-orbit
term is not included in the interaction the relative wavefunction takes the simpler form

$$
\begin{align*}
\Phi_{L, S, T}^{r e l} & =\sum_{L_{1}, \ldots L_{2}} A_{l_{1}, \ldots, l_{r}}^{L M_{L}}\left[\underset{i}{\otimes} \Phi_{l_{i}}\left(r_{\alpha i}^{\vec{r}}\right)\right]_{M_{L}}^{L} R\left(\left\{r_{i j}\right\}\right) \times\left[\stackrel{\left.\underset{i=1}{\otimes} \chi_{\sigma_{i}}\right]_{M_{S}}^{S} \times\left[\stackrel{r}{\otimes} \chi_{i=1}^{r} \chi_{T_{i}}\right]_{M_{T}}^{T}}{ }\right. \\
& \equiv \Phi_{L}^{r e l}\left(\left\{\bar{r}_{i}\right\}\right) \chi_{\sigma \tau}(S, T), \chi_{\sigma \tau}(S, T)=\left[\stackrel{r}{\otimes} \chi_{i=1} \chi_{\sigma_{i}}^{s}\right]_{M s} \times\left[\stackrel{r}{\otimes} \chi_{i=1} \chi_{\tau_{i}}^{T}\right]_{M_{T}} .
\end{align*}
$$

where the relative wavefunctions are coupled to a total orbital momentum $L$, which $S$, is the total spin. In the $L-S$ coupling scheme the wavefunction can be "inner product" of a spatial with a spin-orbit part, something that will be described in detail later.

$$
\begin{equation*}
\Phi_{L, S, T}^{r e l}=A\left\{\Phi_{\alpha 1} \Phi_{\alpha 2} \ldots \Phi_{o k} \Phi_{L, S, T}^{r e l}\right\} \ldots \tag{3-8}
\end{equation*}
$$

The next step is to consider more than one alpha-particle. For z-alpha-particles and $k$ additional nucleons the wavefunction of equation (3.1) changes to:
where $\Phi_{L, S, T}^{\text {rel }}$ must be extended to include the correlations between different alpha-particles a part from the ones between alpha-particles and weakly-bound nucleons and between weakly-bound nucleons. Contrary to the case above where we have only one alpha-particle, this case is much harder to generalize and we only consider the situation of two alpha-particles. Alone (corresponding to ${ }^{8} \mathrm{Be}$ and two alpha-particles with one additional nucleon ${ }^{9} \mathrm{Be}$.

In the case of two alpha-particles the spatial part $\Phi_{L}^{\text {rel }}$ of the wavefunction $\Phi_{L, S, T}^{\text {rel }}$ becomes:

$$
\begin{equation*}
\Phi_{L, S, T}^{\text {rel }}=\Phi_{L}^{\text {rel }}\left(r_{\alpha_{1} \alpha_{2}}^{\overrightarrow{ }}\right) \chi_{\sigma \tau}(S, T) . \tag{3-9}
\end{equation*}
$$

Where

$$
\Phi_{L}^{r e l}\left(r_{\alpha_{1} \alpha_{2}} \quad \overrightarrow{ }\right)=R\left(r_{\alpha_{1} \alpha_{2}}\right) Y_{M_{i}}^{L}(\theta, \phi) .
$$

$\qquad$
, $r_{\alpha_{1} \alpha_{2}}^{\rightarrow}$ is the coordinated vector between the two alpha-particles. This will be the type of correlation that will be used between alpha-particles.

### 3.2.1. RGM- like wavefunction

The RGM provides an accurate microscopic description of collisions between light nuclei. The wavefunctions are based on an assumed simplified structure for the colliding nuclei. They are fully antisymmetric and posses exact angular momentum and parity quantum numbers. [Hes02]

The RGM formalism is the technique developed in [Gua01]. In this method the wavefunction is described by a similar reference state as in the $\mathrm{J}-\mathrm{TICI}(2)$ model, but instead of using a linear correlation operator the reference function is described by a linear expansion, where each amplitude corresponds to a different set of the variational parameters used to describe the separation between individual clusters. In our formalism this corresponds in expanding the function $\Phi^{\text {rel }}$ of equation (3-2) in terms of a set of variational parameters. We shall describe this in more detail in chapter 5 , when we consider individual cases.

Both the $\mathrm{J}-\mathrm{TICI}(2)$ and RGM like methods will be applied in a later chapter. The J-TICI(2) is a more natural consequence of our previous work on the alphaparticles.

## 3-3 Nucleon-Nucleon Interactions

The atomic nucleus turns out to be a complicated interacting many body system, governed by the nucleon-nucleon interaction active inside the nucleus [Ann05].

Although the effective nucleon-nucleon interaction (active in some limited part of the full Hilbert space and within a nuclear medium)

Will be largely different from the form of the free nucleon-nucleon interaction [Ann05].

Although the description of the nuclear force problem is beyond our purpose, a general discussion of the basic characteristic of the most common realistic interactions used is given below. The term "realistic interactions" refers to
interactions depending on all particles labels but obtained from an incomplete theory in order to reproduce some experimental results.

At first approximation realistic interactions are given as two-nucleon potential terms. These potentials are builded by fitting deuteron properties and nucleon-nucleon scattering data. An example of a realistic type of potentials is the Argonne V14 [Wir84] and its extended Version Argonne V18 [Wir95]. The potential (V14) is written as a sum of 14 operator components [Fab97]

$$
\begin{equation*}
V(i j)=\sum_{p=1}^{14} v^{p}\left(r_{i j}\right) O^{p}(i j) \tag{3-11}
\end{equation*}
$$

where $v^{p}\left(r_{i j}\right)$ are terms depending only on the relative distance and the $O^{p}(i j)$ are operators. These are given as: [18]

$$
O^{p=1,14}(i j)=\left\lfloor 1, \sigma_{i}^{\vec{~}} \cdot \sigma_{j}^{\vec{j}}, S_{i j},\left(L^{\rightarrow} \cdot S^{\rightarrow}\right)_{i j}, L^{2}, L^{2}\left(\sigma_{i} \cdot \overrightarrow{\sigma_{j}}\right),\left(L^{\rightarrow} \cdot S^{\rightarrow}\right)_{i j}^{2}\right\rfloor \otimes\left[1, \tau_{i}^{\vec{i}}, \tau_{j}^{\vec{j}}\right] \ldots \ldots \ldots .(3-12)
$$

where $\sigma_{i}^{\rightarrow}$ and $\tau_{i}^{\rightarrow}$ indicate the usual Pauli spin and isospin operators and

$$
\begin{aligned}
& S_{i j}=3\left(\sigma_{i}^{\rightarrow} \cdot r_{i j}^{\wedge}\right)\left(\sigma_{j}^{\rightarrow} \cdot r_{i j}^{\wedge}\right)-\sigma_{i}^{\rightarrow} \cdot \overrightarrow{\sigma_{j}} \\
& S_{i j}=\left(3 r_{i j}^{\wedge} \cdot \sigma_{i}^{\rightarrow} r_{i j}^{\wedge} \cdot \sigma_{j}^{\vec{~}}-\overrightarrow{\sigma_{i}} \cdot \overrightarrow{\sigma_{j}}\right)
\end{aligned}
$$

The factor $S_{i j}$ is the tensor operator. [Ann05, Bis07]
The non-local terms arise because of the inclusion of the non-local spin $\operatorname{orbit}\left(L^{\rightarrow} \cdot S^{\rightarrow}\right)_{i j}$, where $L$ is the relative orbital angular momentum and $S^{\rightarrow}$ is the total spin of the pair. [Fab97] In our calculations we shall only consider local interactions, that is interactions independent of the nucleon velocities. Because of transitional invariance, the interaction involves only the relative distance $r_{i j}=r_{i}-r_{j} .[$ Ann05] Furthermore, it can be separated into interactions depending only on the magnitude of $r_{i j}$, termed central forces, and forces that dependent also on the direction.

The separation distance $r_{i j} \simeq 1.5-2 \mathrm{fm}$ but the actual interaction becomes repulsive (in coordinate space) at distances $r_{i j} \leq 0.5 \mathrm{fm}$ [Ann05].

These types of potentials are most realistic ones currently present as result of their rich operator structure, although a calculation should include as many potential terms as possible, approximations are usually taken and a subset of the
operators is taken. However this will require to us a different type of realistic interactions than the Argonne ones, which are adapted for a smaller set of operators.

The central forces are local forces since they do not depend on the velocity, and contain only scalar products of the major nucleon variables $\sigma_{i}$ and $\overrightarrow{\tau_{i}} . \overrightarrow{\tau_{i}}$. [Ann05].

$$
\begin{equation*}
V_{c}(i, j)=V_{o}\left(r_{i j}\right)+V_{\sigma}\left(r_{i j}\right) \sigma_{i}^{\vec{~}} \cdot \sigma_{j}^{\overrightarrow{ }}+V_{\tau}\left(r_{i j}\right) \tau_{i}^{\rightarrow} \cdot \tau_{j}^{\vec{j}}+V_{\sigma \tau}\left(r_{i j}\right) \sigma_{i}^{\vec{~}} \cdot \sigma_{j}^{\rightarrow} \tau_{i}^{\vec{~}} \cdot \tau_{j}^{\vec{j}} . \tag{3-14}
\end{equation*}
$$

This form can be rewritten using certain exchange operators. One defines the spin exchange operator $\quad P_{i j}^{\sigma}$ [Ann05].

$$
\begin{equation*}
P_{i j}^{\sigma}=\frac{1}{2}\left(1+\sigma_{i} \cdot \sigma_{j}^{\vec{~}}\right) . \tag{3-15}
\end{equation*}
$$

And, likewise, the isospin exchange operator $P_{i j}^{\sigma}$ [Ann05].

$$
\begin{equation*}
P_{i j}^{\tau}=\frac{1}{2}\left(1+\tau_{i}^{\rightarrow} \cdot \tau_{j}^{\rightarrow}\right) . \tag{3-16}
\end{equation*}
$$

The central potential can be written in terms of the Wigner, Majorana, Barlett and Heisenberg components (denoted by their initials), given the form:

$$
\begin{equation*}
V_{C}(i j)=V_{W}\left(r_{i j}\right)+V_{M}\left(r_{i j}\right) P_{i j}^{\sigma} P_{i j}^{\tau}+V_{B}\left(r_{i j}\right) P_{i j}^{\sigma}+V_{H}\left(r_{i j}\right) P_{i j}^{\tau} \cdots \tag{3-17}
\end{equation*}
$$

In the case of projection operators, the potential is defined in term of singlet or triplet spin-isospin channels and even or odd spatial parts [Ann05].

The coefficients of the different terms in (3-14) and (3-17) fulfill the following relation

$$
\begin{aligned}
& V_{W}\left(r_{i j}\right)=V_{0}\left(r_{i j}\right)-V_{\sigma}\left(r_{i j}\right)-V_{\tau}\left(r_{i j}\right)+V_{\sigma \tau}\left(r_{i j}\right) \ldots \ldots . . . . . . . . . . . . .(3-18) \quad \text { (Wigner force) }
\end{aligned}
$$

With the Yukawa type radial dependence for all radial dependences $V_{0}(r), V_{\tau}(r)$, $V_{\sigma}(r)$ and $V_{\sigma \tau}(r)$

$$
V(r)=-\lambda_{A} \frac{e^{-\mu_{A} r}}{r}+\lambda_{R} \frac{e^{-\mu_{R} r}}{r} . .
$$

$\mathrm{V}(\mathrm{r})$ is the strength of the radial dependence [Ann05]
The Afnan and Tang [Afn98] potentials $S 3$ and its modified version [Gua81] MS3, are other examples of V4 potentials, where a sum of three Gaussians is used for each for each channel. The channels used for the $S 3$ potential are the same as the previous case, while the (MS3) potential is adjusted to include channels of total add parity which can be extended to include non-local terms of spin-orbit coupling, The Gongy [Gog70] potential is composed of a V6 part and a spin-orbit coupling part, containing both, first and second order terms V8. It is given by:

$$
\begin{equation*}
V(i j)=V_{V 6}(i j)+V_{L S}\left(r_{i j}\right) L^{\rightarrow} . S \rightarrow+V_{L L}\left(r_{i j}\right) L_{i j} . \tag{3-23}
\end{equation*}
$$

Where in term of exchange operators the general form of a V6 potential

$$
\begin{equation*}
V(i j)=V_{c}\left(r_{i j}\right)+V_{\tau}\left(r_{i j}\right) P_{\tau}^{i j}+V_{\sigma}^{i j}\left(r_{i j}\right) P_{\sigma}^{i j}+V_{\sigma \tau}\left(r_{i j}\right) P_{\sigma}^{i j} P_{\tau}^{i j}+V_{T_{0}}\left(r_{i j}\right) S_{i j}+V_{T_{\tau}}\left(r_{i j}\right) P_{i j}^{\tau} \tag{3-24}
\end{equation*}
$$

And

$$
L_{i j}=\left(\sigma_{i}^{\wedge} \cdot \sigma_{j}^{\wedge}\right) L^{2}-\frac{1}{2}\left[\left(\sigma_{i}^{\wedge} \cdot L^{\rightarrow}\right) \cdot\left(\sigma_{j}^{\wedge} \cdot L^{\rightarrow}\right)+\left(\sigma_{j}^{\wedge} \cdot L^{\rightarrow}\right)\left(\sigma_{i}^{\wedge} \cdot L^{\bullet}\right)\right] .
$$

$\qquad$ .(3-25)

Being a second order spin-orbit interaction. The radial parts of the Gogny potential are expressed as summation of Gaussians.

In general there is a large number of realistic nucleon-nucleon interaction. We shall mainly make use to the $S 3$ and MS3 V4-type interactions. These provide any easy ground for a first approximation and can be referred to as semi-realistic interactions since they are composed of Gaussians and are finite at zero nucleon separation.

The nice analytic properties of these interactions do not imposes any immediate problems for the numerical evaluation of the Hamiltonian expectation value.

One of the focal points of all physics is symmetry. The nucleon-nucleon interaction and all effective interactions used in practice have certain symmetries.

They are invariant by translation (changing the frame of reference so that directions are not altered), by rotation (turning the frame of reference around some axis), or parity (changing the sense of axes) in the sense that the interaction does not change funder any of these operations [Kat08].

## 3-4- Symmetry and Quantum Mechanics

Symmetry considerations dominate modern fundamental physics, both in quantum theory and in relativity

The application of the theory of groups and their representations for the exploitation of symmetries in the quantum mechanics of the 1920s undoubtedly represents the second turning point in the twentieth-century history of physical symmetries. It is, in fact, in the quantum context that symmetry principles [Kat08].

Their most effective. Winger and Weyl were among the first to recongnize the great relevance of symmetry groups to quantum physics and the first to reflect on the meaing of this. As Winger emphasized on many occasions, one essential reason for the "increased effectiveness of invariance principles in quantum theory" (Winger, 1967, p.47) is the linear nature of the state space of a quantum physical system, corresponding to the possibility of superposing quantum states.

This give rise to, among other things, the possibility of defining states with particularly simple transformation properties in the presence of symmetries [Kat08].

## 3-4-1 The Concept of Symmetry

the term "symmetry" derives from the Greek words sun (meaning "with" or 'together') and metron ('measure')

We arrive at a definition of the symmetry of geometrical figure in terms of its invariance when equal component parts are exchanged according to one the specified operations. [Kat08]

The next key step was the generalization of this notion to the group-theoretic definition of symmetry, which arose following the nineteenth-century development
of the algebraic concept of a group, and the fact that the symmetry operations of a figure were found to satisfy the conditions for forming a group.

Finally, we have the resulting close connection between the notion of symmetry, equivalence and group

## 3-4-2 Symmetry of States

One important part of any quantum mechanical calculation is the inclusion of the correct symmetry, since it will effect the expectation value of any observable. In most case the Hamiltonian of a system commutes with a number of operators. The set of operators with the Hamiltonian commutes can be the elements of finite groups or the generators of continuous groups (e.g., $\mathrm{SO}(3), \mathrm{SU}(2)$ ) which are the elements of Lie algebras, consider the set of orthogonal transformation. The group $\mathrm{SO}(3)$ of orthogonal transformation in 3-dimensions. The group-theoretic notion of symmetry is the one that has proven so successful in modern science. Note, however, that symmetry remains linked to beauty (regularity) and unity: by means of the symmetry transformations, distinct (but "equal" or, more generally, "equivalent") elements are related to each other and to the whole, thus forming a regular "unity" [Kat08]. And if the determinant of the group $U(2)$ equal to unity then it is called special unitary $\mathrm{SU}(2)$.

According to the symmetry of the Hamiltonian each space of degenerate eigenstates (eigenspace) belonging to some eigenvalue of the Hamiltonian can be labeled by a distinct set of quantum numbers, which correspond to conserved quantities. The properties of the states in a particular eigenspace are important for evaluation of expectation values of different operators.

In the case of the nuclear many-body problem and particularly when the nuclear forces do not depend strongly on the spin we can written the wavefunction as the product of an orbital function and a function of the spin and isospin variables, this is the case corresponding to the local-scalar V4 realistic interaction described earlier. The spatial part will obey rotational invariance and will thus belong to the $\mathrm{SO}(3)$ group. The spin-isospin has overall $\mathrm{SU}(4)$ symmetry that is described by

Wigner multiples [Win37], we shall discuss this in more detail latter on in section (3.4.5).

In addition to the individual symmetries of the spatial and spin-isospin parts we require that the full wavefunction is antisymmetric in the exchange of particle labels. This implies that the wavefunction belongs to a one-dimensional representation of the permutation group. This condition requires the orbital and spin-isospin parts to belong to conjugate representations of the permutation group instead of being confined to the antisymmetric one-dimensional irrepresentations. This is a subject that requires special attention when exchange operators are involved and we examine it in the next section.

## 3-4-3 Totally Antisymmetric Product Functions

As was already stated, in the absence of spin-orbit coupling the total wavefunction is constructed in a product space of the spatial and spin-isospin parts. We demand the full wavefunction to be totally antisymmetric which in turn implies that each space is invariant under the permutation group and the full wavefunction is given by Clebsh-Gordan coefficients of the permutation group. Since each state is also described by other continues symmetries there must be a connection between functions belonging to the irrepresentation of these groups and the irrepresentation of the permutation group. [Jin98]

The first non-spactiotemporal symmetry to be introduced into microphysics, and also the first symmetry to be treated with the techniques of group theory in the context of quantum mechanics, was permutation symmetry (or invariance under the transformations of the permutation group). This symmetry "discovered" by W. Heisenberg in 1926 in relation to the indistinguishability of the "identical" electrons of an atomic system.[Kat08]

For the moment we can describe in simple terms the process by which we can construct a totally antisymmetric product function. By $S_{n}$ we denote the permutation group on order $n$ [Kat08]. The basis functions of irrepresentation $\mu$ of $S_{n}$ for the spatial part are the $\Phi_{i}^{\mu}$ while those of the spin-isospin part are the $\chi_{i}^{\mu}$.

The "inner product" between the spatial and spin-isospin part is the linear combination of product of wavefunctions with definite symmetry in the overall degrees of freedom.

Thus a function $\Psi^{\nu}$ belonging to the inner product space of the irrepresentation $\alpha$ and $\beta$ can be written as:

$$
\begin{equation*}
\Psi_{i}^{\nu}=\sum_{j, k}^{\eta_{\alpha}, \eta_{\beta}} C_{\alpha j, \beta k}^{\nu, i} \Phi_{j}^{\alpha} \chi_{k}^{\beta} . \tag{3-26}
\end{equation*}
$$

where $C_{\alpha_{j}, \beta_{k}}^{v, i}$ are the Clebsh-Gordian coefficients. There is usually one additional multiplicity label associated with $v$ that can ignore because it does not appear in the spin-isospin state we shall consider. $\eta_{\alpha}$ and $\eta_{\beta}$ are the dimensions of $\alpha$ and $\beta$.

In order for the full wavefunction to be totally antisymmetric we want $\Psi_{i}^{\nu}$ to be invariant with respect to permutations p a part from a phase factor $\left((-)^{\mathrm{P}}\right)$. This means that $\Psi_{i}^{v}$ belongs to the one-dimensional irrepresentation of $S_{n}$ denoted as $\Psi^{\left[1^{n}\right]}$

$$
\begin{equation*}
C_{\alpha_{i} \beta_{j}}^{[n], 1}=\frac{1}{\sqrt{\eta_{\alpha}}} \Lambda_{j}^{\alpha} \delta_{\alpha \beta^{\rightarrow}} \delta_{j k} . \tag{3-27}
\end{equation*}
$$

, where $\left[1^{n}\right]$ is the tableau consisting of a column of $n$ boxes. For this case the Clebsh-Gordan coefficients taken the simple form

And $\Lambda_{j}^{\alpha}$ is a phase factor that can be either $( \pm 1)$, while $\left(\alpha^{\rightarrow}\right)$ denotes the irrepresentation conjugate to $\alpha$. The action of a permutation P on $\Psi$ gives

$$
\begin{align*}
P \Psi & =\sum_{i} \Lambda_{i}^{\alpha}\left(P \Phi_{i}^{\alpha}\right)\left(P \chi_{i}^{\alpha^{\lrcorner}}\right) \ldots . . . . . . . . . . . . . . . . . . . . . . . ~ \tag{3-28}
\end{align*}
$$

Where $U^{\alpha}(P)_{k}$ is a matrix element of the ${ }^{\alpha} t h$ irreducible representation of $P$, which can be assumed to be real and orthogonal. The demand that $\Psi$ is antisymmetric with respect to $P$ requires the condition
which in turn requires that:

Therefore, having a totally antisymmetric wavefunction implies having a linear combination of products with the form:

$$
\begin{equation*}
\Psi=\sum_{I} \Phi_{i}^{\alpha} \chi_{i}^{\alpha^{\top}} . \tag{3-31}
\end{equation*}
$$

Where the transformation of these sets $\Phi_{i}^{\alpha}$ and $\chi_{i}^{\alpha \rightarrow}$ under a permutation is given as:

$$
P \Phi_{i}^{\alpha}=\sum_{i} U^{\alpha}(P)_{j i} \Phi_{j}^{\alpha} \quad, P \chi_{i}^{\alpha^{\star}}=(-)^{p} \sum_{j} U^{\alpha}(P)_{j i} \chi_{j}^{\alpha} .
$$

## 3-4-4 Representation of Groups

In general, if G is a symmetry group of a theory describing a physical system (that is, the fundamental equations of the theory are invariant under the transformations of G), this means that the states of the system transform into each other according to some "representation " of the group G. in other words, the group transformations are mathematically represented in the state space by operations relating the states to each other. In quantum mechanics, these operations are generally the operators acting on the state space that correspond to the physical observables, and any state of a physical system can be described as a superposition of states of elementary systems, that is, of systems the states of which transform according to the "irreducible" representations of the symmetry group. Quantum mechanics thus offers a particularly favourable framework for the application of symmetry principles. The observables representation the action of the symmetries of the theory in the state space, and therefore commuting with the Hamiltonian of the system, play the role of the conserved quantities; furthermore, the eigenvalue spactra of the invariants of the symmetry group provide the labels for classifying the irreducible representations of the group: on this fact is grouded the possibility of associating the values of the invariant properties characterizing physical systems wit the labels of the irreducible representations of symmetry group, i.e. of
classifying elementary physical systems by studying the irreducible representations of the symmetry groups.[Kat08]

## 3-4-5 SU(4)Quantum Nnumbers

An antisymmetric wavefunction that is a linear superposition of spatial and spin-isospin functions can be labeled by several quantum numbers that are related to the transformation of the spatial and spin isospin parts under rotations in coordinate, spin and isospin space.These are the orbital momentum quantum number $L$, the total spin $S$ and the total isospin $T$. Furthermore, additional quantum numbers or labels are required to uniquely specify the state of the system as a result of permutation symmetry, The fact that we require the spin-isospin functions to be of conjugate permutation symmetry to the spatial one implies some restrictions on the possible sets of quantum numbers. We provide an analysis of the decomposition of the wavefunction since its important for the expectation value of the Hamiltonian.

In the case of total angular momentum $J$, the requirement is that the spatial part $\Phi_{i}^{v}$, belonging to the $v$ irrepresentation of $S_{N}$ is restricted to representations compatible with the group $\mathrm{SO}(3)$. In our case the situation is simple since we shall only couples pair of particles. This can be applied by the usual way of coupling two integer representations of the $\mathrm{SU}(2)$ algebra, with $l_{1}$ and $l_{2}$ quantum numbers, into an irrepresentation. With $L=l_{1}+l_{2}$ and definite parity $(-1)^{L-l_{1}-l_{2}}$. Therefore the labels for spatial part are the irrepresentation of $S_{n}$. In general more labels are needed to uniquely specify the spatial symmetry since for some $L$ with the same irrepresentation labels of $S_{n}$ we can find several linear combinations of coordinate tensor-product functions. This way the spatial functions of expansion equa.(3-31) can be written as:

$$
\begin{equation*}
\Phi_{i}^{v} \rightarrow \Phi_{L, i}^{v} . \tag{3-33}
\end{equation*}
$$

Apart from conjugate permutation symmetry to the spatial part, the spin-isospin part belongs to $S U(4)$ symmetry. This is a result of the fact that the

Hamiltonian is invariant under rotations in spin as well as in isosopin space. The invariance is expressed by the following commutation relations:

$$
\begin{equation*}
\left[\hat{H}, \sum_{i=1}^{n} s_{k}(i)\right]=\left[\hat{H}, \sum_{i=1}^{n} t_{k}(i)\right]=\left[\hat{H}, \sum_{i=1}^{n} s_{k}(i) t_{k}(i)\right]=0, k, l=1,2,3, \ldots, n \tag{3-34}
\end{equation*}
$$

Here $s_{k}(i)$ and $t_{i}(i)$ are the $k t h$ spin and isospin components, respectively, for nucleon $i$. The first two commutators imply that the states can also be labeled by the total spin $S$ and isopspin $T$ of $\mathrm{SU}(2)$. Apart from $S$ and $T$ the basis states have one additional label. Resulting from the third commutation relation (3-34). This additional label classifies the permutation symmetry to which the spin-isospin state belongs, that has to be conjugate to that of the spatial part.

The symmetry of the spin-isospin state leads to the general problem of the direct product $S U(m) \times S U(n)$ of two unitary groups in a subgroups of $S U(m n)$ [Itz96]. Therefore, we need the $S U(m n) \supset S U(m) \times S U(n)$ irreducible basis. This is equivalent to the inner products of two irrepresentations of the permutation group $S_{n}$ into an irrepresentation of $S_{n}$ [Jin98]. The spin-isospin function is given as:

$$
\begin{equation*}
\chi_{i}^{v}=\left|s^{[\nu] i} M_{s}, T M_{T}\right\rangle=\sum_{j, k} C_{\left[v_{1}\right]_{j},\left[v_{2}\right]_{k}}^{[v]}\left|s^{\left[\nu_{1}\right], j} M_{s}\right\rangle\left|T^{\left[v_{2}\right] k} M_{T}\right\rangle \tag{3-35}
\end{equation*}
$$

where $C_{\left.\left.\left[v_{1}\right]\right]_{j}, \nu_{2}\right] k}^{[\eta]_{i},}$ are the Clebsh-Gordon coefficients of $S_{n}$ for the Coupling to the irreducible basis $[v]$ of $\left[v_{1}\right] \times\left[v_{2}\right]$.

In the case of the V4 interaction this is evident from the fact that the exchange operators $P_{i j}^{\sigma}, P_{i j}^{\tau}$ and $P_{i j}^{\sigma \tau}$ can be used in the place of the terms $\sigma_{i}^{\rightarrow} \cdot \sigma_{j}^{\overrightarrow{ }}, \tau_{i}^{\rightarrow} \cdot \tau_{j}$ and $\left(\sigma_{i}^{\rightarrow} \cdot \sigma_{j}^{\vec{j}}\right)\left(\tau_{i}^{\rightarrow} \cdot \tau_{j}^{\vec{j}}\right)$.

The total spin operators, $\hat{S}^{2}=\left(\sum_{i=1}^{N} \hat{S}_{i}\right)^{2}$
and

$$
\hat{T}^{2}=\left(\sum_{i=1}^{N} \hat{T}_{i}^{2}\right)^{2}
$$

Correct permutation symmetry in the many-body wavefunction is equivalent to having the right quantum numbers. The eigenfunctions $\Psi$ for the $\operatorname{SU}(4)$ Hamiltonian can be written as:

$$
\begin{equation*}
\Psi=|[v], L, S, T\rangle=\sum_{i}\left|L^{[v] i}, M_{L}\right\rangle\left|S^{[\nu \overrightarrow{ }] i} M_{S}, T M_{\tau}\right\rangle \tag{3-36}
\end{equation*}
$$

where the eigenvalues depend on the set of labels $\{\nu\rangle, L, S, T\}$. The structure provided by the permutation symmetry is expectation values.

## 3-5- Expectation values

We have to deal with the expectation value of an operator $O^{\wedge}$ in the totally antisymmetric wavefunction. A part from state dependence in $O^{\wedge}$ in general we have to consider the state dependence in the wavefunction resulting from the correlation operator as it was previously shown the state dependence will appear in terms of exchange operators.

$$
\begin{equation*}
\Psi=|[\nu], L, S, T\rangle . \tag{3-37}
\end{equation*}
$$

For the matrix elements of the Hamiltonian and normal matrices we require the matrix elements of a single or a number of pair spin-exchange operators with respect to the wavefunction of equa. (3-36)

The expectation values require knowledge evaluation of the matrix elements for the spin-exchange operators in the irrepresentation of Sn provided by the spinisospin states:

$$
\begin{align*}
& \left\langle s^{\left[\nu^{\rightarrow}\right]{ }_{i}} M_{s}, T M_{T}\right| P_{i j}^{\sigma}\left|s^{\left[\nu^{\bullet}\right]{ }^{2}} M_{s}, T M_{T}\right\rangle, \\
& \left\langle S^{[\hat{\nu}]_{i}} M_{s}, T M_{T}\right| P_{i j}^{\sigma} P_{k l}^{\sigma}\left|s^{\left[\nu^{\bullet}\right]{ }_{i}} M_{s}, T M_{T}\right\rangle \tag{3-38}
\end{align*}
$$

In order to avoid explicitly dealing with the different particle pairs we shall represent the above exchanges as a general permutation of the spin label that will be denoted as $P_{\sigma}$ and the associated function as $F_{\sigma}$. These matrix elements are:

$$
\begin{aligned}
& \equiv M_{s, T}^{v_{i, i}}\left(P_{\sigma}\right)
\end{aligned}
$$

where knowledge of the Clebsh-Gordan coefficients and of the irrepresentation of $S_{n}$ are required. Similarly for isospin exchanges we have :

$$
\begin{array}{r}
\left\langle S^{[\nu \rightarrow]_{i}} M_{S}, T M_{T}\right| P_{\tau}\left|S^{[\nu \rightarrow]_{i}} M_{S}, T M_{T}\right\rangle=\sum_{j k l} C_{\left.\left[v_{1}\right]\right]_{j, l}\left[\nu_{2}\right] k}^{[\nu] i} U_{k m}^{\left[\nu_{1}\right]}(P) C_{\left[\nu_{1}\right],\left[\nu_{2}\right] m}^{[\nu], i} .  \tag{3-40}\\
\equiv M_{S, T}^{\nu, i, i}\left(P_{\tau}\right)
\end{array}
$$

The notation $M_{S, T}^{v, i, i}(P)$ is introduced for later convenience.
A part from purely spin or isospin exchanges will have to deal with mixed exchanges, such as:

$$
\left\langle S^{\left[\nu^{\bullet}\right] i} M_{S}, T M_{T}\right| P_{i j}^{\sigma \tau}\left|S^{\left.\left[\nu^{\rightarrow}\right]\right]^{i}} M_{S}, T M_{T}\right\rangle,\left\langle S^{\left.\left[\nu^{\prime}\right]\right]_{i}} M_{S}, T M_{T}\right| P_{i j}^{\sigma} P_{k l}^{\tau}\left|S^{\left.\left[\nu^{\prime}\right]\right]_{i}} M_{S}, T M_{T}\right\rangle
$$

In general this will result in the product of two permutations, one in spin space $P_{\sigma}$ and one in isospin space $P_{\tau}^{\prime}$. The prime is important since part from acting in different spaces the two permutations will in general be different. For this mixed case the matrix element become:

$$
\begin{aligned}
& \left\langle S^{[\nu \rightarrow] i} M_{S}, T M_{T}\right| P_{\sigma} P_{\tau}^{\prime}\left|S^{[\eta \rightarrow] i} M_{S}, T M_{T}\right\rangle=
\end{aligned}
$$

$$
\begin{aligned}
& \equiv M_{S, T}^{v, i, i}\left(P_{\sigma} P_{\tau}^{\prime}\right)
\end{aligned}
$$

Therefore the Clebsh-Gordan coefficients and the representation matrices of the symmetric group carry the action of the spin, isospin and spin-isospin permutation on the fully antisymmetric wavefunction.

## 3-5-1 Spatial Integrals

As described in chapter 2, the variational principle for the ground state energy leads to a $4 M \times 4 M$ dimensional generalized eigenvalue problem (where $M$ is the number of components used to expand the correlation functions)
$\left[\begin{array}{cccc}H_{0}^{0} & H_{\sigma}^{0} & H_{\tau}^{0} & H_{\sigma \tau}^{0} \\ H_{0}^{\sigma} & H_{\sigma}^{\sigma} & H_{\tau}^{\sigma} & H_{\sigma \tau}^{\sigma} \\ H_{0}^{\tau} & H_{\sigma}^{\tau} & H_{\tau}^{\tau} & H_{\sigma \tau}^{\tau} \\ H_{0}^{\sigma \tau} & H_{\sigma}^{\sigma \tau} & H_{\tau}^{\sigma \tau} & H_{\sigma \tau}^{\sigma \tau}\end{array}\right]\left[\begin{array}{c}C_{0} \\ C_{\sigma} \\ C_{\tau} \\ C_{\sigma \tau}\end{array}\right]=E_{0}\left[\begin{array}{cccc}N_{0}^{0} & N_{\sigma}^{0} & N_{T}^{0} & N_{\sigma \tau}^{0} \\ N_{0}^{\sigma} & N_{\sigma}^{\sigma} & N_{\tau}^{\sigma} & N_{\sigma \tau}^{\sigma} \\ N_{0}^{\tau} & N_{\sigma}^{\tau} & N_{\tau}^{\tau} & N_{\sigma \tau}^{\tau} \\ N_{0}^{\sigma \tau} & N_{\sigma}^{\sigma \tau} & N_{\tau}^{\sigma \tau} & N_{\sigma \tau}^{\sigma \tau}\end{array}\right]\left[\begin{array}{c}C_{0} \\ C_{\sigma} \\ C_{\tau} \\ C_{\sigma \tau}\end{array}\right]$
the Hamiltonian has the decomposition:

$$
\begin{equation*}
\hat{H}=\hat{K}+V_{0}+V_{\sigma}+V_{\tau}+V_{\sigma \tau} ; V_{k}=\sum_{i<j} v_{k}\left(r_{i j}\right) P_{i j}^{k} \tag{3-43}
\end{equation*}
$$

The kinetic energy operator and the Wigner-part of the potential, $V_{o}$ are the only state-independent terms entering the Hamiltonian. If we denote the different particle pairs by $r$ and $r^{\left(r \equiv\left(r_{1}, r_{2}\right)\right)}$; the matrix elements of the kinetic energy matrix become:

$$
\begin{equation*}
\left(K_{k}^{k}\right)_{l} m=\left\langle[\nu], L, S, T \mid F_{l}^{k} K^{\wedge} F_{k}^{m}[V], L, S, T\right\rangle . . \tag{3-44}
\end{equation*}
$$

with

$$
\begin{equation*}
\left\langle L^{[v] i}, M_{L}\right| f_{k}^{l}(r) K^{\wedge} f_{k}^{m}\left(r^{\prime}\right)\left|L^{[v] i}, M_{L}\right\rangle=\int \Phi_{L, M_{L}}^{[v] i}\left(r_{1}, \ldots ., r_{n}\right) f_{k}^{l}(r) K^{\prime} f_{k}^{m}(\bar{r}) \Phi_{L, M_{L}}^{[[\nu]}\left(r_{1}, \ldots r_{n}\right) d \Omega \tag{3-45}
\end{equation*}
$$

The result is the same for the overlap and potential (Wigner part) matrices, where in the form $K^{\wedge}$ is replaced by 1 while in the latter by $V_{0}$. In the case of state-dependent operators, such as the spin-dependent part of the interaction the situation is similar:

$$
\begin{equation*}
\left(\left(V_{\sigma}\right)_{k^{\prime}}^{k}\right)_{l m}=\sum_{i, j^{\prime}} \sum_{r, r^{\prime}} M_{s, T}^{v, i, i^{\prime}}\left(P_{r}^{k} P_{r}^{\sigma} P_{r,}^{\bar{k}}\right)\left\langle L^{[v] i}, M_{L}\right| f_{k}^{l}(r) v_{\sigma}\left(r^{\prime}\right) f_{k}^{m}\left(r^{\prime \prime}\right)\left|L^{[l] i}, M_{L}\right\rangle . \tag{3-46}
\end{equation*}
$$

The number of required integrals can be further reduced by considering an alternative form of expansion (3-37) for the ket state:

$$
\begin{equation*}
\Psi \equiv|[v], L, S, T\rangle=\sum_{i}\left|L^{[v] i}, M_{L}\right\rangle\left|S^{[\nu \neg] i}, M_{S}, T M_{T}\right\rangle=A|[\nu] 1\rangle\left|\left[v^{\sim}\right] 1\right\rangle \tag{3-47}
\end{equation*}
$$

where $A$ is an antisymmetrizer and for simplicity the quantum numbers are ignored. Because $A$ is Hermitian and independent the expectation value of an operator $O^{\wedge} \equiv F_{k}^{\wedge} O^{\wedge \wedge} F_{k^{\prime}}^{\wedge} \quad$ becomes:

$$
\begin{aligned}
\left\langle O^{\wedge}\right\rangle= & \left.\left.\left.\left\{A\langle[v]|\left|\left\langle\left[v^{\sim}\right]\right|\right|\right\} O^{\wedge} A \mid[v]\right]\right\rangle\left[v^{\sim}\right] 1\right\rangle \ldots \ldots . . . . . . . . . . . . . . . . ~
\end{aligned}, \begin{aligned}
& \left.\left.\left.\left\langle O^{\wedge}\right\rangle=\frac{N!}{n_{v}}\left\{A\langle[v]|\left|\left\langle\left[v^{\sim}\right]\right|\right|\right\} O^{\wedge}|[v]\rangle\right\rangle\left[v^{\sim}\right]\right]\right\rangle
\end{aligned}
$$

In all case the presence of state-dependent correlations increases the number of the required integrals for a particular matrix element. The number of required integrals is proportional to the number of relative coordinates $\left(\left(\frac{n(n-1)}{2}\right)^{3}\right)$. This can be a serious draw back for large systems. The above display of the integrals for the matrix elements are in the most general form. According to the system under examination there can be simplifications such as the case of the alpha-particle. This with the cases of ${ }^{5} \mathrm{He},{ }^{6} \mathrm{He},{ }^{8} \mathrm{Be}$ and ${ }^{9} \mathrm{Be}$ are examined in the next section.

## 3-5-2 Alpha-particle

In our approximation the correct permutation symmetry for the alpha-particle ground-state is straight forward. Since the spatial part is totally symmetric the only possibility to obtain an antisymmetric wavefunction is by considering a totally antisymmetric spin-isospin state.

The alpha particle represents the core ${ }_{2}^{4} \mathrm{He}_{2}$
In general the orbital momentum quantum number $\mathrm{L}=0$, the spin and isospin ( $\mathrm{S}=0, \mathrm{~T}=0$ ) for the alpha-particle

The tableau describing the symmetry of the wavefunction is called Young tableaus

$$
\psi \equiv|[4], L=0, S=0, T=0\rangle=\left|\begin{array}{cc}
{[4]} & 1 \\
0 & 0
\end{array}\right|\left|\begin{array}{cc}
{\left[1^{4}\right]} & 1 \\
S=0, & T=0
\end{array}\right\rangle
$$

$$
=\left|\begin{array}{cc}
{[4]} & 1  \tag{3-50}\\
L=0 &
\end{array}\right\rangle \sum_{i=1}^{4}\left|\begin{array}{c}
{\left[2^{2}\right]} \\
S=0
\end{array}\right\rangle\left|\begin{array}{c}
{\left[2^{2}\right] i} \\
T=0
\end{array}\right\rangle
$$

where the spin-isospin part belongs in the inner-product space of a self conjugate irreprepresentation of $S_{4}$ :

$$
\left|\begin{array}{cc}
{\left[1^{4}\right]} & 1  \tag{3-51}\\
S=0, & T=0
\end{array}\right| \in \square \square \square \square
$$

The only state dependence in the alpha-particle appears in terms of spin (or isospin) exchange operators. The expectation value of spin exchange operators becomes:

$$
\begin{align*}
\left\langle\begin{array}{cc}
{[1]^{4}} & 1 \\
S=0, & T=0
\end{array}\right| P_{\sigma}\left|\begin{array}{cc}
{\left[1^{4}\right]} & 1 \\
S=0, & T=0
\end{array}\right\rangle & =\sum_{i, i^{\prime}}\left\langle\begin{array}{c}
{\left[2^{2}\right] i} \\
S=0
\end{array}\right|\left\langle\begin{array}{c}
{\left[2^{2}\right]} \\
T=0
\end{array}\right| P_{\sigma}\left|\begin{array}{c}
{\left[2^{2}\right] i^{\prime}} \\
S=0
\end{array}\right\rangle\left|\begin{array}{c}
{\left[2^{2}\right] i^{\prime}} \\
T=0
\end{array}\right\rangle  \tag{3-52}\\
& =\sum_{i} U_{i i}^{\left[2^{2}\right]}(P)=\operatorname{Tr}^{\left[2^{2}\right]}(P)
\end{align*}
$$

where the effect of a spin-permutation is the trace of the permutation in the irrepresentation of the spin-space. where the trace of the permutations depends on the cycle structure. The non-zero traces of interest are those of the products of two transpositions that can belong to either of two classes: the first one is when the transpositions do not commute and give a cycle structure of order (e.g. , $P_{12} P_{13}=P_{123}$ ) that has a trace equal to ( -1 ) and the second one is when the transpositions commute (e.g. , $P_{12} P_{34}$ ) that gives a trace equal to 2 .

The above result for the alpha-particle could have been generalized to an arbitrary spin-isospin state $\left|\begin{array}{c}{[v] i} \\ S, T\end{array}\right\rangle$ of an $n$-particle system, provided that is given by the inner product of spin and isospin parts belonging to a self conjugate irrepresentation of $S_{n}$ i.e.,

$$
\left.\left|\begin{array}{l}
{[V] i}  \tag{3-53}\\
S, T
\end{array}\right\rangle=\sum_{i}|[\alpha] j ; S\rangle\left[\alpha^{\sim}\right] j ; T\right\rangle .
$$

However this kind of simplification does not appear beyond $S_{4}$ for the $S U(4) \subset S U(2) \times S U(2)$ classification. Because of the above simplification the alpha-particle wavefunction in the $\mathrm{SU}(4)$ approximation shares no resemblance with any other wavefunction of more than 4 particles. The calculation of the matrix elements is straight forward.

## 3-5-3 ${ }^{5} \mathrm{He}$

The first case we have an alpha-particle accompanied by a number of neutrons is that of ${ }^{4} \mathrm{He}$. In our approximation there is only one possibility for the tableau describing the permutation symmetry of the spatial part:

$$
[4,1] \equiv \square \square \square
$$

The tableau describing the conjugate permutation symmetry for the spin-isospin part is

$$
\left[2,1^{3}\right] \equiv \begin{array}{|}
\square  \tag{3-55}\\
\square
\end{array}
$$

There is only one possible decomposition of the spin-isospin compatible with $S U(2) \times S U(2)$ [Itz96]:

$$
\begin{equation*}
\left|\left[2,1^{3}\right] i\right\rangle \in \square \times \square\left(s=\frac{1}{2}, T=\frac{1}{2}\right) . . \tag{3-56}
\end{equation*}
$$

This corresponds to an alpha-particle accompanied by a single neutron (or proton with charge independent interaction) since this is the only configuration that can be reduced to that of the alpha-particle by removing a neutron (or proton). The simplification of exchange operators in term of traces can not be applied, but the irrepresentations describing the spin and isospin states are identical the matrix elements of spin and isospin exchange operators coincide. This means that we can either use spin or isospin exchange operators and not both. The potential and correlation operators reduce to

$$
\begin{array}{r}
V=V_{o}+V_{\sigma}+V_{\tau}+V_{\sigma \tau}=V_{o}^{\prime}+V_{\sigma}^{\prime}+V_{\sigma \tau}^{\prime} .  \tag{3-57}\\
F^{\wedge}=F_{o}^{\wedge}+F_{\sigma}^{\wedge}+F_{\tau}^{\wedge}+F_{\sigma \tau}^{\wedge} \rightarrow F_{o}^{\wedge}+F_{\sigma}^{\wedge}+F_{\sigma \tau}^{\wedge} \cdots \ldots \ldots . . . . . . . . . . . . ~
\end{array}
$$

## 3-5-4 ${ }^{6} \mathrm{He}$

The next case is that of ${ }^{6} \mathrm{He}$. There are two possible spatial states associated with the following partitions


The associated conjugate spin-isospin states are $\left|\left[2^{2}, 1\right]\right\rangle$ and $\left|\left[3,1^{3}\right]\right\rangle$ respectively, unlike the case of ${ }^{5} \mathrm{He}$ only one of these spin-isospin states has a unique $S U(2) \times S U$ (2) decomposition in terms of spin and isospin states.

## 3-5-5 ${ }^{8} \mathrm{Be}$ and ${ }^{9} \mathrm{Be}$

After introducing additional neutrons to an alpha-particle we can consider the case of two alpha-particles and that of two-alpha-particles accompanied by a neutron. These two cases correspond to the nuclei ${ }^{8} \mathrm{Be}$ and ${ }^{9} \mathrm{Be}$ respectively.

In our approximation there is only one possibility for the tableau describing the permutation symmetry of the ${ }^{9} B e$ spatial part:

$$
\begin{equation*}
[4,4] \equiv \square \square \square \tag{3-60}
\end{equation*}
$$

The tableau describing the conjugate permutation symmetry for the spin-isospin part is

$$
\begin{equation*}
\left[2^{4}\right] \equiv \square \tag{3-61}
\end{equation*}
$$

There is only one possible decomposition of the spin-isospin state compatible with $S U(2) \times S U(2)$
$\left.\left[2^{4}\right] j\right\rangle \in$


$$
\begin{equation*}
(S=\mathrm{o}, T=0) \tag{3-62}
\end{equation*}
$$

The case ${ }^{9} \mathrm{Be}$ is very similar of ${ }^{5} \mathrm{He}$. By adding one more neutron to the above configuration of ${ }^{8} \mathrm{Be}$ there is only one possibility for the permutation symmetry of the spatial part:


The tableau describing the conjugate permutation symmetry of the spin-isospin part is :


There is only one possible decomposition of the spin-isospin states compatible with $S U(2) \times S U(2)$ with quantum numbers $S=1 / 2, T=1 / 2$

The cluster-like variational model we wish to examine preserves the full microscopic nature of the nuclear many-body problem. The approximations imposed are of two types: One concerning the actual wavefunction and the other concerning the type of interaction used. In the latter approximation we restrict ourselves in the study of central local interactions. Although such terms have been examined for the closed shell alpha-particle, we do not wish to pursue them at this stage for the lightly bound systems to be examined. In principle is always possible to include such terms

The approximations chosen for the wavefunctions are such that lead to a linear variational problem where the solution is well known. The J-TICI(2) method has the advantage over the RGM-Like method that it can incorporate state-dependent correlation. The fact that we are allowed to have a spin-isospin saturated structure due to the exclusion of spin-isospin coupling. This results in $\operatorname{SU}(4)$ symmetry for the spin-isospin part of the wavefunction should have a decomposition in to $\mathrm{SU}(2)$ irrepresentations. for the spin and isospin labels respectively, something related with the permutation symmetry.

The incorporation of the antisymmetry condition, appropriate, for fermions has been given spatial attention. It was shown that the complexity greatly increases in going from the alpha-particle to ${ }^{5} \mathrm{He},{ }^{6} \mathrm{He},{ }^{8} \mathrm{Be}$, and ${ }^{9} \mathrm{Be}$. Some simple group-theoretical results can simplify the expectation values. In general the antisymmetry condition can be applied without any difficulty to the alpha-particle, where only either spin or isospin exchange required. Beyond that there are no radical simplications.

In any-case the present model is as an extension of previous related work concerning the closed shell alpha-particle into the area of halo nuclei. A major drawback can be the closed shell alpha-particle structure since it restricts the possible configurations of the reference function. In practice the bound system might require a superposition of different reference function having to the alphaparticle "broken"

## 4-1 Introduction

As described in the previous chapters we will approximately solve the manybody schrödinger equation through a linear variational principle. Although the theoretical background is fairly simple a numerical evaluation of the matrix elements is usually required, due to complexity of the many-body expectation values, therefore to explain VM and MC [Gua96].

The most important task of the analysis provided in this chapter is to ensure the validity of the error estimate and in particular as applied to the linear eigenvalue problem, we shall make use of a number of statistical concepts, most of which can easily be found in the literature such as [Kla86].

We also describe the application of a method that is used to improve the performance of VMC.

## 4-2 Variational method

There are many problems of wave mechanics which can not be conveniently treated either by direct solution of the wave equation.

Therefore, the variation method is one of the most powerful approximation methods of quantum mechanics.Historically the VM derives from a general method putting in 1959 by Ritz[Bri35,Has ].

## 4-2-1 Mathematical Review of vairational method

The basic idea behind the variational method is this expectation value of the Hamiltonian gives the average energy of the system. In a state corresponding to the particular function used in evaluating the expectation value.

Clearly, this average energy must be greater than or equal to the lowest energy state of the system:

$$
\begin{equation*}
\langle\widehat{H}\rangle=\langle\Psi| \hat{H}|\Psi\rangle \geq E_{o} \tag{4-1}
\end{equation*}
$$

That the lowest energy state is lower bound on the expectation value enable us to choose a trail wavefunction containing a number of parameters and then to
minimize the expectation value by varying these parameters; hence the name vairational method. [Dic60, Han65].Let Schrodinger equation of the system is

$$
\begin{equation*}
\widehat{H} \Psi_{n}=E_{n} \Psi_{n} \tag{4-2}
\end{equation*}
$$

Where
En = true (exact) energy
$\Psi_{n=}$ true (exact) wavefunction
$\mathrm{n}=1,2,3 \ldots$, and
$\mathrm{E} 1<\mathrm{E} 2<\mathrm{E} 3, \ldots<\mathrm{En}, \mathrm{E} 1=$ exact ground state energy
Let $\Phi_{\mathrm{n}}$ be a trial wavefunction then

$$
\begin{equation*}
H=\frac{\left\langle\Phi_{\mathrm{t}} \hat{\hat{H}} \mid \Phi_{\mathrm{t}}\right\rangle}{\left\langle\Phi_{\mathrm{t}} \mid \Phi_{\mathrm{t}}\right\rangle} \tag{4-3}
\end{equation*}
$$

$H=\left\langle\Phi_{\mathrm{t}}\right| \hat{\mathrm{H}}\left|\Phi_{\mathrm{t}}\right\rangle$, if $\Phi_{\mathrm{t}}$ is normalized since $\Psi_{\mathrm{m}}$ forms a complete set of or the normal eigenfunction state, we can expand $\Phi_{\mathrm{t}}$ in terms of $\Psi_{m}$ i.e.

$$
\begin{equation*}
\Phi_{\mathrm{t}}=\sum_{n} \mathrm{a}_{\mathrm{n}} \Psi_{\mathrm{n}} \tag{4-4}
\end{equation*}
$$

$\widehat{H}_{\text {min }}$ is found by making differential equation
$o=\frac{\partial H}{\partial a}=\frac{\partial w}{\partial b}=\cdots$
, and then the values of $\mathrm{a}, \mathrm{b}, \mathrm{c} \ldots$ are found to make
$\widehat{H}_{\text {min }}=H(a, b, c, \ldots)$
$\widehat{H}_{\text {min }}$ is the best energy that can be found from $\Phi_{t}$
The improved wave function is found :
$\Phi_{t}($ improved $)=\Phi_{t}(a, b, c, \ldots)$
So, to obtain the best result of Hamiltanin must be choose the trail wave function approach to the form real wave function

## 4-3 Monte Carlo method

Many problems are to complicated to analyse mathematically. However, some of these processes can be analysed using a probability technique known as the Monte Carlo method [Joh03] Monte Carlo methods are used to solve problem by using random numbers to simulate interaction probabilities for various physical processes [Cod01,Dav ].

The Monte Carlo method is now the most powerful and commonly used technique for analyzing complex problems [Reu81].

Therefore, the Monte Carlo method is a numerical solution to a problem that models objects interacting with other objects or their environment based upon simple object - object or object environment relationships. The Monte Carlo method is essentially simple in its approach- a solution to a microscopic system trough simulation of its microscopic interactions.

A solution is determined by random sampling of the relationships, or the microscopic interactions, until the result converges [Bie01]

The Monte Carlo method provides approximate solutions to a variety of mathematical problems by performing statistical sampling experiments on a computer . The Monte Carlo method can be used to closely approximate the solutions to many probability problems [Dav ].

The terms "Monte Carlo methods" derives from the name of the town in Monaco on the Mediterranean know for its gambling casinos. Historically the name Monte Carlo was used as a code name during WWII [Dav ].

In general, Monte Carlo method are used in mathematics to solve various problems by generating suitable random numbers and observing that fraction of the numbers obeying some property or properties. The method is useful for obtaining numerical solutions to problems which are too complicated to solve analytically

## 4-4 Variational Mote Carlo method

The first application of Monte Carlo methods to nuclei interacting with realistic potentials was a (VMC) [Bar03].

The variational Monte Carlo algorithm is limited to treating small systems optimistically up to $\mathrm{A}=8$. For the spin independent interactions in condensed matter physics [Car90].

## 4-4-1 Nuclear Hamiltonian

Before studying the VMC methods discussing the nuclear Hamiltonian and the difficulties involved in determining its eigenstates. We will employ the traditional description of the nucleus as a system of non-relativistic nucleons interacting through spin and isospin dependent nuclear interactions. The solutions of the schroedinger equation equa.(1-1), Can then used, to determine many properties of the nucleus[Car90]. The two-body interaction can be written as a sum of spinisospin dependent operator Okij multiplied by functions of the pair separation rij

$$
\begin{equation*}
V_{i j}=\sum_{i<j j} V_{(r i j)}^{k} O_{i j}^{k} \tag{4-5}
\end{equation*}
$$

Where the operators $\mathrm{O}^{\mathrm{k}}{ }_{\mathrm{ij}}$ are
$O^{k}(i j)=\left|1, \sigma_{i}^{\rightarrow} \cdot \sigma_{j}^{\rightarrow}, S_{i j},\left(L^{\rightarrow} \cdot S^{\rightarrow}\right)_{i j}, L^{2}, L^{2}\left(\sigma_{i}^{\rightarrow} \cdot \sigma_{j}^{\rightarrow}\right),\left(L^{\rightarrow} \cdot S^{\rightarrow}\right)_{i j}^{2}\right| \otimes\left[1, \tau_{i}^{\rightarrow}, \tau_{j}^{\rightarrow}\right]$
Variational Monte Carlo (VMC) studies of light nuclei of ten employ a generalized Jastrow form for the wavefunction

$$
\begin{equation*}
\left|\Psi>=S\binom{\pi}{i<j} F_{i j}\right| \Phi> \tag{4-7}
\end{equation*}
$$

Where, $\Phi$ is antisymmetric slater determinant of one particle states, and the Fij are pair correlation operations[Car90].

## 4-4-2 variational Monte Carlo for light nuclei

variational Monte Carlo calculations of light nuclei are somewhat more complicated because of the spin-isospin dependence of the interaction and wavefunction [Car90]. Variational Monte Carlo calculations are constructed so that they will be more efficient for better trial wavefunction.

In fact, if the trial wavefunction is an exact eigenstate of the Hamiltonian the energy's statistical error will be zero. In this ideal case every sample of H. used the operator acting on the trial wavefunction $\mathrm{O}(\mathrm{R})$

$$
\begin{equation*}
O(R)=\frac{\Psi_{T}^{*}(R) O \Psi_{T}(R)}{\Psi_{T}^{*}(R) \Psi_{T}(R)} \tag{4-8}
\end{equation*}
$$

The initially the minimize energy in a variational calculation where O is the Hamiltonian. In nuclear physics, the Hamiltonian (and also the wave function) will depend up on the spin and isospin of the nucleons [Car90]

## 4-4-3 The variational problem

The vairiational Monte Carlo method (VMC) 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

We are going to make use of the time-independent Schrodinger equation,

Where in general we approximate $\Psi(x)$ as

$$
\begin{equation*}
\Psi(x)=\sum_{n} C_{n} f^{n}(x) \tag{4-10}
\end{equation*}
$$

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 digresses of freedom are ignored here. Multiplying equation (4-9) on the left by the complex conjugate wavefunction and integrating over the appropriate variable, the equation takes the form

$$
\begin{equation*}
\sum_{n} C_{k}^{*}\left(\int f_{k}^{*} H^{\wedge} f_{n} d \Omega\right) C_{n}=E \sum_{n} C_{k}^{*}\left(\int f_{k}^{*} f_{n} d \Omega\right) C_{n} \tag{4-11}
\end{equation*}
$$

where $d \Omega$ is the volume element. The above equation can now be written as

$$
\begin{equation*}
E=\frac{\sum_{n} C_{k}^{*} H_{k n} C_{n}}{\sum_{n} C_{k}^{*} N_{k n} C_{n}} . \tag{4-12}
\end{equation*}
$$

where $H_{k n}$ and $N_{k n}$ represent the Hamiltonian and overlap matrix elements with

$$
\begin{gather*}
H_{k n}=\int f_{k}^{*} H f_{n} d \Omega .  \tag{4-13}\\
N_{k n}=\int f_{k}^{*} f_{n} d \Omega \ldots .
\end{gather*}
$$

The coupled equations of the form.

$$
\sum_{n} H_{k n} C_{n}-E \sum_{n} N_{k n} C_{n}=0 .
$$

That constitute a generalized eigenvalue problem.

## 4-4-4 Error estimate

The matrix elements entering the eigenvalue problem might well be evaluated numerically 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 equation (4-15) can be obtain from the linear perturbation of the eigenvalue problem

$$
\begin{equation*}
\sum_{n}\left(H_{k n}+\delta H_{k n}\right)\left(C_{n}+\delta C_{n}\right)=(E+\delta E) \sum_{n}\left(N_{k n}+\delta N_{k n}\right)\left(C_{n}+\delta C_{n}\right) . \tag{4-16}
\end{equation*}
$$

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

$$
\begin{equation*}
\delta E=\frac{1}{C_{k} N_{k n} C_{n}}\left(C_{k} \delta H_{k n} C_{n}-E C_{k} \delta N_{k n} C_{n}\right) . . \tag{4-17}
\end{equation*}
$$

with summation convention implied.
Since in reality the errors in the Hamiltonian and overlap matrix elements are likely to be correlated. Away 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.

A real symmetric matrix of the from

$$
C=\left|\begin{array}{llll}
\sigma^{2}\left(H_{l l}\right) \ldots \operatorname{cov}\left(H_{l l} H_{n n}\right) & \operatorname{cov}\left(H_{l l} N_{1 l}\right) \ldots \operatorname{cov}\left(H_{l l} N_{n m}\right)  \tag{4-18}\\
& & & \\
\operatorname{cov}\left(H_{n n} H_{l l}\right) \ldots & \sigma^{2}\left(H_{n n}\right) & \operatorname{cov}\left(H_{n n} N_{1 l}\right) \ldots & \operatorname{cov}\left(O_{n n} N_{n n}\right) \\
\operatorname{cov}\left(N_{l l} H_{l l}\right) \ldots \operatorname{cov}\left(N_{l l} H_{l l}\right) & \sigma^{2}\left(N_{l l}\right) \ldots \ldots . . \operatorname{cov}\left(N_{l l} N_{n n}\right) & \ldots \\
& & & \\
\operatorname{cov}\left(N_{n n} H_{l l}\right) \ldots \operatorname{cov}\left(N_{n n} H_{n n}\right) & \operatorname{cov}\left(N_{n n} N_{l l}\right) \ldots & \sigma^{2}\left(N_{n n}\right)
\end{array}\right|
$$

with dimensions $\left(2 n^{2}\right) \times\left(2 n^{2}\right)$. 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. Diagonalizing the covariance matrix is equivalent to obtaining a new set of uncorrelated observables that each is a linear combination of the old ones.

The conventional approach to calculating the estimated error is as follow

1. Assume that the calculation calls for the smulation of N particle
2. Calculate the mean value of (expectation value) [Bie01].

$$
\begin{align*}
\langle O\rangle=\lim _{n \rightarrow \infty} & \frac{1}{n} \sum_{i=1}^{N} O(x i) \\
<O> & \approx O^{-} \ldots \ldots \ldots \ldots \ldots \ldots . . . . . . . . . . . . . . . . . . ~ \tag{4-20}
\end{align*}
$$

where the $x_{i}$ represents the set of appropriate coordinates that are distributed according to a probability density $\omega(x)$ [Bie01

The expectation value $<O>$ corresponds to the average of the quantity $O$ over an infinite ensemble of statistically independent trials.

The random walk that is actually performed in simulations provides an average over a finite sequence of measurement. This sample average or mean will be denoted by $\bar{O}$. In the case of $N$ samples taken from a distribution.
3.Estimate the variance associated with the distribution of the xi [Bie01]

$$
\begin{equation*}
\sigma^{2}=\frac{1}{N} \sigma_{o}^{2} . \tag{4-22}
\end{equation*}
$$

with

$$
\begin{equation*}
\sigma_{o}^{2}=\left\langle O^{2}\right\rangle-\langle O\rangle^{2} \tag{4-23}
\end{equation*}
$$

The fact that there is a correlation between individual measurements corresponds to the case where

$$
\begin{equation*}
<O_{i} O_{j}>\neq<O_{i}><O_{j}> \tag{4-24}
\end{equation*}
$$

When the above is taken into consideration the variance of the mean becomes

$$
\begin{align*}
& \sigma^{2}\left(O^{-}\right)=<\left(O^{-}-\langle O>)^{2}>\right. \\
&=<\left(O^{-}-\left\langle O^{-}>\right)^{2}>.\right.  \tag{4-25}\\
&=<O^{2}>-<O^{-}>^{2} \\
&=\frac{1}{N^{2}} \sum_{i j}\left(<O_{i} O_{j}>-<O_{i}><O_{j}>.\right.
\end{align*}
$$

This described the deviation of the calculated mean from the theoretical expectation value, the true variance for the mean can be written as [Dan84].

$$
\begin{equation*}
\sigma^{2}(\bar{O})=\frac{1}{N}\left[\sigma_{0}+2 \sum_{t=1}^{N-1}\left(1-\frac{t}{N}\right) \rho_{t}\right] \tag{4-26}
\end{equation*}
$$

Where

$$
\begin{align*}
& \rho_{t} \equiv<O_{i} O_{j}>-<O_{i}><O_{j}>\quad t=|i-j| \\
& =\left\langle O_{i} O_{i+t}>-\left\langle O_{i}\right\rangle\left\langle O_{i+t}\right\rangle\right. \tag{4-27}
\end{align*}
$$

the covariance between the means of two different quantities, $O$ and $\left(O^{\prime}\right)$, since

$$
\begin{align*}
\operatorname{cov}\left(\bar{O} \bar{O}^{\prime}\right) & =\left\langle\bar{O} \bar{O}^{\prime}\right\rangle-\langle\bar{O}\rangle\left\langle\bar{O}^{\prime}\right\rangle \\
& =\frac{1}{N^{2}} \sum_{i j}\left(\left\langle O_{i} O_{j}^{\prime}\right\rangle-\left\langle O_{i}\right\rangle\left\langle O_{j}^{\prime}\right\rangle\right)  \tag{4-28}\\
& =\frac{1}{N}\left[\gamma_{0}+2 \sum_{t=1}^{N-1}\left(1-\frac{t}{N}\right) \gamma_{t}\right]
\end{align*}
$$

where similarity to equation (4-27) we define

$$
\begin{equation*}
\gamma_{t} \equiv\left\langle O_{i} O_{j}^{\prime \prime}\right\rangle-\left\langle O_{i}\right\rangle\left\langle O_{j}^{\prime \prime}\right\rangle \tag{4-29}
\end{equation*}
$$

## 4-4-5 Estimating auto- and cross correlation

An estimate for $\rho_{t}$ and $\gamma_{t}$ can be obtained through the auto-and crosscorrelation coefficients.

The auto correlation coefficients are intrinsic properties of the Marko chain, closely related to the eigenvalues. They determine the error limits on the sample averages and also the optimal sampling interval length, it is important to have a reasonable estimate for them [

The auto-correlation coefficients, $C_{t}$ is defined in the case of $N$ samples as:

$$
\begin{equation*}
C_{t}(O)=\frac{1}{N-1} \sum_{i=1}^{N-t}\left(O_{i}-O^{-}\right)\left(O_{i+t}-O^{-}\right) . . \tag{4-30}
\end{equation*}
$$

While the cross-correlation coefficients as

$$
\begin{equation*}
C_{t}\left(O, O^{-}\right)=\frac{1}{N-1} \sum_{i=1}^{N-t}\left(O_{i}-O^{-}\right)\left(O_{i+t}^{\prime}-O^{-{ }^{-}}\right) \tag{4-31}
\end{equation*}
$$

The variable $t$ will be referred to as the correlation time. These two coefficients provided biased estimators for $\rho_{t}$ and $\gamma_{t}$, in the sense that they underestimate the actual values, this is expressed as

$$
\begin{align*}
& \left\langle C_{t}(O)\right\rangle=\rho_{t}-\sigma^{2}(O)+\Delta_{t} \ldots . .  \tag{4-32}\\
& \left\langle C_{t}\left(O, O^{-}\right)\right\rangle=\rho_{t}-\sigma^{2}(O)+\Delta_{t}^{\prime} \tag{4-33}
\end{align*}
$$

Where the terms $\Delta_{t}$ and $\Delta_{t}^{\prime}$ are given as

$$
\begin{gather*}
\Delta_{t}=2\left(\sigma^{2}\left(O^{-}\right)-\frac{1}{N(N-t)} \sum_{i=1}^{N-t} \sum_{j=1}^{N} \gamma_{i j}\right) \ldots \ldots .  \tag{4-34}\\
\Delta_{t}^{\prime}=2\left(\operatorname{cov}\left(O^{-} O^{-}\right)-\frac{1}{N(N-t)} \sum_{i=1}^{N-t} \sum_{j=1}^{N} \gamma_{i j}^{\prime}\right) . . \tag{4-35}
\end{gather*}
$$

With

$$
\begin{aligned}
& \gamma_{i j}=\left\langle O_{i} O_{j}>-\left\langle O_{i}>\left\langle O_{j}\right\rangle\right.\right. \\
& \gamma_{i j}^{\prime}=\left\langle O_{i} O_{j}^{\prime}\right\rangle-\left\langle O_{i}>\left\langle O_{j}^{\prime}\right\rangle\right.
\end{aligned}
$$

However, in most applications the largest correlation time in $\rho_{t}$ and $\gamma_{t}$ is finite, meaning that equations (4-26) and (4-28) can be approximated by

$$
\begin{gather*}
\sigma^{2}(\bar{O}) \approx \frac{1}{N}\left[\sigma_{0}^{2}+2 \sum_{t=1}^{T}\left(1-\frac{t}{N}\right) \rho_{t}\right]  \tag{4-36}\\
\operatorname{cov}\left(O^{-}, O^{-}\right) \approx \frac{1}{N}\left[\operatorname{cov}\left(O, O^{\prime}\right)+2 \sum_{t=1}^{T} 2\left(1-\frac{t}{N}\right) \gamma_{t}\right] \tag{4-37}
\end{gather*}
$$

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 $\left\langle O_{i} O_{j}\right\rangle-\left\langle O_{i}\right\rangle\left\langle O_{j}\right\rangle$ and $\left\langle O_{i} O_{j}^{\prime}\right\rangle-\left\langle O_{i}\right\rangle\left\langle O_{j}^{\prime}\right\rangle$ become zero for large enough correlation time $t=|i-j|$. The parameter $T$ in the above equations represents a cut off 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 $\Delta_{t}^{\prime}$ in equations (4-32) and (4-33) will become arbitrarily small for sufficiently large number of samples $n$.

Provided that $\left(\frac{T}{N}\right)$ is sufficiently small, the variance and covariance can be Approximated by:

$$
\begin{align*}
\sigma^{2}(0) \approx & \frac{\sigma_{0}^{2}+2 \sum_{t=1}^{T} C_{t}}{N} \\
& =\left(1+2 \frac{\sum C_{t}}{\sigma_{0}^{2}}\right) \frac{\sigma_{0}^{2}}{N}  \tag{4-38}\\
\operatorname{cov}(O, \bar{O}) \approx & \frac{C_{0}+2 \sum_{t=1}^{T} C_{t}}{N} \\
= & \left(1+2 \frac{\sum C_{t}}{C_{0}}\right) \frac{C_{0}^{2}}{N} \tag{4-39}
\end{align*}
$$

The above equations provide as with a way of measuring the strength of correlations in a particular simulation through the 'normalized' correlation coefficients, $C_{t} / \sigma_{o}^{\tau}$ and $C_{t} / C_{o}$. these can be obtained for a particular simulation as a function of the correlation time $t$.

The variance of equation (4-38) and the normalized auto and cross correlation coefficients of (4-30) and (4-31) were sampled as functions of correlation-time. This way done for the matrix elements of both the Hamiltonian and overlap matrices. The result is shown in figure (4-1). We can see in the upper part of the figure that the variance strongly depends on the correlation coefficients, starting from a minimum 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. This is backed up by sampling the correlation coefficient rapidly decays as the correlation time increases. According to the figure we can safely assume 50 samples as the value of the cutoff.

In the alpha-particle calculation we do not have knowledge of the exact simulation variance, since this would require the expectation value of the sample
average. We assume that the value obtained through the approximate equations (4-38) and (4-30) is sufficiently accurate.

Since we can obtain the numerically exact value for $H_{k n}$ and $N_{k n}$ 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. Such ashe variance for the each matrix element. For example the variance for the Hamiltonian matrix element is given as

$$
\begin{align*}
& \frac{\sigma^{2}\left(H_{k n}\right)}{N}=\left\langle\left(\bar{H}_{k n}-E_{k n}\right)^{2}\right\rangle \\
& \approx \sum_{i=1}^{n}\left(\bar{H}_{k n}^{i}-E_{k n}\right)^{2} \tag{4-40}
\end{align*}
$$

Where $E_{k n}$ corresponds to the exact value while the summation is over a number of distinct random walks with $\bar{H}_{k n}^{i}$ denoting the distinct average obtained in ith walk consisting of $N$ samples.

The approximation symbol becomes equality in the limit of large $n$.

Show figure (4-2) the relationship between the exact value of the variance and the correlation time and comparision between the statistical value and estimator value


Figure 4-1: The variance (upper part) and the normalized auto-and cross-correlation coefficients (lower part) as a function of correlation time. These results for the Hamiltonian and overlap matrices of the alpha-particle J-TICI(2) calculation.


Figure(4.2) 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 $\mathbf{t}$ 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

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 take use both of intermediate moves and the correlation coefficient.

## 4-4-6 Variance reduction

In this section explain a method to reduce the variance on the Monte Carlo sample averages used is techniques is to reduce the lime it takes to calculate a result with a given variance. Hence, with the calculated result is associated an estimated variance $\sigma^{2}$ [Bie01]

The so called 'zero variance principle' is a way of increasing the efficiency of a Monte Carlo algorithm by reducing the variance. The method is described in [Ass99] where applications of the zero-variance principle were shown to be very powerful. This variance reduction technique is examined in order to establish its application for the case of many-body cluster models.

Although the variance reduction technique in principle can reduce the variance of an observable

In fig. (4-3) shows the relationship between the variance in the $y$-axis and the number of component in x -axis for the alpha-particle in the $\mathrm{J}-\mathrm{TICI}(2)$ approximation. Although there is a substantial reduction in the variance of the alpha-particle calculation (about $80 \%$ ), this is not a reduction that can be of practical help. Having in mind that the error is given by the standard deviation we have that its value changes with the number of samples as $\frac{1}{\sqrt{N}}$.

Therefore, the variance reduction for the alpha-particle is not sufficient for adding the numerical calculation.

Furthermore, we attempted to apply the variance reduction technique beyond the alpha-particle $e . g$, the for ${ }^{5} \mathrm{He}$ and ${ }^{6} \mathrm{He}$. In these case the wavefunction is no longer given by a $0^{+}$but by a more complicated antisymmetrized product of spatial and spin-isopin parts.


Figure(4.3) The variance of the various matrix element 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 was plotted against the number of components used to approximate the trial function.

In terms of accuracy we are interested in obtaining the results that are accurate within $(0.1 \%)(\sim 10-50 \mathrm{KeV})$. Although the linear approximation of the 'zero variance principle' seems not to be of any substantial help for systems more complicated than the alpha-particle. We can always obtain the required accuracy within reasonable time-limits. In principle we could have looked for a more complicated approximation than the one at hand, but this is beyond our purpose since it over complicates an already complicate problem.

Is a numerical Monte Carlo method used to find solutions to mathematical problems which may have many variables) that cannot easily be solved. Its efficiency relative to other numerical methods increases when the dimension of the problem increases.

The error provided by the Monte Carlo method is of statistical nature (variance). This was analyzed in detail in the main body of this chapter. As indicated by a number of results we can obtain a reliable error estimate. The work
provided by this chapter ensures a reliable numerical method and we are confident that the results obtained are within the error bounds, the work in this chapter depends on the woke of the scientist N.Walet on the field of VMC method.

## 6-1 Conclusions

The subject of this thesis was the approximate solution of the few-body schrödinger equation in terms of a linear variational problem with application to light nuclei. The most basic ingredient in such an approximation is the construction of the trail wavefunction. So, In this thesis study some physical properties of the light nuclei. The ground state energy and the one -two body densities have been calculated. The variational wavefunction consists of three factors: a central Jastrow term, a spinisospin term and a model wavefunction. One type of such parametrization is given by the Coupled-Cluster Model (CCM). The basic principle of the CCM is that the exact wavefunction can be obtained by correlating a starting reference function. The CCM in this study dependent on the alpha - partical, a microscopic CCM is well adapted to halo nuclei.

In chapter 5 We could demonstrate the applicability of our model to open-shell system by initially making use of the same semi-realistic interactions that bind the alpha-particle. Although this could not produce bound-state for 6 He and 9 Be our calculations demonstrated the several aspects of our model.

We except that our sample version of the nuclear interaction is not adequate to reproduce what is expected for halo nuclei from experimental evidence. This conclusion was drawn from the variational character of the results. Since could not find any of the nuclei examined to be bound, i.e., to poses a variational stationary point. A part from the nuclei of 5 He and 8 Be the experimentally are unbound, those of 5 He and 8 Be are known halo nuclei. The general behaviour obtained was that the energy approached a minimum, as the separation between the several constituents increased. This could be monitored by observing the spherically averaged one-and two-body density distributions. We could clearly see that the energy was minimized as the one-body distribution broadened with the center shifting a way from the origin. The two-body density distribution separated into two parts: a main body similar to the alpha-particle and a small tale effect. We used algorithmic scaling in order to distinguish the two parts.

Despite the fact our interaction is not adequate for the light halo nuclei of 6 He and 9Be we demonstrated that our model can produce bound state for such open-shell systems by modifying the inter-nucleon force. This was done by artificially altering the Wigner part of the S3 interaction, where we could obtain bound states for both 5 He and 6 He .

In this study show the relationships between the energy and the width of shell, the energy and the distance parameters and compared with 5 He the calculation for 6 He is substantially more complicated, Since the number of parameters is too many for the entire set to be displayed in an eligible plot, the general behaviour of the 6 He calculation through some selected configurations, that nevertheless are conclusive. Although, this is one of the simplest possible configurations it is conclusive for the case of ( $\mathrm{S}=0, \mathrm{~T}=1$ ) spin and isospin quantum numbers. the variational behaviour is similsr to that of 5 He , where for large enough $\omega$ the dependence on the distance parameters becomes negligible, while the value for the ground state energy approaches that of the alpha-particle as the value of $w$ increases show in fig. $\{(5-$ $6),(5-7),(5-8),(5-9)\}$.

Finally one and two body densities obtained for the nuclei studied with approximations of the wavefunctions, the probability finding two - particle in the short range is very small this is caused by the correlation function, but in one- body the probability is large because the probability of finding the particle approach to the center is very large.

For the one-body density we can clearly see that the effect of either moving the dineutron away from the alpha-particle or the two-neutron away from each other or both shifts the average probability away from the center-of-mass (the origin) and furthermore broadens the distribution. This is again a similar behavior to 5 He . The tail effects for 6 He are more profound that those of figure (5-3) for 5 He , particularly from more localized configurations. The non-existence of a variational minimum suggests an unbound structure. Furthermore, this is supported by the fact that the value for the ground-state energy never goes below that of the alpha-particle. Despite the fact that
we have a rich configuration space, the importance of the variational parameters is only significant for a well localized system. The value obtained for the binding energy of a well localized wavefunction is well above that of the alpha-particle. Thus our approximation of 6 He as an $\alpha+\mathrm{n}+\mathrm{n}$ (alpha-particle+neutron+neutron) system is not adequate to construct the Borromen system in the absence of a spin-orbit force. show fig. $\{(5-3)(5-10)$ and fig.(5-11) $\}$.

The calculation for 9Be did not show any different behavior from the previous cases. Again there is not a variational stationary point and at the limit of large separation between the two alpha-particles and the additional neutron the energy approaches its minimum.
the error bars of figure (5-15) are considerably bigger than any of the previous cases, since we restricted the number of Monte-Carlo samples due to the rapid increase in computation time. Never the less, the restricted sampling did not effect the clarity of the results, although in principle we could always allow for more computer time.
In that case we did not fully antisymmetrize the reference state between the two alphaparticles. Although the remaining antisymmetry forces the wavefunction to be unbound at relatively small separations, there appears a strong minimum, including that 8 Be is bound. This is in contradiction from we found when we correctly imposed the full antisymmtry [figure (5-19)]. We worked in the L-S coupling scheme and assumed that the alpha-particle remained in the $0+$ state. The incorporation of the antisymmetry condition, appropriate for fermions, has been given special attention where it was found that the complexity greatly increases in going beyond the alphaparticle.
The general conclusion is that our simple version of a variational approach to light halo nuclei is capable of producing bound states to the open-shell systems. However, this required a small modification of the potential function. In the case where direct use of available semi realistic interactions was made we could not find any of the nuclei examined to be bound, i.e., to poses a variational stationary point. A part from the nuclei of 5 He and 8 Be are known halo nuclei. It seems that the absence of spin
orbit coupling is critical for these nuclei. It seems that the absence of spin-orbit coupling is critical for these nuclei.

In addition to the absence of spin-orbit terms in the interaction that can alter the symmetry and thus the binding energy of the ground state the form of the wavefunction employed has a number of approximations. Although, this is important for the case of the light halo nuclei and is not necessarily the major approximation for the general many-body problem.

Therefore, the general conclusion is that we have a successful cluster like model that can produce bound states of open-shell nuclei, despite the fact that in reality a spin - orbit term might be necessary.

## 6-2 - Suggestions

The fact that our results, using the semi-realistic V4 introduction introduced in chapter 3 did not provide a bound state for the halo nuclei of interest was expected since the experimental evidence points towards the need for spin-orbit terms. A possible future development is the inclusion of such terms in the interaction. We can both add more terms and investigate some more realistic types of nucleon-nucleon potentials. Future more, working with spin-orbit force will require rethinking the inclusion of permutation symmetry and will increase all allowed configuration.

Another possibility is to include more structure in the reference function. In the J-TICI (2) this can be achieved by providing a multi-linear expansion where we expand both the linear operator and the reference function. However, such a formalism is not as straight forward as the case of a single $0^{+}$alpha-particle state, since it is not clear what type of basis-functions will be used. An adequate alpha-particle $0^{+}$state can be obtained by correlating a Harmonic oscillator ground state. Extra nucleons can then be added by assigning coordinates relative to the alpha-particle center-of-mass. It is not clear how the model will develop if we wish to go beyond the alpha-particle $0^{+}$state. However, this is not the most immediate future development.

We avoided using state-dependent correlations because of simplicity. Another possibility for future work is to examine more closely the effect of these correlations, so that a more economic approach can be found for including them into our calculations. As shown in chapter 3, the number of spatial integrals required greatly increases when state-dependence is included in the correlations. This makes calculations of this type impractical when moving to heavier systems. However, the analysis performed for the alpha-particle greatly simplifies matters, by using some simple results from the theory of the symmetric group. Despite the fact that this simplification is lost when we move away from the alpha-particle, reconsidering the problem might yield further simplifications that are applicable beyond the alpha-particle.

A part from improvements in the current model we can broaden our investigation in order to examine the continuum states provided by our formalism, such as resonance states. This can be done using the method of complex scaling [Rei82]. This reduces the study of resonance to that of bound states by examining complex eigenvalues. The complex scaling method has been shown to be a powerful method for solving resonance of three-body systems [Kiy01], where ${ }^{6} \mathrm{He}$ and ${ }^{11} \mathrm{Li}$ were studied as three-body systems. By studying the unbound states produced by our model we can obtain further information about the structure of the wavefunction.

## Examination Committee Certification

We certify that we have read this thesis and examined the student on its contents, and that in our opinion it is adequate for the partial fulfillment of the requirements of the degree of Ph.D. of Science in Physics

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## االخلاصة

احد الاكتشافات التي حدثت مؤخرا في الفيزياء النووية هي وجودالانوية السحرية(Halo nuclei).
الانوية السحرية هي انوية ضميفة الترابط حيث قلب النواة مع كثافة نووية طبيعية محاطان بمنطقة من مادة نووية مخففة كما في (كالنيوترون السحري). مثل هذه النوى تتواجد بكثافات خفيفة اوثقيلة، ان هذه الانوية موضوع بحث عدد كبير من الاراسات النظرية وكذلك العملية لغرض فهمها بطريقة اكثر وضوحا. ولهذا لوحظ خلال السنوات العشر اللسابقة اتسعت دراسة هذه الانوية. وفي هذه الاراسة تم فصص عدد من الانوية السحرية ومعالجتها بعدة طرق وايجاد بعض الخصائص الفيزيائية لهذه الانوية.
في هذه الاطروحة تم فحص تركيب النوى السحرية الخفيفة من خلال الانموذج المجهزي المتغير، هنا الانموذج هو عبارة عن توسيع لعمل سابق عن القشر

المغلقة.
تم استخدام الانموذج العنقودي المزدوج في هذه الاطروحة بالاعتماد على جسيمة الفا كاساس في الانموذج العنقودي وكذلك النيوترونات التي تظهر من خلال

ها الانموذج.
كما تم معالجة الدالة الموجية بطرق التغاير وطريقة جاسترو للوصول الى دالة موجية اختبارية مقاربة الى الاالة الموجية الحقيقية. الدالة الموجية نحصل عليها من حالة االمصدر والتي تتضمن المتناظرات المطلوبة وتقام وصف انتقالي (ثُابت) للنظام يشكل عناقيد متعددة وغير مترابطة بعد ذلك نستخدم المؤثرات المترابطة ( بنوعيها المدى المتوسط الى الطويل الخطي والمدى القصير اللاخطي ) للحصول على دالة موجية جديدة، كم ان الدالة الموجية في الانموذج العنقودي تسمح بوصف الحركة الاهتزازية بين التجمعات داخل النواة.

ان اهمية هذه الطرق تكمن في ايجاد حل لمعادلة شرودنكر كما تم الاعتماد على تفاعل نوية ـ نوية شبه الواقعية للوصول الى الجهـ المطلوب، وان هنا البحث يتطابق مع مبدآ باولي للاستبعاد.
كما تم استخدام طريقة مونتي كارلو في هذا البحث وذلك لانها تمتاز بدقة رقمية عالية. وتولي اهتمام عالي لمتطبات الانموذج الدقيقة. "والافضل استعمال المترابطات بحالة عشوائية كما يجب الاخذ بنظر الاعتبار تقدير الاخطاء بصورة اكثر دقة"

في هذه الاطروحة تم استخدام الانموذج لفحص الانوية التالية: (5He,6He,8Be,9Be) توزيع الكثافة لجسيم واحد و لجسيمين. بعدها نحصل على صورة نوعية لتوزيع المادة في النواة التي نحصل عليها وتجهيز تحليل معين لحالة مقيدة واحدة تتطب قوة المدار-البرم في خطة مزدوج ( L - S ) ستظهر لنا انموذج قادر على انتاج حالات مقيدة يقترح لانظمة القشر المفتوحة بشكل اصطناعي لتعديل التعبير المركزي للتفاعلات شبه الو اقعية المستخدمة. كما تم ايجاد علاقة الطاقة مع عرض القشرة، وكذلك ايجاد سلوك النواة من خلال ايجاد العلاقة بين الطاقة والمسافة الى مركز كتلة جسيمة الفا. (5He ,8Be) هي انوية سحرية ، نلاحظ اللنوك العام للطاقة تقترب للحد الادنى وهذه يمكن ملاحظتها من المعدل الكروي لتوزيع الكثافة لجسيم و جسيمين،امـا الانوية الخفيفة (6He,9Be)
في هذه الاطروحة تم كتابة البرامج باستخدا لغة الفورتران (77).


جمهورية العراق
وزارة التُليم العالي والبحث العلمي جامعة النهرين كلية العلوم
قسم الفيزياء

تطبيقات الانموذج العنقودي المزدوج في الانوية الخفيفة

## رسالة

مقدمة إلى كلية العلوم في جامعة النهرين و هي جزء من متطلبات نيل درجة دكتور اه فلسفة

في
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باشراف كل من
الدكتور ليث عبد العزيز العاني الدكتور سعد ناجي عبود

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# APPIIEATIONS OF GOUPLED CIUSTER MODEL IN LIEHT NUGLEI 

A Thesis<br>Submitted to the College of Science of AL-Nahrain University in Partial Fulfillment of the Requirements for the Degree of Doctor of Philosophy<br>in<br>Physics<br>by<br>Alyaa $\mathcal{H}$ usain Al-Se6ahe<br>(B.Sc.2000)<br>(M.Sc.2002)

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