Vibrations and potential energy surfaces (with Argonne V18) of ^{4}He and ^{3}He

Lorenzo Fortunato

Dipartimento di Fisica e Astronomia "G.Galilei" - Università di Padova
I.N.F.N. - Sez. di Padova,
via F.Marzolo 8, I-35131 Padova, Italy

E-mail: `fortunat@pd.infn.it`

Abstract.   A potential energy surface is constructed for ^{3,4}He with the two-body Argonne V18 potential. The minimization suggests a semi-rigid asymmetric top structure for ^{4}He, where the appropriate point-group symmetry is C_2. We calculate the Hessian matrix, determining the 6 normal modes of vibration (in the range 300-700 MeV). The breathing mode is found to lie at too high an energy to be observable and the nature of the 0_2^+ excited states of the alpha particle at 20 MeV should probably be sought elsewhere. Similar investigations have been carried out for the A=3 system, finding a planar C_s configuration (scalene triangle) and three excited vibrational states (in the range 600-1900 MeV).

1. Introduction

In this contribution, the application of methods and techniques of quantum chemistry and molecular physics to the realm of nuclear physics is explored. This somewhat unconventional approach to nuclear structure has a tradition that goes back to early works in nuclear theory, such as those of Wheeler [1], Hafstad and Teller [2] and many others. Several studies on clusterization and exotic states of nuclear systems have relied on the same approach, for example the works of von Oertzen and collaborators [3, 4] where a Linear Combinations of Nucleonic Orbitals has been used, or works on the two center shell model [5]. Most of these approaches are nicely reviewed in Ref. [6] where details can be found about cluster models, Ikeda rules and several phenomenological approaches. Recently Bijker and Iachello have developed an algebraic version of cluster models that incorporates point-group symmetries and gives very interesting results on ^{12}C and ^{16}O [7, 8].

The common criticism to the application of molecular-type approaches to nuclei, revolves around the different stiffness of the two systems: most molecules are rigid (although there are examples of floppy molecules and of fluxional or super-rotor [9] molecules that baffle this traditional approach), while nuclei are 'liquid', in the sense that one expect large fluctuations inside the strongly interacting system, that forbid 'rigid' structures. Nevertheless, one normally adopts certain well-defined two-body interaction potentials, derived from phase-shifts analysis, between constituents of the nucleus that are deep enough to justify the calculation of a global potential energy surface (PES) built by using these interactions between all pairs of nucleons. This can be minimized giving equilibrium configurations that

have a precise geometric shape (or none). It is the equilibrium configurations, not the actual position of the nucleons, that displays symmetry properties that should be reflected in the symmetry of the wavefunctions and in the character of the vibrational states. We will analyze the cases of ^{4}He and ^{3}He (^{3}H is essentially equivalent), finding equilibrium shapes and their point-group symmetry and discussing the consequences on the vibrational spectrum. The energies of these modes will be found by applying the normal modes analysis (Hessian matrix) for the sake of simplicity, even though this is not the ideal approach because, despite the depths of the potential well being of the order of hundreds of MeV, the bound states are only a few MeV from the separation threshold, therefore they cannot be seen as deep lying states. It is instructive anyway to look at the results.

2. PES equilibrium configuration of ^{4}He

Let's consider the potential energy surface obtained by using the Argonne V18 potential between all the constituents of the α particle:

$$PES(\vec{r}_1, \vec{r}_2, \vec{r}_3, \vec{r}_4) = \sum_{i<j}^{4} V_{ij}(|\ \vec{r}_i - \vec{r}_j\ |) \tag{1}$$

where the vector coordinates $\vec{r}_i$ are not all independent in center of mass or intrinsic system, but they are constrained as follows:

$$\sum^{4} m_i \vec{r}_i = 0 \tag{2}$$

Of course the specific potentials are different for each type of interaction, i.e. they depend on the spin-isospin of each pair ij and on the orbital angular momentum. If we set 1 as the proton spin up, 2 as the proton spin down, 3 as the neutron spin up and 4 as the neutron spin down, the possible potential terms are listed in Table 1:

		spins	terms
1	2	p↑ p↓	$^1S_0^{T=1}$, $^3P_J^{T=1}$, $^1D_2^{T=1}$, $\cdots$
1	3	p↑ n↑	$^3S_1^{T=0}$, $^3P_J^{T=1}$, $^3D_J^{T=0}$, $\cdots$
1	4	p↑ n↓	$^1S_0^{T=1}$, $^1P_0^{T=0}$, $^1D_2^{T=1}$, $\cdots$
			$^3S_1^{T=0}$, $^3P_J^{T=1}$, $^3D_J^{T=0}$, $\cdots$
2	3	p↓ n↑	as in 1 4
2	4	p↓ n↓	as in 1 3
3	4	n↑ n↓	as in 1 2

Table 1. List of possible potential terms for each pair. Notice that the antisymmetry of the total wavefunction limits the possible combinations. The index J stands for all possible vector couplings between S and L.

The static picture that we adopt is that of looking for the minima of the potential energy surface with the combinations of potentials that minimize the energy. These are to be intended merely as equilibrium configurations for the nucleons, that nevertheless possess high momenta and have large fluctuations around these minima (as large as the nucleus itself). The dynamical picture instead is that of nucleons that are continuously scattered inside the α particle, and the scattering is described by the appropriate potential term. One might wonder if the PES corresponding to the lowest potentials (S-waves) ever cross
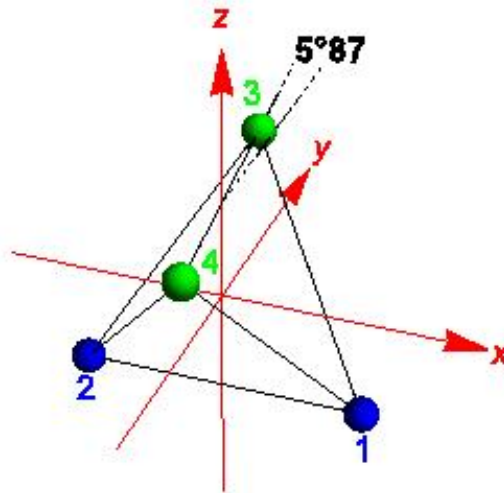
Figure 1. Equilibrium positions of protons (blue) and neutrons (green) in the α particle. Notice that the bond connecting 3 and 4, while perpendicular to the z-axis, is tilted 5^o87 away from the y-axis. This implies that the point-group symmetry is simply C_2.

(or has conical intersections) with higher order terms and this might lead to reaction paths, i.e. to loci of the potential energy surface that might allow a transition (chemists would call it isomerization) from a given geometric configuration (local minimum) to a different one (another local minimum) given a sufficient activation energy.

Let's use for the moment only the deepest possible S-wave potentials, i.e. those corresponding to the first configuration given in Tab. 1 for each pair. For the sake of simplicity I do not consider the $^3S_1^{T=0}$ configuration for the 1-4 and 2-3 pairs, because the depth of this potential is about one half of the $^1S_0^{T=1}$ one, therefore it does not affect the following search for the absolute minimum. Similarly, potentials with higher values of L have shallower pockets and can be disregarded for the present search. The PES depends in general on 4 vector positions, that correspond to 12 variables. A brute force minimization of Eq. (1) with constraints given by Eq. (2), gives an absolute minimum at -557.531 MeV. This minimum is spatially quite stiff with respect to small changes in each of the 12 variables and very easy to locate. It gives a somewhat simple geometric structure. A closer scrutiny of the coordinates that minimize the PES function reveals that a few simple rigid rotations can be made without altering this structure, nor the energy of the minimum. The following list of constraints can be imposed on minimization without loosing the minimum:

$$x_1 = -x_2 \quad x_3 = -x_4$$
$$y_1 = -y_2 \quad y_3 = -y_4$$
$$z_1 = z_2 \quad\;\; z_3 = z_4$$

The resulting geometric structure is depicted in Fig. 1: the equilibrium points of the two protons are

contained in the xz plane and are parallel to the x axis, while those of the two neutrons lie in a line perpendicular to the z axis, but tilted 5.87^o away from the yz plane. The coordinates of the equilibrium points are:

$$x_1 = -0.437648 \text{ fm} \qquad y_1 = 0 \text{ fm} \qquad z_1 = -0.31883 \text{ fm}$$
$$x_3 = 0.0446687 \text{ fm} \quad y_3 = -0.43476 \text{ fm} \quad z_3 = 0.318391 \text{ fm}$$

Note that one can be chosen to be zero without altering the minimization, in the c.m. frame it corresponds to rotate the whole system until the line connecting two particles lies in the $y = 0$ plane.

This shape is not a tetrahedron (it cannot be, the two protons repel each other more than the neutrons even neglecting spin), therefore T_d is excluded. If the inter-neutron bond would have been parallel to the y-axis a C_{2v} symmetry would have resulted, but this is not the case and the only possible symmetry operations are identity and a 180° rotation around the z-axis, therefore the point-group symmetry is simply C_2. The representations of this groups are very simple: A and B have positive and negative character with respect to the C_2 rotation. As far as we know, the only hint to non-tetrahedral shape of ^{4}He, was obtained in calculation of photonuclear sum rules using AV18 +UIX (notice that we don't have three-body potentials here) [10]. The authors conclude that helium-4 should look like a slightly deformed tetrahedron exactly as we find directly from the minimization.

> 1st *Claim: the geometric shape of equilibrium positions of the nucleons composing the α particle, obtained by minimizing the the Potential Energy Surface (1) with the two-body AV18 potentials, is that of an asymmetric top with C_2 symmetry.*

3. Vibrational spectrum in the harmonic approximation

We can perform a normal mode analysis in order to see the symmetry-type and energy of the fundamental vibrations. Even if the potentials are quite stiff, all of the following analysis is most certainly just an academic exercise that little has to do with reality: in fact, while in molecules masses distances and interactions often allow for the presence of tens of excited vibrational states, the nucleons in the α particle have such a different relationship between masses, distances and interactions that the energy of excited vibrational bands lies outside of the potential well. It is instructive anyway to take a look at this approach. If the potential energy is expanded in a Taylor series around the minimum, the first order derivatives vanish at the minimum and the mass-weighted Hessian matrix can be computed as

$$\tilde{H}_{lk} = H_{lk}/\sqrt{m_l m_k} = (\partial^2 PES/\partial q_l \partial q_k)/\sqrt{m_l m_k} \qquad (3)$$

From group theory, after subtraction of translations and rotations, one should expect $3N - 6$ normal modes, all non-degenerate: $\Gamma_{3N} - \Gamma_{rot} - \Gamma_{tra} = 4A \oplus 2B$. Of these, 4 are symmetric and 2 antisymmetric. We have obtained the explicit expressions for the displacements (eigenvectors of the Hessian) and energies (linked to the eigenvalues of the Hessian). The fundamental vibrations are all at very high energies, namely A 689.056 MeV, B 526.534 MeV, A 525.475 MeV, B 392.526 MeV, A 388.906 MeV, A 285.293 MeV, possibly too high to ever be observed as they are an order of magnitude higher than the various particle emission thresholds. They are depicted in Fig. 2. The first and higher in energy is the symmetric breathing mode. This is a very important result because in Ref. [11] the relevant and poignant question was asked whether the first excited 0_2^+ state of the alpha particle, lying at about 20 MeV might be interpreted as a breathing mode. Our analysis seems to exclude such a possibility, but it should be noted that a proper full calculation of the vibrational energy should be attempted before one can answer
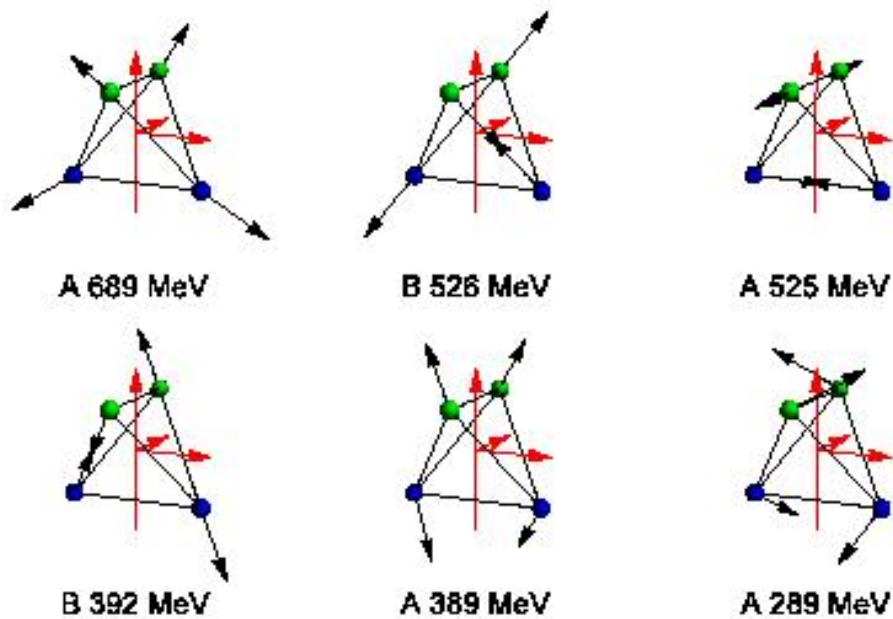
Figure 2. Normal modes of vibration of the C_2 configuration of the α particle.

this question with confidence. The two B modes at 526 and 392 MeV are both pn asymmetric stretches (one pn bond gets smaller, while the other gets stretched) that mix and repel, the A mode at 525 MeV is a pp asymmetric stretch (the pp bond gets smaller, while the other gets stretched and viceversa) and the two lowest A modes at 389 and 285 MeV are torsions that lift and simultaneously rotate the two neutrons away from the protons. The six sets of 4 displacement vectors form a system of normal coordinates, that could be taken as a symmetry-adapted basis for further calculations.

> 2st *Claim: the fundamental vibrations of the C_2 configuration of the α particle, in the normal mode approximation, are too high in energy to be observed. Accordingly, the first excited 0_2^+ state at 20 MeV is probably not the breathing mode of this structure.*

4. ^{3}He - C_s symmetry

Let's apply the same methods to helium-3. Analogous results can be obtained for the mirror system ^{3}H, that will not be reported here. The neutron and the two protons in the nucleus ^{3}He can be represented with three coordinates and three spin vectors: the two protons spin-up and down are assigned to 1 and 2 and the neutron (spin up or down is irrelevant) to 3. Thus the total PES can be written as:

$$PES(\vec{r}_1, \vec{r}_2, \vec{r}_3) = \sum_{i<j}^{3} V_{ij}(|\,\vec{r}_i - \vec{r}_j\,|) \tag{4}$$
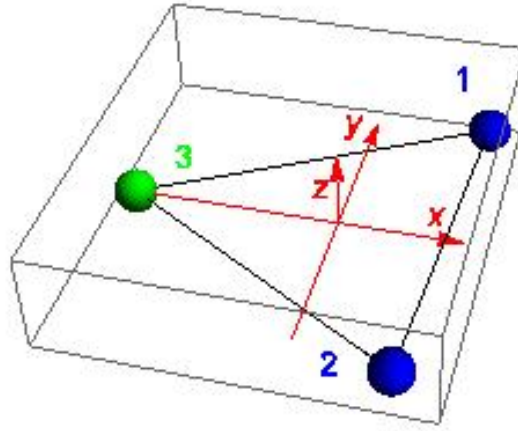
Figure 3. Equilibrium positions of 2 protons (blue) and a neutron (green) in ^{3}He. The point-group symmetry is simply C_s. Notice that the bond connecting 1 and 2 is not quite parallel to the y-axis, but tilted 3.31^o away from it.

The equilibrium configuration can be found by minimizing the above PES with the center of mass constraint, i.e.

$$\sum_{}^{3} m_i \vec{r}_i = 0 \ . \tag{5}$$

The result of the minimization, with the minimum lying at -277.67 MeV, is not affected if we set some additional geometrical constraints, for example that all the three particles are in the $z = 0$ plane and that the neutron lies on the x-axis, namely :

$$y_1 = -y_2$$
$$z_1 = z_2 = z_3 = 0$$

The resulting geometric structure is depicted in Fig. 3: the triangle is not equilateral, as one could have expected from the fact that one of the particle is different from the other two, but surprisingly is not even isosceles, all sides are dissimilar. This is due to the fact that the interactions of the n with the p's is slightly different depending on the relative spin orientations. The coordinates of the equilibrium points are:

$$
\begin{array}{lll}
x_1 = 0.283102 \text{ fm} & y_1 = 0.436916 \text{ fm} & z_1 = 0. \text{ fm} \\
x_2 = 0.232502 \text{ fm} & y_2 = -0.436916 \text{ fm} & z_2 = 0. \text{ fm} \\
x_3 = -0.514895 \text{ fm} & y_3 = 0. \text{ fm} & z_3 = 0. \text{ fm}
\end{array}
$$

The point-group symmetry is just C_s, i.e. the group of identity and reflection upon the horizontal plane, with the possible representations A' and A'' that differ because of the sign under reflection.
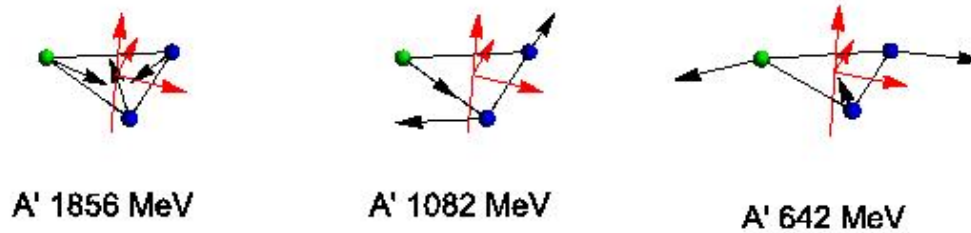
Figure 4. Normal modes of vibration of the C_2 configuration of the ^{3}He nucleus. Notice that all displacement vectors have unequal lengths and that their orientations are not interchangeable by any rotation.

The group theoretical analysis of the normal modes after subtraction of translations and rotations, gives $3N - 6$ normal modes: $\Gamma_{3N} - \Gamma_{rot} - \Gamma_{tra} = 3A'$, all symmetric, therefore all preserving the overall scalene shape.

> 3rd Claim: the geometric shape of equilibrium positions of the nucleons composing ^3He, obtained by minimizing the the Potential Energy Surface (4) with the two-body AV18 potentials, is that of a scalene triangle with C_s symmetry.

The energies of the fundamental vibrations obtained from diagonalization of the Hessian matrix are: 642.033, 1081.92 and 1856.07 MeV. The three sets of displacement vectors shown in Fig. 4 indicate that the lowest vibration is a sort of bending mode, the intermediate one is a sort of stretching mode and the higher one is a sort of breathing mode. We have slavishly repeated the words 'sort of' to underline that, in general, all nucleons have displacements of different lengths, for example the two protons in the breathing mode don't move in the same way or to the same extent. The above energies of the excited vibrational states are very high for low-energy nuclear structure, far beyond proton or neutron separation threshold and pion production threshold. Probably one could wonder if the harmonic approximation makes any sense, but I expect that the normal modes analysis gives results that are at least of the same order of magnitude as the full ab initio calculation of eigen-energies. These states could exist as resonances, but their width would be extremely large and therefore I do not expect that they could ever be observed in scattering or photoabsorption experiments.

5. Conclusions

The exact ab initio calculations of the vibrational energies would be a major step forward in this approach, because it might tell (by exclusion for instance) if any of the observed excited states of the α particle has anything to do with a breathing mode. Extensions of the present approach to heavier systems are in principle not difficult, provided that one considers also higher order interaction terms that go beyond $L = 0$. It would be very nice to explore if the PES with at least one D interaction term give energy differences with the ground state PES that are in the range of 20 MeV and if there is any conical intersection, i.e. if two different geometrical equilibrium shapes have PES that touch or cross each other (they have a locus of degenerate energies) where interesting phenomena might appear.

References

[1] Wheeler J A 1937 *Phys. Rev.* **52** 1083-1106
[2] Hafstad L R and Teller E 1938 *Phys.Rev.* **54** 681
[3] von Oertzen W 1970 *Nucl. Phys. A* **148** 529
[4] von Oerzen W and Bohlen H G 1975 *Phys. Rep. C* **19** 1
[5] Freer M and Merchant A C 1997 *J. Phys. G* **23** 261
[6] von Oertzen W, Freer M and Kanada-En'yo Y 2006 *Phys. Rep.* **432** 43-113
[7] Bijker R and Iachello F 2014 *Phys. Rev. Lett.* **112** 152501
[8] Bijker R and Iachello F 2017 *Nucl. Phys. A* **957** 154176
[9] Schmiedt H, Jensen P and Schlemmer S 2017 *Chem. Phys. Lett.* **672** 34-46
[10] Gazit D, Barnea N, Bacca S, Leidemann W and Orlandini G 2006 *Phys. Rev. C* **74** 061001(R)
[11] Bacca S, Barnea N, Leidemann W and Orlandini G 2105 *Phys. Rev. C* **91** 024303