Theoretical studies of nuclei at the proton drip-line

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**Abstract.** Proton emission from drip-line nuclei has provided a unique possibility to probe nuclear structure at the extremes of stability. In the present work, we discuss some results obtained in our studies of these exotic decays.

1. Introduction

The production in the laboratory of nuclei with an excess of protons or neutrons is increasing at a very fast rate in recent years, due to the appearance of new experimental facilities and technologies. Not only the limits of stability were reached in some areas of the nuclear chart, but many nuclei were produced along the path of the proton and neutron capture reactions, that are supposed to lead to the process of formation of heavier elements in the universe, therefore, of great relevance for nuclear astrophysics. An important progress in the field, was also the capability of observing some features of the bulk properties, of these extremely unstable nuclei. The extraordinary development of trapping techniques, the use of storage rings and new detection procedures, have provided high precision measurements of masses, and decay observables which form a basic testing ground for the nuclear structure models and underlying fundamental theories. Whereas on the neutron rich side, exotic nuclei with neutron skins and halos [1] were found, on the proton rich side, nuclei that could spontaneously decay by emitting one[2] or two protons[3, 4], were found beyond the drip line. Proton radioactivity has provided a way to define completely the proton drip line in the region of nuclear charges between Z=50 and Z=83.

Data gathered from decay to ground and excited states, which includes the decay widths, branching ratios, the proton energy and in some cases the spectrum of the decaying nucleus, provide valuable information on the structure of the nuclei involved in the process. In previous studies, [5, 6, 7, 8] we have proved that a theory that accounts for the data, is also able to predict the spin and parity of the decaying state, and the nuclear shape and deformation parameters. The breaking of axial symmetry, for example, hinted in some experimental data, was confirmed by the theory[9, 10]. Proton emission has been thoroughly studied within non
relativistic models based on phenomenological mean field descriptions of the nucleus, obtained by fitting the single particle properties of stable nuclei. Decay of deformed odd–even and odd–odd nuclei were interpreted, and the importance of the Coriolis and residual interaction studied. More recently, spherical emitters were interpreted within a self–consistent relativistic density functionals theory[11]. It is the purpose of the present work to review some aspects of the models we have developed and what we have achieved in the interpretation of these exotic decays.

2. Nuclear structure at the proton drip-line
Proton emitters exist beyond the drip line, as resonances in the nuclear mean field. Since the proton escapes with a very low energy of 1-2 MeV, these resonances are essentially single particle resonances, and the continuum becomes unimportant. According to scattering theory, the half-life for decay by one particle emission is given by

\[ T_{1/2} = \frac{\hbar \ln 2}{\Gamma} \]

where the decay width can be found [5] from the relation:

\[ \Gamma = \frac{S \hbar k^2 \alpha^2}{m} \]

with \( m \) and \( k \) standing for the mass and wave number of the proton. \( S \) is a spectroscopic factor, and the quantity \( \alpha \) the asymptotic normalization of the proton wave function. If nuclei are spherical, the tunneling process can be treated within the semi-classical WKB approach, or using perturbation theory, like the distorted wave Born Approximation (DWBA) or two potential model [12]. The structure enters in the spectroscopic factor that measures the probability that, after the decay, the daughter nucleus is left in the ground state, and carries information on the structure of the two nuclei. Usually, it is calculated within the BCS approach, that is, the probability \( u^2 \) that the decaying level is empty in the daughter nucleus.

For an unambiguous interpretation of the data, the proton wave function has to be calculated with great precision, with a realistic interaction. Therefore, a basic ingredient for these studies is the nuclear mean field. Some models [13, 14, 15], obtain the mean field by a folding of an effective two-body force extracted from a microscopic calculation, with the nuclear density of the daughter nucleus as described in Ref. [11, and references therein.

However, most models use standard phenomenological parameterizations of the nuclear mean field available in the literature [16, 17, 18, 19, 20, 21], which fit single particle properties of stable nuclei. They are essentially described by Woods-Saxon shapes but the radius of these potentials is the most sensitive parameter, since it directly controls the magnitude of the decay width. A potential with a small radius will lead to a large half-life and vice-versa. Certainly, this does not mean that one can change the radius arbitrarily to interpret decay, but gives a hint to understand the results obtained from different interactions. We found[22] that different interactions available in the literature that provide a good fitting of nuclear properties, give similar results for the calculation of the decay widths, and the differences are within experimental uncertainties.

A self-consistent description of the nucleus based on Lorentz invariant density functionals is a better approach, since some contributions to the interaction are included from first principles. The treatment of the spin-orbit interaction, arises in a natural way without any additional adjustable parameters, and is consistent with the non linear realization of chiral symmetry. Consequently, a relatively small number of parameters adjusted to reproduce a set of bulk properties of finite nuclei, are required to define the interaction. Covariant density functional theory (CDFT) has been quite successful in a microscopic descriptions of nuclear structure of spherical and deformed nuclei over the entire nuclear chart [23] [24]. Therefore, we have applied CDFT to the study of proton emission from spherical nuclei [11]. A fully self-consistent relativistic calculation was performed, based on relativistic density functionals derived from meson exchange NL3 [25] and density dependent point coupling DD-PC1 [26] models. For
details, see Ref. [11]. The spectroscopic factor needed, according to Eq. 1, came from the BCS approach.

In this calculation, the experimental half lives for decay to ground state, were calculated and compared with the experimental data, showing an overall agreement between theory and experiment. The data were consistently interpreted, showing a clear evidence for a mixing of configurations, in nuclei where the number of protons or neutrons is far from a magic number, which in the region of proton emitters corresponds to Z or N ≈ 82. In such cases, it is possible to find a strong mixing of wave functions or a coupling to phonon states. In addition, for open proton and neutron shells, deformations will set in. The spectroscopic factor will become smaller than the one derived from the BCS model, since pairing will not be the only effective interaction, leading to theoretical half-lives longer than the experimental ones. With such calculations, one could identify deviations from spherical symmetry at the proton drip line. In fact, there is new evidence that $^{161}$Re and $^{145}$Tm should be deformed[9, 10, 27, 28].

When neutrons and protons are away from magic numbers, one has to take into account also the residual quadrupole interaction between unlike particles. This interaction gives rise to rotational bands, and can be treated by a transformation similar to the Bogoliubov one for the pairing. The symmetry that is broken is the rotational invariance, giving rise to a deformed mean field and to the so-called Nilsson levels. The decaying state will be a Nilsson resonance in a deformed mean field [5, 6, 29], and the spectroscopic factor does not depend only on the $u^2$ of the BCS, but depends also on the amplitude of the component of the Nilsson wave function with angular momentum equal to the one of the ground state. Therefore, in addition to the position of the Fermi surface, it is possible to get detailed information on components of the wave function that can be quite small, and not detectable by other means.

The calculation of decay from deformed nuclei have been done in the adiabatic approximation, which is the simplest way to include the structure of the emitter, assuming it has an infinite moment of inertia, and therefore, a frozen spectrum. The residual interaction is included through the spectroscopic factor. The inclusion of the Coriolis interaction, that takes into account the finite moment of inertia, was done in the non-adiabatic quasi-particle model[8], where the pairing residual interaction was also included. The Coriolis force is then diagonalized in the quasi-particle basis states, and the correlations in the medium make the decaying state appear as the lowest in energy.

The adiabatic approach can be justified on the theoretical point of view, when the deformation is very large, and the decaying state has a low spin. In this case, the decaying state can be predicted and the data reproduced. But, it can happen that a state that is far from the Fermi surface in the adiabatic approach, due to correlations as a result of the Coriolis and residual interactions, could become the decaying state. This is the case of 121Pr, a nucleus with a large prolate deformation $\beta_2 \approx 0.318$, and where [30] the 3/2$^-$ state was identified as the decaying data in the adiabatic approach, but it is the 7/2$^-$ that in the quasi-particle approach reproduces the experimental half-life and becomes the ground state, providing evidence for partial rotational alignment in this nucleus. Not all isotopes of odd-A Praseodymium are known from stability up to the proton drip line, but one can already see half way from stability a trend for the 7/2$^-$ to decrease to lower energies as deformation increases towards the drip-line, supporting our prediction.

Recent observation of the excitation spectrum of some proton emitters through recoil-decay tagging technique, provided strong evidence of axial symmetry breaking [31], as predicted by mass model calculations[32]. Islands of triaxiality should appear in this region of the nuclear chart, since a gain in nuclear binding can be achieved by the breaking of axial symmetry.

Triaxial degree of freedom can be included in the non-adiabatic quasi-particle formalism, by generalizing the collective Hamiltonian in order to encompass $\gamma$ deformations. The partial decay
width becomes,
\[
\Gamma_{ij}^{IR}(r) = \frac{\hbar^2}{\mu} 2 \left( \frac{2R + 1}{2I + 1} \right) \sum_{\sigma,K} u_{ij} \langle j\Omega RK_R | I K \rangle \\
\times g_{R K_R}^{j} a_{\sigma,K}^{j} \phi_{ij}^{\sigma\Omega}(r) | G_{I}(kr) + iF_{I}(kr) |^{2},
\]
(2)

with \( g_{0,0}^{\tau} = 1 \) and, considering the decay to the lowest \( 2^+ \) state (\( \tau = 1 \)),
\[
g_{2,K_R}^{1} = \frac{1}{\sqrt{1 + |K_R|^2}} \left[ \frac{1}{2} + (-1)^{K_R/2} F(\gamma) \right]^{1/2},
\]
(3)

where
\[
F(\gamma) = \frac{\sin \gamma \sin 3\gamma + 3 \cos \gamma \cos 3\gamma}{2 (9 - 8 \sin^2 3\gamma)^{1/2}}.
\]
The symbol \( \sigma \) specifies the single-particle states included as basis states in the Coriolis diagonalization and the prime in the summation in Eq. (2) stands for the constraint that \( K - \Omega \) must be an even integer. The coefficients \( a_{\sigma,K}^{j} \) are the components of the eigenvectors of the Coriolis matrix and \( \phi_{ij}^{\sigma\Omega}(r) \) are the radial components of the eigenfunctions of the triaxial Nilsson Hamiltonian that includes a deformed spin-orbit term and the residual pairing interaction. The quantity \( |u_{ij}^{\sigma}|^2 \) gives the probability that the proton single-particle level in the daughter nucleus is empty and is obtained from the BCS calculation. For given angular momentum of the decaying nucleus \( I \), and of the core \( R \), the width can be calculated according to the relation,
\[
\Gamma^{IR} = \sum_{j=|R-I|}^{R+I} \Gamma_{ij}^{IR},
\]
(4)

and the branching ratio between the decay to the ground and first excited \( 2^+ \) states follows in a straightforward way as \( \Gamma^{I2}/(\Gamma^{I2} + \Gamma^{00}) \). All details of the formalism can be found in Ref. [9].

In practice to determine the decay widths, one starts by getting the Nilsson resonance states in a well established non-axial mean field, by solving the Schrödinger equation imposing outgoing wave boundary conditions. The pairing residual interaction is treated in the BCS approach, and the Coriolis interaction is then diagonalized in the quasi-particle states.

There are some standard quantities in the model that need to be discussed. For example, the moment of inertia of the nucleus \( I_\nu \), may change with the angular momentum, and this dependence is usually treated within the variable moment of inertia model(VMI), by including a parameter \( b \) such as [33] \( I_\nu(I) = I_0 \sqrt{1 + b \frac{I(I+1)}{I_0}} \), with \( I_0 \) fixed by fitting the energy of the first excited \( 2^+ \) state of the nucleus. The calculation of the rotational spectrum of the daughter nucleus and the comparison with the experimental data, will determine \( b \). Also, in nuclear structure calculations one inserts sometimes an attenuation factor \( \rho \) for the Coriolis interaction [34]. We have studied the influence of these parameters on the value of the half-lives, but their impact is very much within experimental uncertainties, resulting primarily from the error in the determination of the proton energy.

As an example, we show in Fig. 1 the branching ratio for proton emission from the \( 11/2^- \) state in 145Tm to the ground and first excited \( 2^+ \) state in the daughter nucleus \( ^{144}\text{Er} \). The experimental value is reproduced by a large triaxial deformation with a very narrow window around \( \approx 30^\circ \), a value quite independent of the choice of the various parameters. For details
Figure 1. Branching ratio for proton emission from the 11/2\(^{-}\) state in \(^{145}\)Tm to the ground and first excited 2\(^{+}\) state in the daughter nucleus. Different curves as indicated by legends correspond to different attenuation factor \(\rho\) for the Coriolis interaction, axial deformations \(\beta_2\), and pairing gap parameters \(a_\Delta\), defined such that \(\Delta = a_\Delta \times 12\sqrt{A}\). The grey shaded area corresponds to the experimental value including errors[35]. The error bar at \(\gamma = 20^\circ\) represents the uncertainty in our calculations due to the error in the knowledge of the experimental Q-value.

see Ref.[10]. This is a very precise identification of the breaking of axial symmetry, provided by the observation of fine structure in proton emission.

While decay widths for a specific state might depend strongly on the various parameters of the model, like deformation, radius of the potential and Q-value, branching ratios are practically insensitive to variations of these quantities, but depend strongly only on the difference of Q-values of the two transitions, which usually are known with good accuracy.

For nuclei with \(\gamma\) deformation, the dimension of the Coriolis matrix will be quite large since the third component of the angular momentum \(\Omega\) of the Nilsson particle is not conserved. Thus
Table 1. Breaking of axial-symmetry in the region of proton emission Deformation parameters and decaying state that reproduce the experimental data.

| Nucleus | $\beta$ | $\gamma$ | $J^\pi$   |
|---------|---------|---------|-----------|
| $^{141}$Ho | 0.24   | 20°     | 7/2$^-$ [36] |
| $^{141}$Ho$^m$ | 0.24   | 20°     | 3/2$^+$ [36] |
| $^{145}$Tm | $\approx$ 0.25 | 30° | 11/2$^-$ [10] |
| $^{161}$Re | $\approx$ 0.2  | 30°     | 1/2$^+$ [9]   |

the choice of the decaying level is more complicated than in the axially symmetric case, and the mixing between quasi–particles becomes even more crucial. If besides decay to ground state, fine structure is also observed, the consistent interpretation of the data with the same deformation parameters imposes strong constraints, and usually selects univocally the decaying state.

Until now, few nuclei were found to display non-axial symmetry[28, 31], but $^{141}$Ho was the only known odd-Z even-N deformed nucleus for which fine structure in proton emission from both ground and isomeric states was observed[37]. It provides a very interesting test to a theoretical model, since the widths and branching ratios have to be consistently described for the same $\beta$ and $\gamma$ deformations without any change of parameters of the model.

Applying the formalism discussed above, we could explain the decay widths and branching ratios of proton emission from both ground and isomeric states of $^{141}$Ho assuming a strong triaxial deformation $\gamma \sim 20^\circ$. This assignment of deformation was also consistent with the analysis of the rotational spectra of $^{140}$Dy and $^{141}$Ho, which have been observed.

In Table 1, we show the breaking of axial symmetry and the values of the deformation parameters $\beta_2$ and $\gamma$ which were assigned to nuclei using the formalism discussed above to reproduce the decay data. The corresponding decaying state is indicated in the last column. At the quoted values, our calculation reproduces simultaneously the experimental half-lives, branching ratios and rotational spectra of the nucleus. The attributed $\gamma$ deformations seem to support data expectations.

So far, we have discussed nuclei with an odd number of protons and an even number of neutrons. Odd-odd nuclei pose interesting questions due to the complications involved in the coupling of the valence proton as well as the neutron with the core. Odd–odd emitters have been discussed in the adiabatic approach[7]. The coupling between the odd proton and the odd neutron leads to several possible combinations of spin for the ground state of the nucleus. Therefore, the neutron is not a spectator, but it contributes with its spin to the total angular momentum of the decaying state.

Due to these possible couplings, it is possible to have a few states as candidates for decay, and data from decay to ground state of the daughter or even fine structure, might not be enough to assign a single state for decay.

A non-adiabatic quasi-particle approach to odd-odd nuclei, will give the possibility to study the role of the residual neutron-proton interaction in the Coriolis mixing. However, it is a quite difficult task.

We have preliminary results from such calculation[38], that for the strongly deformed $^{130}$Eu with $\beta_2 \sim 0.3$, confirmed that the decaying state is the $I^\pi = 1^+$ state. We also found that the residual interaction could influence the effect of Coriolis interaction and significantly modify the proton emission half-lives.
3. Conclusions

In conclusion, we have discussed spherical nuclei in the framework of relativistic covariant density functional theory, using the non-linear meson exchange NL3 [25] and density dependent point coupling DD-PC1 [26] interactions, that are well established models, and describe nuclear properties from very light to quite heavy nuclei. All data available of nuclei considered spherical was analyzed, and strong evidence for configuration mixing was found for some nuclei, pointing out to a possible occurrence of deformation or coupling to phonon states. Our studies on deformed nuclei, performed within the non-adiabatic–quasi–particle model, that include the Coriolis and residual interactions were quite successful and established the predictive power of the model. It was possible to observe the effect of correlations in the medium and the importance of very small components of the proton Nilsson state. Through the interpretation of the experimental decay widths, branching ratios and rotational spectra of the emitter, it was possible to identify the decaying state and the axial and non-axial deformation parameters. The most challenging case are the odd-odd emitters treated in the non-adiabatic approach, where not only the nucleus has a finite momentum of inertia, but the residual neutron-proton interaction is also taken into account. The effect of the latter on the Coriolis mixing is quite strong, and detectable in the half–life data.

We were able to obtain nuclear structure information of very unstable nuclei just from the interpretation of the experimental decay data, but with a well founded model, that encloses the forces and mechanism that condition the nuclear structure, and without any freedom for the parameters.

Acknowledgments

This work was supported by the Fundação para a Ciência e a Tecnologia (Portugal), Project: CERN/FP/123606/2011.

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