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# Three-body structure of $^{18}\text{Ne}$ in a microscopic model

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**Abstract.** The structure of  $^{18}\text{Ne}$ , and in particular of the  $1^-$  (6.18 MeV) level, is investigated in a microscopic cluster model involving  $^{16}\text{O}+p+p$  configurations. We use the three-cluster Generator Coordinate Method associated with the hyperspherical formalism. The spectroscopy of  $^{18}\text{Ne}$  and  $^{18}\text{O}$  low-lying states is analyzed. Using the Analytical Continuation in the Coupling Constant (ACCC) method, we determine the width of the  $1^-$  (6.15 MeV) resonance in  $^{18}\text{Ne}$  and find  $\Gamma = 40 \pm 10$  keV. This result is in fair agreement with experiment ( $50 \pm 5$  keV).

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## 1. Introduction

The simultaneous emission of two protons (diproton decay) for nuclei close or beyond the proton drip line is well established since many years [1]. The interest for this decay mode has been recently revived with the availability of intense radioactive beams [2, 3]. Diproton radioactivity has been observed in some nuclei, such as  $^{17}\text{Ne}$  [4] or  $^{19}\text{Mg}$  [5]. This decay mode is, in general, in competition with the sequential decay, where the two protons are emitted through an intermediate nucleus with charge  $Z - 1$ .

Recently, diproton decay of the  $1^-$  excited level of  $^{18}\text{Ne}$  (6.15 MeV) has been reported by the  $^{17}\text{F}+p$  reaction [6] and by Coulomb excitation of a  $^{18}\text{Ne}$  beam on a Pb target [7]. The total width, including one and two-proton decay, was measured to be  $50 \pm 5$  keV [6]. The two-proton partial width is  $21 \pm 3$  eV assuming a diproton emission, and  $57 \pm 6$  eV assuming a three-body decay.

The theoretical analysis of this mechanism requires specific models, able to account for a three-body structure of the nucleus. In addition, the theoretical treatment of three-body resonances is a delicate problem [8, 9]. Various calculations of diproton emission have been done in the shell model [10] or in a non-microscopic three-body model [8]. Here we focus on the  $1^-$  state of  $^{18}\text{Ne}$ , and use a microscopic cluster theory, based on an  $^{16}\text{O}+p+p$  description within the hyperspherical formalism [11, 12]. This approach has

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been already applied to bound states of some nuclei, such as  $^6\text{He}$ ,  $^9\text{Be}$  or  $^{12}\text{C}$  [13, 14]. In a microscopic model, all nucleons are included in the Hamiltonian, and the Pauli principle is exactly taken into account. The model is based on a nucleon-nucleon interaction, and therefore presents a fairly strong predictive power. Of course, the Schrödinger equation cannot be solved exactly for large nucleon numbers, and the cluster approximation is used [15].

The treatment of resonances requires an additional tool, taken here as the Analytical Continuation in the Coupling Constant (ACCC, see Ref. [16]). This method provides an estimate of the energy and width of a resonance. Its main advantage is that it is based on bound-state calculations only, which do not need to account for scattering boundary conditions. The ACCC method was successfully applied in the same microscopic three-cluster model to describe  $^5\text{H}$  and  $^5\text{He}$  ( $T = 3/2$ ) three-body resonances [17]. Of course, the ACCC method only provides the total width of a resonance. A separation between 1p and 2p decays is not feasible in this framework.

Section 2 is devoted to a brief overview of the theory. We describe the microscopic cluster model, and give the main properties of the ACCC method. In Section 3, we present the theoretical  $^{18}\text{O}$  and  $^{18}\text{Ne}$  spectra, and we focus on the proton width of  $1^-$  (6.15 MeV) resonance in  $^{18}\text{Ne}$ . Concluding remarks are discussed in Section 4.

## 2. Theoretical background

### 2.1. The microscopic cluster model

We use here a microscopic description [15], where the Hamiltonian of the system is given by

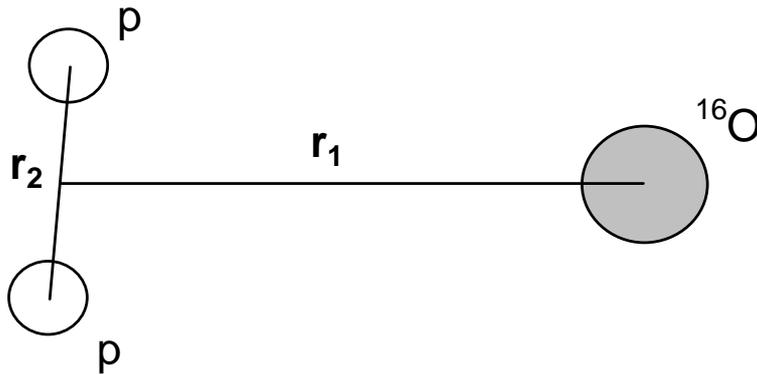
$$H = \sum_{i=1}^A T_i + \sum_{j>i=1}^A V_{ij}, \quad (1)$$

$T_i$  being the kinetic energy of nucleon  $i$ , and  $V_{ij}$  a nucleon-nucleon effective interaction. For large nucleon numbers ( $A \geq 12$ ), and in particular to investigate resonances, the Schrödinger equation associated with Hamiltonian (1) cannot be solved exactly. We use here the cluster approximation [15], where the  $A$  nucleons are assumed to be grouped in clusters. In the present case,  $^{18}\text{Ne}$  is described by a three-cluster wave function, with an  $^{16}\text{O}+p+p$  structure. In a schematic notation, the total wave function reads

$$\Psi = \mathcal{A}\phi_O\phi_p\phi_p G(\mathbf{r}_1, \mathbf{r}_2), \quad (2)$$

where  $\phi_O$  and  $\phi_p$  are  $^{16}\text{O}$  and proton wave functions, defined in the harmonic-oscillator model, and  $G(\mathbf{r}_1, \mathbf{r}_2)$  is a relative function depending on the Jacobi coordinates  $\mathbf{r}_1$  and  $\mathbf{r}_2$  (see Fig. 1). In (2),  $\mathcal{A}$  is the  $A$ -body antisymmetrization operator which enables an exact account of the Pauli principle, not only inside the  $^{16}\text{O}$  core, but also between the core and the external nucleons. The center-of-mass motion is exactly factorized.

The wave function (2) is defined in the hyperspherical formalism, well adapted to three-body systems. Jacobi coordinates  $\mathbf{r}_1$  and  $\mathbf{r}_2$  are therefore transformed into the



**Figure 1.** Three-cluster structure of  $^{18}\text{Ne}$  with the Jacobi coordinates  $r_1$  and  $r_2$ .

hyperangle  $\alpha$  and hyperradius  $\rho$  (see Refs. [11, 12] for details). For a given spin  $J$  and parity  $\pi$  of  $^{18}\text{Ne}$ , the wave function is expanded as

$$\Psi^{JM\pi} = \sum_{K\ell_x\ell_yLS} \Psi_{K\ell_x\ell_yLS}^{JM\pi}, \quad (3)$$

where  $K$  is the hypermomentum,  $\ell_x$  and  $\ell_y$  are the orbital momenta associated with the Jacobi coordinates, and  $L$  and  $S$  represent the total angular momentum and intrinsic spin, respectively. The summation over  $K$  must be truncated at a maximum value, denoted as  $K_{max}$ . Of course, the  $^{18}\text{O}$  wave functions have the same three-cluster structure. Owing to the charge symmetry of the nuclear force, only the Coulomb interaction is changed in (1).

The extension of three-body models to a microscopic version has been proposed in Ref. [13]. In the Generator Coordinate Method (GCM), the partial wave functions (3) are expanded over a Gaussian basis, which enables to express them as linear combinations of Slater determinants. Each component of Eq. (3) is therefore written as

$$\Psi_{K\ell_x\ell_yLS}^{JM\pi} = \int f_{K\ell_x\ell_yLS}^{J\pi}(R) \Phi_{K\ell_x\ell_yLS}^{JM\pi}(R) dR, \quad (4)$$

where  $\Phi^{JM\pi}(R)$  are projected Slater determinants, and  $f^{J\pi}(R)$  the generator functions. Both depend on the generator coordinate  $R$  associated with the hyperradius  $\rho$ . In practice this integral is replaced by a sum over a finite set of  $R$  values (typically 8 ~ 12 values). An approximate solution of the Schrödinger equation can be obtained by the variational principle, using matrix elements of the Hamiltonian (1) between GCM basis functions.

In Ref. [13] we have shown that matrix elements between projected Slater determinants involve seven-dimensional integrals, which are performed numerically. The main part of the calculation is the evaluation of the potential matrix elements. A two-body matrix element between unprojected basis functions involves quadruple sums over individual orbitals [18]. In the applications considered so far [13, 14], this microscopic three-body model was limited to  $s$  clusters (nuclei such as  $^6\text{He}$ ,  $^9\text{Be}$  or  $^{12}\text{C}$  were studied). Under these conditions the development of the model to the three-body continuum was

proposed recently [19], and applied to  $\alpha+n+n$  unbound states. This extension requires large values of the generator coordinate (typically values up to 25 fm must be considered) and, consequently, a large basis. The calculation was made possible by the use of semi-analytical techniques to evaluate the matrix elements. This approach is much faster than the numerical procedure. In contrast, the present calculation involves  $^{16}\text{O}$  as core nucleus, where  $p$  orbitals are included. In that case a semi-analytical treatment raises important difficulties, and a numerical approach must be used. However, the presence of  $p$  orbitals considerably increases the computer time. In a Cartesian representation, the number of individual orbitals is  $N_o = 6$  (1  $s$  and 3  $p$  orbitals for the  $^{16}\text{O}$  core, and 1 for each external nucleon) whereas it is  $N_o = 3$  when only  $s$ -clusters are involved. The quadruple sums mentioned before contain  $N_o^4$  terms, and the computer times therefore increase by a factor 16 when going from an  $\alpha$  core to an  $^{16}\text{O}$  core. We have tested Monte-Carlo methods [20] to evaluate the seven-dimensional integrals, but this approach turns out to be not well adapted since many partial waves ( $K\ell_x\ell_yLS$ ) are treated simultaneously. It was not possible to achieve a good accuracy for all partial waves simultaneously, and therefore standard quadratures have been adopted.

## 2.2. The ACCC method

In contrast with the approach of Ref. [19] which provides three-body phase shifts at any energy, the ACCC method [16] is limited to resonances. However it provides resonance properties from bound-state calculations, which do not require very large values of the generator coordinate (here  $R_{max} = 12$  fm, see Sect. 3.1). Its application to microscopic calculations has been shown in the past to be very efficient [21, 17]. We briefly give here the main principles and refer the reader to Ref. [16] for more detail.

To apply the ACCC method, the Hamiltonian is written as

$$H(\lambda) = H_0 + \lambda H_1, \quad (5)$$

where  $\lambda$  is a linear parameter, and where  $H_1$  is supposed to be attractive. In cluster models, the nucleon-nucleon effective interaction often involves a linear parameter which has a standard value, but can be slightly modified to reproduce important properties of the system, such as a resonance energy. This parameter is the natural choice for the linear parameter  $\lambda$ .

Let us define  $\lambda_0$  as  $k(\lambda_0) = 0$ , where  $k$  is the wave number (throughout the paper, energies are determined from the three-body threshold). For negative energies (i.e.  $\lambda > \lambda_0$ ), the wave number is imaginary and is parametrized in a Padé approximant of degree  $(M, N)$  as

$$k(x) = i \frac{c_0 + c_1x + \dots + c_Mx^M}{1 + d_1x + \dots + d_Nx^N}, \quad (6)$$

where  $x = \sqrt{\lambda - \lambda_0}$  is real. The calculation is performed for  $M + N + 1$  values of  $\lambda$ , each of them providing a bound-state energy. This procedure allows to determine the Padé coefficients  $c_j$  and  $d_j$ .

For a resonance, the physical value  $\lambda$  is lower than  $\lambda_0$ . Then the resonance energy  $E_R$  and width  $\Gamma$  are obtained by using (6) for an imaginary value of  $x$ . One defines the complex energy  $E$  as

$$E = \frac{\hbar^2 k^2}{2m_N} = E_R - i\Gamma/2, \quad (7)$$

$m_N$  being the nucleon mass. This method only needs bound-state calculations, but is limited to the total width of a resonance. The associated wave function is not available in this approach. In addition it requires a high accuracy of the variational basis. In particular, the sensitivity with respect to the Padé parameters ( $M, N$ ) should be checked by considering various sets of  $\lambda$  values.

### 3. The $^{18}\text{O}$ and $^{18}\text{Ne}$ nuclei

#### 3.1. Conditions of the calculation

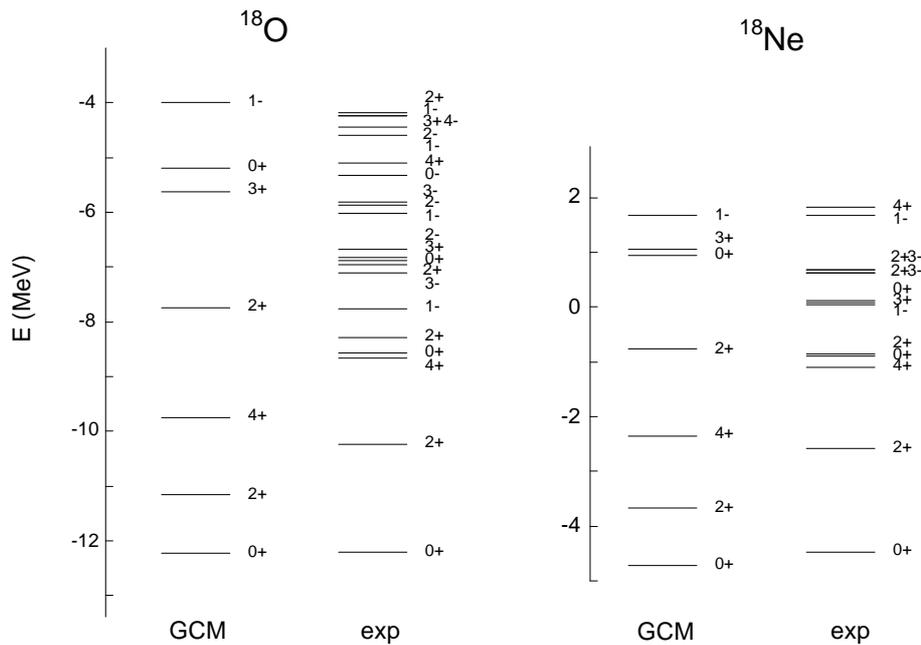
The  $^{16}\text{O}$  wave function  $\phi_O$  (see Eq. (2)) is defined in the shell model, with harmonic-oscillator orbitals involving the oscillator parameter  $b$ . This parameter determines the properties of the  $^{16}\text{O}$  ground state. Its value is chosen as  $b = 1.6$  fm, which corresponds to a compromise between the minimum energy and the experimental radius. The nucleon-nucleon interaction is taken as the Volkov force V2 [22], which involves the exchange parameter  $M$  (the standard value is  $M = 0.6$ ). Here it is adjusted on the ground-state energy of  $^{18}\text{O}$  for positive parity ( $M = 0.620$ ), and on the  $1^-$  (6.15 MeV) level of  $^{18}\text{Ne}$  for negative parity ( $M = 0.589$ ). Reproducing the energy of a resonance is crucial to derive realistic values for its width. The Coulomb interaction is treated exactly.

We also include a zero-range spin-orbit force [23]. The amplitude is adopted as  $S_0 = 40$  MeV.fm<sup>5</sup>, a standard value in this mass region. The generator coordinates  $R$  have been selected from 1.5 fm to 12 fm with a step of 1.5 fm. The summation over the hypermoment  $K$  [see Eq. (3)] has been truncated at  $K_{max} = 20$ . As we will show below, this value provides an accurate convergence.

#### 3.2. Energy spectra

The  $^{18}\text{O}$  and  $^{18}\text{Ne}$  energy spectra are displayed in Fig. 2, and compared with experiment [24]. In both nuclei, the excitation energy of the  $2_1^+$  state is underestimated by about 1 MeV. This problem is common to most nuclei in this mass region. The level density beyond 4 MeV excitation energy is quite large, in particular for  $^{18}\text{O}$ . This property represents a challenge for microscopic models, since experimental states may have a different cluster structure. However most of the GCM states can be unambiguously assigned to experimental candidates. In particular we do reproduce the  $2_2^+$  state. A  $0^+$  level is predicted near  $E_x \approx 7$  MeV. Most likely it can be assigned to the experimental  $0_3^+$  state since the  $0_2^+$  state is expected to present an  $\alpha$  cluster structure [25].

In negative parity the lowest GCM state is  $1^-$ ; other negative-parity states are at higher excitation energies. The  $1_1^-$  experimental level is known to have an  $\alpha + ^{14}\text{C}/\alpha + ^{14}\text{O}$



**Figure 2.**  $^{18}\text{O}$  and  $^{18}\text{Ne}$  spectra (experimental data are taken from Ref. [24]). The zero energy is taken as the  $^{16}\text{O}+n+n$  and  $^{16}\text{O}+p+p$  thresholds, respectively.

cluster structure [25] and cannot be described by the present model which includes  $^{16}\text{O}$  as a core. The first theoretical  $1^-$  state therefore corresponds to the  $1_2^-$  experimental level at 6.15 MeV.

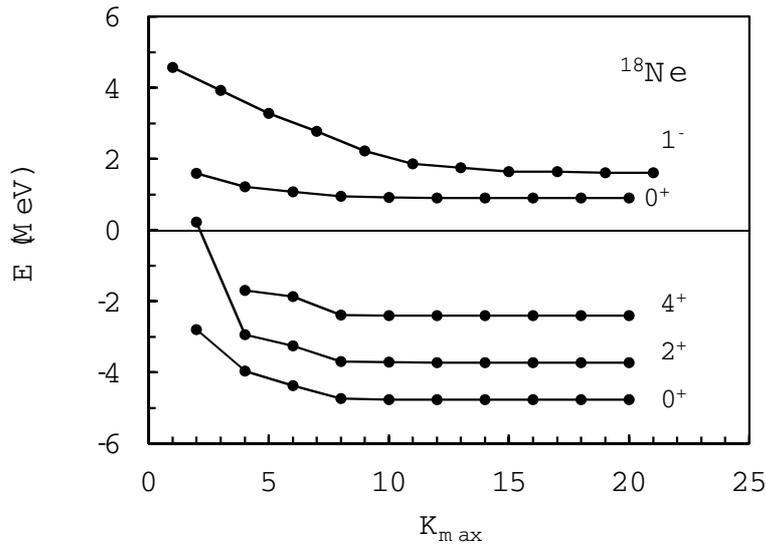
In Fig. 3, we analyze the energy convergence of various states as a function of  $K_{max}$ . In positive parity, the convergence is reached near  $K_{max} \sim 12$ . The energy difference between  $K_{max} = 20$  and  $K_{max} = 18$  is lower than 1 keV. As expected for unbound states, the  $1^-$  resonance presents a slower convergence. Going up to large  $K_{max}$  values (i.e. larger than 15) is necessary to obtain precise properties.

### 3.3. Decay of the $1^-$ (6.15 MeV) state in $^{18}\text{Ne}$

The ACCC method has been applied to determine the width of the  $1_2^-$  state in  $^{18}\text{Ne}$ . As mentioned in Sect. 2.2, the ACCC presents some sensitivity with respect to the conditions of the calculation [i.e. the degree of the Padé approximant, and the  $\lambda$  values used to parametrize the wave number (6)]. Consequently convergence tests must be performed, and the resonance properties cannot be determined without some uncertainty. In particular, the width, which is zero at negative energies, is somewhat sensitive to the conditions of the calculation.

In Fig. 4, we show the energy and width for various degrees ( $M = N$ ) of the Padé approximant (6). In addition, different sets of  $\lambda$  values have been adopted and defined as

$$\lambda_n = \lambda_0 + n\Delta\lambda, \quad (8)$$



**Figure 3.** Convergence of various  $^{18}\text{Ne}$  states as a function of the maximum hypermomentum  $K_{max}$ .

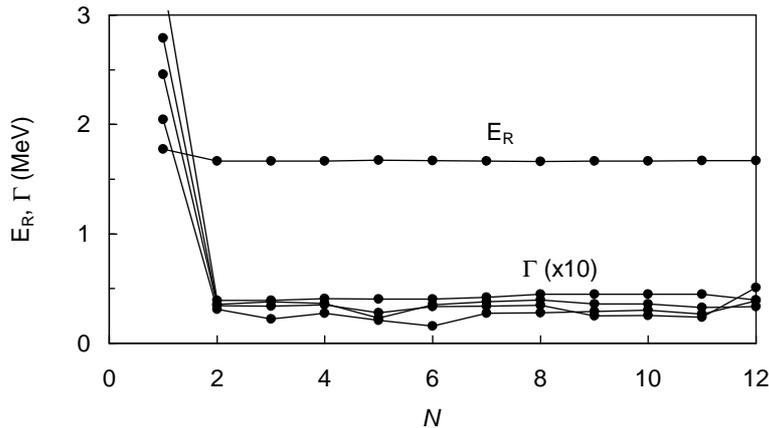
where  $\Delta\lambda$  is a constant step. Variations of the resonance properties against  $N$  and  $\Delta\lambda$  provide an estimate of the uncertainty, which is unavoidable with the ACCC method. Small  $N$  values do not give accurate Padé approximants. Conversely, when  $N$  is large (typically beyond  $N \approx 10$ ), round-off errors become more and more important. The energy is very stable and corresponds to the value obtained in the bound-state approximation, i.e. by a simple diagonalization of the Hamiltonian matrix. The width, related to the imaginary part of the wave number is somewhat less stable.

Fig. 4 provides  $E_R = 1.67 \pm 0.01$  MeV and  $\Gamma = 40 \pm 10$  keV. The energy has been adjusted by the nucleon-nucleon interaction, and is of course very close to experiment. Conversely the width is an output of the model, and is in fair agreement with experiment ( $50 \pm 5$  keV, see Ref. [6]).

#### 4. Conclusion

This work represents a first attempt to describe the three-body decay of  $^{18}\text{Ne}$  in a microscopic approach. The GCM is known for a long time to be well adapted to the spectroscopy of light nuclei, and to low-energy reactions. Its application to unbound states is however a challenge, as it raises several difficulties. A realistic treatment requires a three-body model. In addition, the unstable nature of the initial state requires to go beyond the bound-state approximation, and to complement the GCM by an additional tool, able at dealing with unbound states. We have used here the ACCC method, which is based on standard variational calculations. Even if the resonance properties cannot be derived without some uncertainty, the method should be considered as a very powerful tool.

The GCM width is found as  $\Gamma = 40 \pm 10$  keV, in good agreement with the



**Figure 4.** Energy and width of the  $1^-$  (6.15 MeV) resonance in  $^{18}\text{Ne}$ , as a function of the degree of the Padé approximant ( $M = N$ ). The curves correspond to different sets of  $\lambda$  values [see Eq. (8)].

experimental value  $\Gamma = 50 \pm 5$  keV. This result demonstrates that the theoretical description of the  $1_2^-$  unbound state is realistic. Of course the ACCC method only provides the total width. Determining the (small) diproton branching ratio would require to use more sophisticated methods, providing the partial widths as well.

Other proton-rich nuclei with a marked three-body structure, such as  $^{17}\text{Ne}$  or  $^{19}\text{Mg}$ , might be considered in the future. The  $^{16}\text{O}+p+p$  system is however simpler since the  $^{16}\text{O}$  core is a closed-shell nucleus. The hyperspherical formalism applied to the GCM requires seven-dimension integrals for the matrix elements. The numerical evaluation of these integrals need very long computer times, and going beyond this limitation represents a challenge for the future.

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