INFLUENCE OF LEFT RIGHT ASYMMETRY DEGREES OF FREEDOM IN SELF-CONSISTENT CALCULATION OF ^{20}Ne

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Abstract

Within a constrained Hartree-Fock calculation we investigate the effects of left right asymmetric degrees of freedom associated with the channel $^{16}O + {}^{4}He \leftrightarrow {}^{20}Ne$. We find a large softness of ^{20}Ne against octupole deformation. The optimal solution after restoration of the parity by means of a projection shows a pronounced $^{16}O + {}^{4}He$ clustering. A generator coordinate calculation along the collective path confirms this conclusion. Once center of mass motion effects are taken into account a good agreement with experiment is found.

1. INTRODUCTION

The energy of the α decay threshold of ^{20}Ne is remarkably low (4.75 MeV). This distinctive feature which is a consequence of the magicity of both of the decay products has been studied in several cluster model investigations. Those were able to reproduce the spectra, the B(E2) values and α width of the ground state band and of some excited bands of ^{20}Ne (for a recent review see ref.1). The interplay between shell model and cluster configurations has been studied by Tomoda and Arima [2]. Combining wave functions of two different model spaces they were also able to reproduce most of the characteristics of the spectrum of ^{20}Ne. Surprisingly the same quality of results has never been achieved in projected [3-5] or cranked Hartree-Fock calculations [6,7]. The moment of inertia of the ground state band is in general overestimated by a factor two. This discrepancy has sometimes been attributed to a wrong velocity dependence of the nuclear interaction [5,6]. However only left right symmetric configurations of ^{20}Ne were considered in these calculations. The successes of cluster model calculation on the other hand suggests that this restriction of the variational space is unphysically drastic. The aim of this work is to investigate the influence of additional asymmetric degrees of freedom on the results of self consistent calculations.

In section 2 we present a constrained Hartree-Fock calculation which describes the collective path from the symmetric configuration of ^{20}Ne to the asymptotic channel with two well separated ^{16}O and ^{4}He fragments. The collective path is defined in terms of a combination of quadrupole and octupole moments and the self consistent equations are solved on a three dimensional rectangular mesh. In section 3 we investigate the effect of restoring the parity by a simple projection

and discuss the results of a variation after projection. In section 4 we perform a generator coordinate calculation which mixes the slater determinants along the collective path. Finally in section 5 we estimate the uncertainty associated with the spurious relative motion of the center of mass of the fragments in the asymptotic channel.

2. CONSTRAINED HARTREE-FOCK CALCULATION

2.1 Method

Since a detailed account can be found elsewhere [7] we shall mainly outline the method, introduce the notations useful for the rest of the paper and insist on the aspects specific to the present calculation.

The interaction energy between the ^{16}O and ^{4}He nuclei has been calculated as a function of their interdistance. To do so we minimized the energy associated with a hamiltonian composed of a constraining operator, a one body kinetic energy operator, and a two body effective interaction. For the latter we choose the BKN force [8] supplemented by the coulomb interaction. The corresponding Hartree-Fock energy reads

$$E = \int d^3r \left(\tau(\vec{r}) + \frac{3}{8} t_0 \rho^2(\vec{r}) + \frac{1}{16} t_3 \rho^3(\vec{r}) \right) + \int d^3r \, d^3r' \rho(\vec{r}) \rho(\vec{r}') \frac{2 a V_0 e^{-\frac{|\vec{r}-\vec{r}'|}{a}} + e^2}{4 |\vec{r} - \vec{r}'|} \quad (1)$$

In formula (1) t_0, t_3, a and V_0 are parameters of the BKN force, e is the electron charge and ρ and τ are respectively the total density and the kinetic energy density defined as

$$\rho(\vec{r}) = 4 \sum_{\alpha} \left| \Phi_{\alpha}(z, \vec{r}) \right|^2 \quad (2)$$

$$\tau(\vec{r}) = 4 \sum_{\alpha} \left| \vec{\nabla} \Phi_{\alpha}(z, \vec{r}) \right|^2 \quad (3)$$

The index α which appears in the definitions of ρ and τ labels the individual orbits $\Phi_{\alpha}(z,\vec{r})$ associated with an interdistance z. Since we assumed

spin-isospin symmetry only the spacial part need be considered and a degeneracy factor 4 must be introduced.

We want to study a collective path leading from the H.F. ground state of ^{20}Ne to the asymptotic channel with two well separated nuclei ^{16}O + ^{4}He. In most H.F. calculations [3-7] the ^{20}Ne ground state is described as an axially symmetric Slater determinant with an additional left-right plane symmetry. In the present work we intend to study the effects resulting from the breaking of the latter symmetry. For technical reasons we did not enforce axial symmetry and imposed only symmetry with respect to the two perpendicular planes x = 0 and y = 0. The individual wave functions Φ_α are therefore characterized by two quantum numbers (with values $\pm$ 1) associated with these symmetries. It is easy to check that the description of the symmetric ^{20}Ne wave function and the asymptotic ^{16}O + ^{4}He channel requires the same set of quantum numbers.

The constraining operator must ensure a smooth transition between ^{20}Ne and the ^{16}O + ^{4}He system. As such a transition involves both quadrupole and octupole deformations we selected a linear combination of Q_{20} and Q_{30} as operator of constraint. Asymptotically the values of Q_{20} and Q_{30} are simple functions of the interdistance z between the fragments. When the two nuclei come into contact the interdistance z and therefore its relationship to Q_{20} and Q_{30} are no longer unambiguous. We therefore relied on a schematic model to provide us with a reasonable definition of the interdistance. We consider a system of two non overlapping sections of spheres (figure 1). The volume of each section is kept constant as a function of the interdistance z between the centers and proportional to the masses of ^{16}O + ^{4}He. The quadrupole and octupole moments of the total system assigned to a given value of z are then

easily calculated. In addition we take into account the intrinsic deformation of the H.F. ground state of ^{20}Ne, by modifying the value of Q_{20} with a linear interpolation which varies from 0 for the non overlapping and touching spheres ($z \geq 5$ fm) to the intrinsic mass quadrupole moment of symmetric ^{20}Ne ($Q \simeq 100$ fm^2) for $z = 0$. This procedure determines the collective path in the (Q_{20}, Q_{30}) plane as a parametric function of the interdistance z. It then remains to adjust the strength of the constraining quadrupole and octupole operators so that their expectation value in the self consistent solutions follows the same path. From the above discussion it is clear that the interdistance z provides only a convenient parametrization (although it recovers physical meaning asymptotically) and that the Hartree-Fock results will depend only on the collective path and not on its parametrization.

The solution of the Hartree-Fock equations was performed on a three dimensional cartesian mesh by means of the imaginary time step method [9].

2.2 Results

The critical importance of the octupole degree of freedom is apparent from figure 2 which displays the constrained Hartree-Fock energy curve. The minimum corresponds to $z = 0$ (the results for the symmetric H.F. solution ($z = 0$) are summarized in table 1 ; they compare well with experiment) but the energy varies by less than 1 MeV for interdistances up to 3.5 fm. For larger values of z the energy rises to a maximum attained for $z = 7$ fm at which point the nuclear forces cease to be active. For larger values of z the behavior of the energy is that of a pure monopole coulomb interaction. Compared to the asymptotic energy ($z = \infty$) the height of the barrier is 3 MeV. The unrealistic value for the threshold energy (8.5 MeV compared to 4.73 MeV experimentally) is due to our incomplete correction for the center of mass motion. Indeed it is effected by subtracting from the kinetic energy operator the kinetic

energy associated with the motion of the center of mass of the complete system. In the asymptotic channel this correction does not take into account the relative motion of the centers of mass of the individual ions. In the section 5 we show that most of the discrepancy is removed when one evaluates the energy associated to this relative motion by means of a simple projection.

Contour lines of the density of the system are plotted in figure 3 for three different values of the interdistance. One can note the significant octupole deformation of the density for the value $z = 3.5$ fm, which as we have seen corresponds to an H.F. energy less than 1 MeV above that of the symmetric solution.

3. PROJECTION ON PARITY

When the value of z differs from zero the determinantal wave functions are no longer eigenstates of the parity. This symmetry can be restored by a simple projection. If we denote $|z\rangle$ $(z > 0)$ the constrained Hartree-Fock solution we define $|-z\rangle$ $(z > 0)$ as the left right symmetric state of $|z\rangle$. The positive and negative parity projected states $|\Psi_{\pm}(z)\rangle$ are then defined as

$$|\Psi_{\pm}(z)\rangle = \left(|z\rangle \pm |-z\rangle \right) / \sqrt{2}$$

and the parity projected energy curves as

$$E_{\pm}(z) = \langle \Psi_{\pm}(z) | \hat{H} | \Psi_{\pm}(z) \rangle / \langle \Psi_{\pm}(z) | \Psi_{\pm}(z) \rangle$$

We have plotted on figure 2 the values $E_{\pm}$ as a function of z. The minimum of the positive parity curve no longer occurs for $z = 0$ but at $z = 3.6$ the gain in energy equals 1.27 MeV. The state $|\Psi_{+}(z=3.6)\rangle$ can be considered as the result of the (restricted) variation along the collective path after projection (VAP). Some of its properties are given in table 1. The minimum of the curve E_{-} occurs at a larger interdistance $z = 4.6$ fm. The difference between the energies of the

positive and negative parity minima is 5.48 MeV which compares well with the energy difference between the 0^+ ground state and the first 1^- state of ^{20}Ne (5.8 MeV). Before comparing these results with those obtained in earlier works we note that the energy E_- increases rapidly when z devlates from the optimal value $z \simeq 4.6$ fm in constract with the curve E_+ which except for the shallow minima at $z = \pm 3.6$ fm is rather flat for values of z between -4 fm and + 4 fm. Finally as expected, at large distances the curves E_+ and E_- become identical with the constrained Hartree-Fock curve. In our calculation the ratio $|E_+ - E_-| \; / \; |E_+|$ becomes less than 10^{-4} when z is larger than 6 fm which is slightly larger than the value z = 5.86 fm found in ref.[10]. In our opinion this difference can be explained by the too rapid decrease of the gaussian tail of the wave functions used in ref.[10].

Two different studies of the left right asymmetry properties of ^{20}Ne are available which in some of their aspects bear a strong resemblance to our calculation. In the first calculation Nemoto and Bando investigate a two cluster model consisting of ^{16}O and ^{4}He nuclei built from properly antisymmetrized oscillator shell model wave function with fixed oscillators parameters [11]. Their result (figure 3 of ref.[11] is remarkably similar to ours*. The optimal interdistances for the ^{16}O and ^{4}He clusters are z = 3.5 fm and 4.5 fm for the positive and negative parity states. At smaller interdistances however their positive parity energy curves exhibit a strong repulsion not present in our calculation.

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*Due to the simple properties of the oscillator wave functions the authors of refs.[11,12] can also perform the projection on good states of angular momentum. In this chapter we compare our results for the intrinsic states to those obtained in refs[11,12] for the 0^+ and 1^- states.

This is due to a deficiency of the two cluster model which for z = 0 leads to a promotion of the ^{4}He wave function to an highly excited spherical orbital rather than a deformed orbital of the 1d shell. This feature is not present in the α cluster model used by Nemoto et al. in ref.[12] which describes the left right symmetric state of ^{20}Ne by a regular hexaedron. Their results (figure 4 of ref.12) are qualitatively similar to ours. The positive parity state of lowest energy corresponds to a left right asymmetric configuration and the negative parity minimum occurs for an even larger asymmetry. The symmetric state of ^{20}Ne (fig.4a, b=a=3 fm) is less bound by about 1 MeV compared to the absolute minimum. We could not however compare the location of their minima with ours because we could not find a relationship between our interdistance z and the set of parameters used in the geometrical description of the five α cluster. Finally we note that the height of the ^{16}O + ^{4}He barrier relative to the minimum in their model is about twice higher than ours (see fig.4c of ref.[12]) which may indicate a deficiency of the 5 α cluster description of asymptotic channel. Indeed this feature is absent in ref.[11] which for the same quantity finds a result very similar to ours.

4. GENERATOR COORDINATE METHOD

In the preceding section we showed that a significant improvement on the description of the ground date of ^{20}Ne is achieved by projecting on parity a left right asymmetric determinantal wave function. On the other hand we noticed that the curve $E_+(z)$ does not show pronounced structures over a large interval of values of the interdistance. It seems then appropriate to investigate the effects of a mixing by means of a generator coordinate calculation (G.C.M.) of all the states along the collective path.

In order to solve the GCM equations we used the techniques exposed in ref.[13]. The continuous variable is discretized and the Hill Wheeler integral equation is replaced by the generalized eigenvalue problem

$$\sum_{j=1}^{N} \left(H(z_i, z_j) - E_\lambda N(z_i, z_j) \right) g^\lambda(z_j) = 0 \qquad (4)$$

We checked the stability against a change in the number N and the range of the collective coordinate z of the eigenvalues E_λ and the collective wave functions $f^\lambda(z)$ defined below. The functions $g^\lambda(z)$ associated with different eigenvalues are not orthonormal and cannot be interpreted as collective wave functions. For this reason it is convenient to transform the equation 4 into an ordinary eigenvalue problem. To do so one first performs a diagonalization of the overlap kernel

$$\sum_{j=1}^{N} N(z_i, z_j) h^\mu(z_j) = n_\mu h^\mu(z_i) \qquad (5)$$

and introduces the hamiltonian

$$\mathcal{H}_{\mu\nu} = n_\mu^{-\frac{1}{2}} \sum_{i,j=1}^{N} h^{\mu *}(z_i) H(z_i, z_j) h^\nu(z_j) \, n_\nu^{-\frac{1}{2}} \qquad (6)$$

The GCM equation reduces then to the eigenvalue problem

$$\sum_\nu \mathcal{H}_{\mu\nu} F_\nu^\lambda = E_\lambda F_\mu^\lambda \qquad (7)$$

and the functions

$$f^\lambda(z) = \sum_\mu F_\mu^\lambda h^\mu(z) \qquad (8)$$

which form an orthonormal set can be interpreted as collective wave functions. In fact the equations 5-7 provide also a practical algorithm for solving the GCM equation. The well known redundancy of the GCM basis associated with any continuous variable like z shows up in the appearance

of zero or close to zero eigenvalues $\mathcal{N}_\mu$ in the spectrum of the operator N (eq.5). The subspace corresponding to these eigenvalues can therefore be neglected and the eigenvalue problem (6,7) solved in the subspace of vector $\hat{f}^\mu$ with a non negligible collective norm.

The calculation of the overlap and energy kernel

$$N(z_1,z_j) = \langle z_1 | z_j \rangle$$

$$H(z_1,z_j) = \langle z_1 | \hat{H} | z_j \rangle$$

is easily performed on the rectangular (and fixed) mesh used in all the calculations of the Hartree-Fock solutions. The set of states $|z_i\rangle$ $(z_1>,<\infty)$ used in our GCM calculation included the constrained Hartree-Fock solutions as well as the states $|-z_i\rangle$ resulting from the action of the parity operator. For a simple interaction like BKN the energy kernel can be written as the integral of a local functional of a density $\rho(\vec{r})$ and a kinetic energy density $\tau(\vec{r})$ [13] formally identical to the Hartree-Fock functional (1) with an appropriate definition of the densities ρ and τ

$$\rho(\vec{r}) = \sum_{\alpha,\beta} \Phi^*_\alpha(z_i,\vec{r})\, \Phi_\beta(z_j,\vec{r})\, (\mathcal{N}^{-1})_{\beta\alpha}$$

$$\tau(\vec{r}) = \sum_{\alpha,\beta} \vec{\nabla}_r \Phi^*_\alpha(z_i,\vec{r}) \cdot \vec{\nabla}_r \Phi_\beta(z_j,\vec{r})\, (\mathcal{N}^{-1})_{\beta\alpha}$$

In the above definition the matrix $\mathcal{N}$ is given by

$$\mathcal{N}_{\alpha\beta} = \int d^3r\ \Phi^*_\alpha(z_i,\vec{r})\, \Phi_\beta(z_j,\vec{r})$$

The overlap kernel $\langle z_i | z_j \rangle$ is the determinant of the matrix $\mathcal{N}$.

The results are shown in table 2 and figure 2 for the eigenvalues and figure 4 for the collective eigenfunctions of the first two eigenstates. Due to the symmetry of the kernels under the change $(z_i,z_j) \rightarrow (-z_i,-z_j)$ the eigenstates can be sorted according to their

parity. Compared to the positive parity projected Hartree-Fock energy the GCM ground state energy is lowered by 0.2 MeV. Its collective wave function spreads over an interval $\Delta z \sim 5$ fm indicating a strong admixture of left right asymmetric components. The overall energy lowering compared to the symmetric Hartree-Fock ground state equals 1.6 MeV. The first excited state has a negative parity. Its wave function is peaked at larger interdistance. The energy lowering compared to the optimal negative parity projected Hartree-Fock is 0.5 MeV which leads to an excitation energy of 5.15 MeV (5.8 MeV exp.). The position of the second positive parity state is also in reasonable agreement with that of the first 0^+ excited state having significant α decay width (9.65 MeV calculated, 8.6 MeV exp.).

In ref.[12] the collective GCM wave functions are plotted (fig.7c) on the parameter space of the 5 α model. As said before a simple relationship with our coordinate z does not exist. Nevertheless we can note that the ground state wave function (fig.7a) spreads significantly over the space of collective parameters a result which is similar to ours. The wave functions of the 1^- (fig.7b) is, like ours, more localized in a region of the parameter space corresponding to asymmetric shapes.

5. CORRECTION FOR THE RELATIVE MOTION OF CENTERS OF MASS

In section 2.2 we mentioned that the threshold energy resulting from our constrained Hartree-Fock calculation could not be compared directly with experiment because we had not taken into account the relative motion of the centers of mass of ^{16}O and ^{4}He. To evaluate the correction associated with this relative motion we used the simple projection method discussed by Peierls and Yoccoz [14]. The energy correction is estimated as the difference between the sum of individual center of mass motion energies for ^{4}He and ^{16}O and the center of mass energy for the combined system with a fixed interdistance between the ions.

Each of the three energies is given by

$$\Delta E = \frac{\int d^3R \, \langle \vec{o} | \hat{H} | \vec{R} \rangle}{\int d^3R \, \langle \vec{o} | \vec{R} \rangle} - \langle \vec{o} | \hat{H} | \vec{o} \rangle \qquad (9)$$

where $| \vec{0} \rangle$ denotes the corresponding ground state with center of mass at the origin and $| \vec{R} \rangle$ the same state translated by the vector $\vec{R}$. For ^4He and ^{16}O the ground state is described by the H.F. solution and the overlap and energy kernels $\langle \vec{0} | \vec{R} \rangle$ and $\langle \vec{0} | \hat{H} | \vec{R} \rangle$ are calculated with the techniques described in section 4. The kernels for the system of the two infinitely separated ions are taken as the product of the individual kernels for the same value of R.

$$\langle \vec{o} | \vec{R} \rangle = \langle \vec{o} | \vec{R} \rangle_{^{16}O} \cdot \langle \vec{o} | \vec{R} \rangle_{^4He}$$

$$\langle \vec{o} | \hat{H} | \vec{R} \rangle = \langle \vec{o} | \vec{R} \rangle_{^{16}O} \cdot \langle \vec{o} | \hat{H} | \vec{R} \rangle_{^4He} + \langle \vec{o} | \hat{H} | \vec{R} \rangle_{^{16}O} \cdot \langle \vec{o} | \vec{R} \rangle_{^4He}$$

The identical displacement of the two ions, ensures that the energy correction (9) takes into account the global center of mass motion only. Finally the relative motion energy E_R is obtained as

$$E_R = \Delta E (^{16}O + ^4He) - \Delta E (^{16}O) - \Delta E (^4He)$$

The numbers corresponding to each energy correction are given in table 3 and fig.2.

The calculations are made simpler by the spherical symmetry of the two nuclei which reduces to one the dimensionality of the integrals involved in (9). Such a simplification does not exist for the H.F. ground state of ^{20}Ne and the configurations of the combined system associated with finite interdistances z.

6. DISCUSSION

The results of the present work demonstrate clearly the necessity of including the left right asymmetric degrees of freedom in self consistent calculations aiming at an accurate description of the spectroscopy of ^{20}Ne. There is really nothing to be surprised at such a finding, as it could have been guessed either from experimental information (the very low α decay threshold and large α width of the first 6^+ and 8^+ states) or from earlier calculations using cluster models [1]. Our results can be summarized as follows : the Hartree-Fock solution shows a remarkable softness against the combination of quadrupole and octupole constraint that we used to define the collective path leading to the ^{16}O + ^{4}He channel. The symmetric solution remains however the variational minimum. The parity projection changes drastically the picture. The variation after projection solution corresponds to a left right asymmetric determinant. A generator coordinate calculation using the family of determinants of the collective path improves slightly the binding energy and indicates that the collective wave function is very flat over a large range of values of the interdistances between ^{16}O + ^{4}He.

After correction for the relative motion in the asymptotic ^{16}O + ^{4}He channel, the ground state of the generator coordinate calculation lies 0.6 MeV below the threshold. This is in fair agreement with experiment if one remembers that our calculation provides only information on the intrinsic states associated with rotational bands of different parities. It is generally estimated [15,16] that a 4-5 MeV gain in energy would result from a projection of the 0^+ state. As shown in ref.[16] the excitation of the first 1^- state relative to the ground state is not significantly different from the energy difference between the optimal negative and positive parity intrinsic states. Our result 5.48 MeV compares then

reasonably well with the experimental value for the excitation of the 1^-. The last question which is not answered by our calculation concerns the problem of the moment of inertia of the ground state band. We can only note that in cluster model calculations (refs.[11,16]) the clustering is much more pronounced for the 0^+ state than for states with higher spin. The introduction of the left right asymmetry degrees of freedom in angular momentum projected Hartree-Fock could then lead to a lowering of the 0^+ state compared to the other members of the band and therefore a decompression of the band.

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TABLE CAPTIONS

Table 1 Comparison of theoretical and experimental results for the binding energy, charge radius , and charge quadrupole moment of ^{20}Ne (H.F. for the Hartree-Fock solution, V.A.P. for variation after projection, and G.C.M. for generator coordinate method).

Table 2 Energies in MeV of the H.F. ground state, of the positive and negative optimal solutions resulting from a variation after projection, and of the first four eigenstates of the generator coordinate calculation.

Table 3 Center of mass energy corrections in MeV estimated by the projection method.

Table 1

	E MeV	r_c fm	Q_c fm²
Exp.	-160.65	2.91	56.4 ± 2.7
H.F.	-160.11	2.99	50
VAP	-161.38	3.02	53
GCM	-161.60	3.04	55

Table 2

H.F.	VAP		GCM			
	E_+	E_-	E_{1+}	E_{1-}	E_{2+}	E_{2-}
-160.11	-161.38	-155.90	-161.60	-156.45	-151.95	-149.94

Table 3

$\Delta E(^4He)$	$\Delta E(^{16}O)$	$\Delta E(^4He+^{16}O)$	ε_R
9.5	10.7	10.8	-9.4

FIGURE CAPTIONS

Figure 1 Parameters of the schematic model used to specify the constraining operator of the collective path (see text)

Figure 2 Deformation energy curves as a function of the interdistance z between the nuclei ^{16}O and ^{4}He. The full curve corresponds to H.F. while the dashed and dotted curves correspond respectively to the energy of the plus and minus parity projected states. Also shown are the position of the intrinsic states associated to the first and second positive parity bands and the first negative parity band as predicted by the generator coordinates. In the central part of the figure are indicated the value of the threshold as deduced after correction for the relative motion of the ions. On the right part of the figure we show the position of the first experimental positive and negative parity band heads relative to the threshold.

Figure 3 Contour lines of equidensity of the constrained Hartree-Fock solutions corresponding to three distincts values of the interdistance z between ^{16}O and ^{4}He. The lines are determined in a symmetry plane containing the elongation axis z. The interval between two lines corresponds to a density variation $\Delta\rho = 0.02$ fm^{-3}.

Figure 4 Collective wave functions of the intrinsic ground state (positive parity) and first excited state (negative parity).

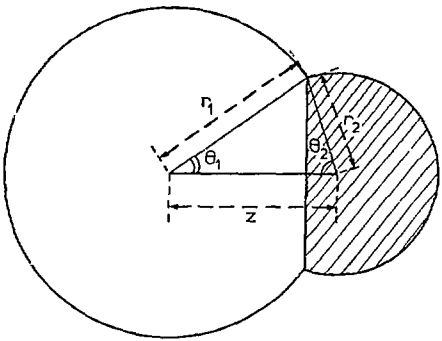

Fig.1

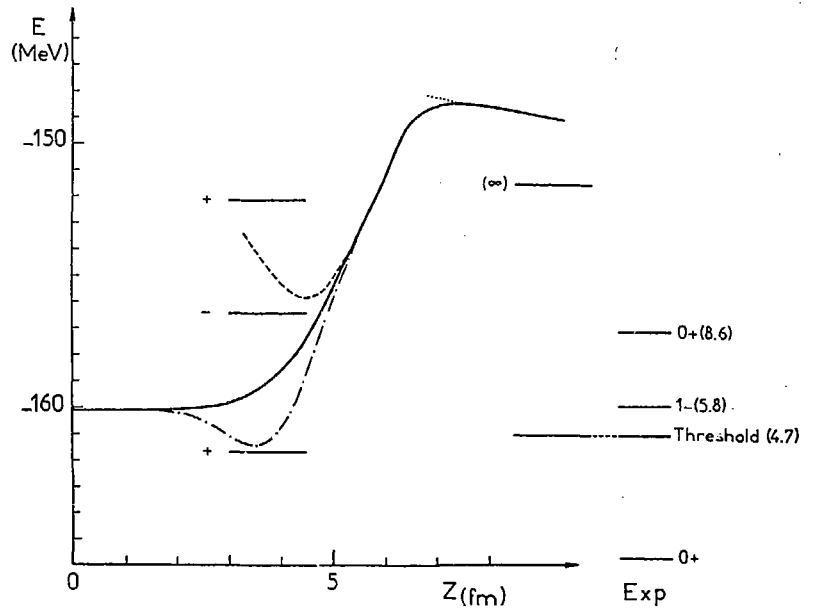

Fig.2

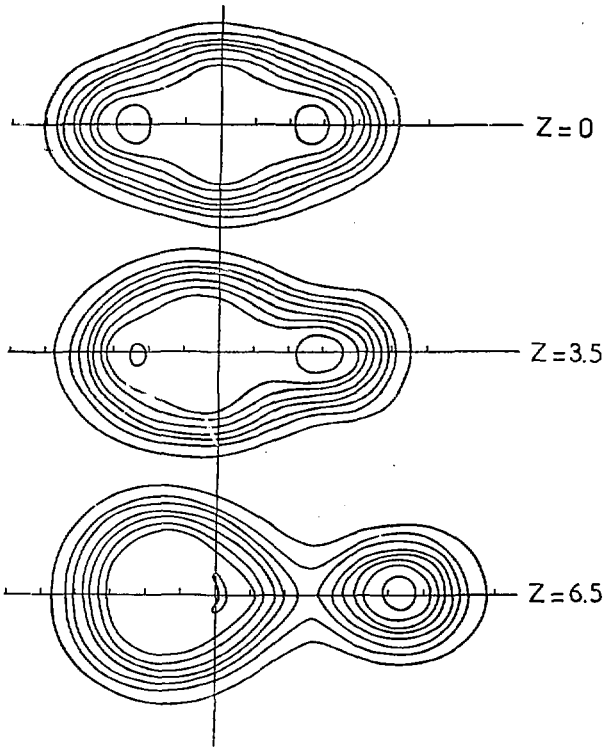

Fig.3

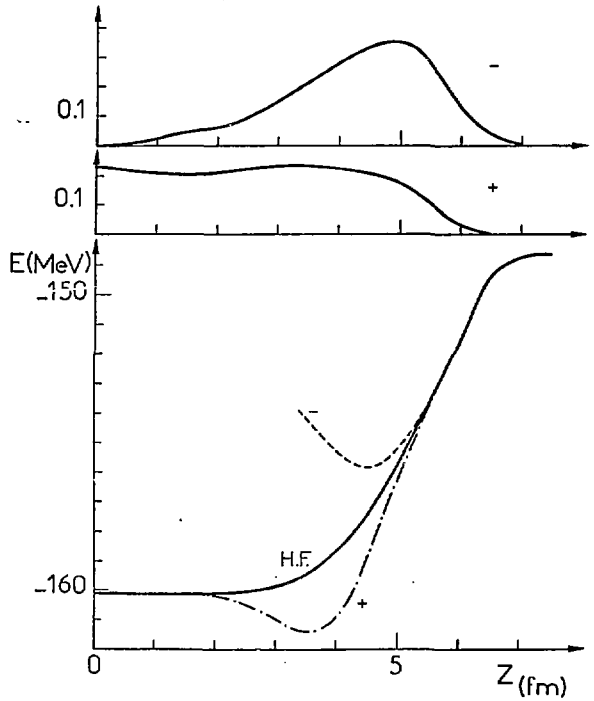

Fig.4