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Covariant density functional theory for decay of deformed proton emitters: A self-consistent approach

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ABSTRACT

Proton radioactivity from deformed nuclei is described for the first time by a self-consistent calculation based on covariant relativistic density functionals derived from meson exchange and point coupling models. The calculation provides an important new test to these interactions at the limits of stability, since the mixing of different angular momenta in the single particle wave functions is probed.

1. Introduction

The fast development of Radioactive Ion Beam (RIB) facilities, and new technologies on multi-particle detection, are leading to the production and detection for the first time in a laboratory of many nuclei far from stability, that should have been formed in the stellar synthesis of the elements. Nuclei at the extremes of stability present various exotic decays [1] which are probes to their definite structure. The observation and interpretation of these decays and level structure will provide a basis to understand the changes in shell structure away from the stability region, and the mechanisms of nucleosynthesis.

On the proton rich side of the nuclear chart, the observation and interpretation of proton radioactivity have been the only possibility to obtain information on the structure of proton drip-line nuclei, since this decay is the only feature that allows to select, in an experiment, drip-line nuclei from all the other nuclei produced in the reaction. With tagging techniques, their spectra can also be studied [2]. One proton emission from the ground and isomeric states was observed for nuclei with charges in the range $50 < Z < 83$, and mapped the drip-line in this region. Below $Z = 50$, two-proton emission [3], beta delayed proton emission [4], and few cases of proton emission from excited states [1] have been observed. This is a region of great experimental activity at the moment, and of great relevance, since the rp-synthesis proceeds along the $N = Z$ line involving proton drip-line nuclei. However, it is a challenging task, since it involves extremely short life times, difficult to observe experimentally. Therefore, a great part of the knowledge on the structure of these nuclei relies on theoretical extrapolations.

Theoretical models for proton emission explain very well the measured half-lives for spherical as well as deformed nuclei. Simple non-relativistic models are based on semi-classical WKB methods [5], while the deformed proton emitters can be studied more rigorously by identifying that the decay proceeds from single-particle resonances [6,7]. Microscopic studies of deformed proton emitters allow to test the details of the nuclear wave function to which the half-lives are quite sensitive. The most consistent non-relativistic theoretical approach for proton emission is the non-adiabatic quasiparticle approach which is very successful [8] in bringing out several interesting features of deformed odd–even proton emitters including the triaxially deformed ones [9]. Its extension to odd–odd nuclei [10] suggested that it is possible to test the residual neutron proton interaction and to determine the neutron Nilsson level even if the neutron does not participate actively in the decay.

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In all of the above non-relativistic microscopic models, the nuclear potential is described in terms of phenomenological Wood–Saxon type forms, with parameters fitted to global nuclear properties. In a recent investigation [11], we have performed self-consistent relativistic mean field calculations (RMF) for spherical nuclei, using interactions derived from density functional theory (DFT) that requires only a minimal number of parameters. The calculation was very successful in reproduction the experimental data. It is the purpose of this work to extend these previous calculations in order to account for deformation.

Nuclear density functionals provide a successful description of ground-state properties and of collective excitations of atomic nuclei, from relatively light systems to super-heavy nuclei, and from the valley of stability to the particle drip-lines. They are usually implemented in terms of self-consistent mean field models. The energy density functional (EDF) is constructed as a functional of the one-body nucleon density matrix that corresponds to a product wave function of single-particle or single-quasiparticle states. This approach is analogous to Kohn Sham DFT [12], that enables a description of quantum many-body systems in terms of universal density functionals. Nuclear DFT models effectively map the many-body problem onto a one-body problem, and the exact EDF is approximated by simple functionals of powers and gradients of ground-state nucleon densities and currents, representing distributions of matter, spins, momentum and kinetic energy [13].

A particular class of DFT models are those based on covariant density functional theory (CDFT). In the past decades, CDFT has been proven to be a very powerful tool in nuclear physics [14–17]. It exploits basic properties of QCD at low energies, in particular, symmetries and the separation of scales. These functionals provide a consistent treatment of the spin degrees of freedom, they include the complicated interplay between the large Lorentz scalar and vector self-energies induced on the QCD level by the in medium changes of the scalar and vector quark condensates [18] and they include the nuclear currents induced by the spatial parts of the vector self-energies. In particular, Lorentz invariance puts stringent restrictions on the number of parameters.

At present nuclear density functionals are not yet fully derived from ab-initio calculations. They are usually adjusted to a variety of finite nuclei and infinite nuclear matter properties. Although all these effective interactions are based on the mean-field approach, some differences will generally appear among them due to the specific ansatz of the density dependence adopted for each interaction. For instance, predictions in the isovector channel of existing functionals differ widely from one another and, as a consequence, the density dependence of the symmetry energy is far from being fully determined. This has an impact on finite nuclei properties such as, for example, the neutron skin thickness. A universal density functional theory should be derived in a fully microscopic way from the interactions between bare nucleons [18,19]. At present, however, attempts in this direction provide only qualitative results since the methods to derive them are not yet precise enough, and the three-body term of the bare interaction is not well known.

The above discussion points out the interest in applying the various modern density functionals available in the literature at the extremes of proton rich matter, and describe the properties of proton radioactive nuclei. It will provide another test to these interactions, and will be a step in the direction of achieving a more fundamental and consistent description of nuclear structure from stability up to the extremes of bound matter.

In the present work we discuss a self-consistent relativistic calculation of proton emission from deformed nuclei, based on relativistic density functionals derived from meson exchange and point coupling models, and apply it to interpret the structure of deformed proton drip-line nuclei.

2. Covariant density functional theory for structure and decay of deformed nuclei

Proton radioactivity probes single particle states since the proton is in a resonance state very low in the continuum, corresponding essentially to a single particle excitation, that decays. The ordering of these states in the nucleus changes with deformation and may be modified by the increasing asymmetry in the proton–neutron ratio and the coupling to continuum states. The half-lives for decay from the single particle resonances are strongly dependent on the angular momentum of the state, and on deformation, and can change by orders of magnitude with small variations of these quantities. Therefore, they are a sensitive test to details of the nuclear mean-field.

The investigations presented in this manuscript are based on covariant density functional theory, derived from old ideas of Teller and Dürr [20,21] and the Walecka model [22]. The essential idea, however, which allowed successful applications of such models to realistic finite nuclei was the use of a density dependence through non-linear meson couplings [23–26]. Based on the success of relativistic Brueckner theory [27], later on these somewhat unphysical non-linear couplings have been replaced by linear models with density dependent coupling constants [28–31]. Although being very successful, these models use forces with finite range and are therefore relatively complicated in numerical applications, in particular for deformed nuclei. Therefore, recently the meson exchange has been replaced by relativistic interactions of zero range [32–35]. These versions of covariant density functional theory are equivalent to Skyrme forces in the non-relativistic scheme: Besides the two-body interactions and derivative terms they contain three- and four-body terms, which are on the mean field level equivalent to density dependent two-body forces.

In the present paper we use two different relativistic point-coupling models. Both are relatively successful and differences between them have been investigated recently on a systematic global scale [36,37]. The functional PC-PK1 of the Peking group [35] contains besides the two-, three-, and four-body terms of zero range also several derivative terms. It contains 11 phenomenological parameters which are determined by a fit to the binding energies and radii of a large number of spherical semi-magic nuclei all over the periodic table. On the contrary, the functional DD-PC1 of the Munich–Zagreb group [34] contains 10 parameters which are fitted to masses of 64 heavy deformed nuclei and a few nuclear matter properties. As a consequence there is a difference between the description of spherical and deformed nuclei in these two models. It turns out that the masses of deformed nuclei are considerably better reproduced by DD-PC1. On the contrary the masses of spherical nuclei are usually somewhat over-bound.

In a first step we determine the scalar and vector potentials $S(\boldsymbol{r})$ and $V(\boldsymbol{r})$ of the deformed nuclei in a fully self-consistent way by solving the relativistic mean field equations (RMF) equations for the even–even daughter nuclei including pairing correlations in the BCS approximation. For reasons of numerical simplicity we use the method of an expansion of the Dirac spinors in oscillator space discussed in Refs. [38,39]. The maximal major oscillator quantum number is $N_F = 20$. The Coulomb potential is, as usual, determined by its Greens function. By comparing the resulting Coulomb-potential in the asymptotic region with its analytic form we could verify that this method provides a very good approximation for the potential of the protons even for large radii.

In a second step we expand the resulting self-consistent axial potentials $S(\boldsymbol{r})$ and $V(\boldsymbol{r})$ in spherical harmonics with different L-values, obtaining the corresponding potentials $S_L(r)$ and $V_L(r)$ on a fine mesh in r-space.

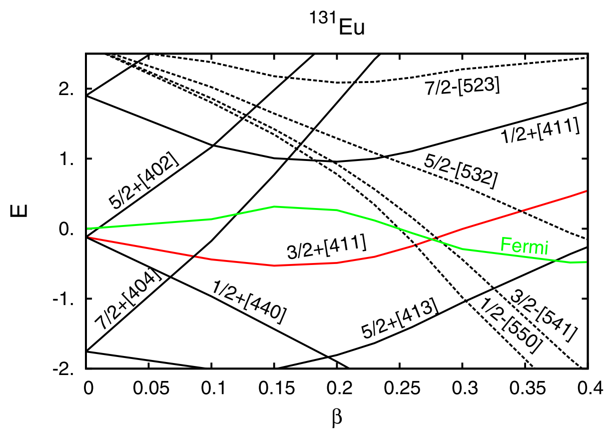

Fig. 1. Nilsson proton levels in ^{131}Eu as a function of quadrupole deformation (β_2) using the DD-PC1 field. The Fermi energy is represented by the green line, and the $3/2^+[411]$ level (red line) corresponds to the decaying state. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

In a deformed emitter, the state of the outgoing proton is a single-particle Nilsson resonance, that can be determined from the solutions of the Dirac equation in the deformed fields S and V imposing outgoing wave boundary conditions. This was done by solving a full coupled channel problem in coordinate space, for the relativistic interactions discussed above, leading to a precise description of the energy, width and wave function of the proton resonances. This is a complex problem, and was solved previously only for $K = 1/2^+$ resonant states by the Beijing group [40], using a Woods Saxon interaction. The energies and widths of resonances in deformed nuclei were also obtained [41] from an extension of the complex scaling method to the relativistic framework. We have solved the full relativistic coupled channel problem for any value of the angular momentum in coordinate space using similar techniques as in the non-relativistic case [42], and the Nilsson diagram for resonances in ^{131}Eu is presented in Fig. 1 for the self-consistent density dependent point coupling DD-PC1 [34] interaction. The interaction for each deformation, different from the self-consistent one, was obtained doing a constrained minimization through a Lagrange multiplier for the deformation. Similar figures can be drawn for the point coupling interaction PC-PK1 [35].

The half-life for decay by one particle emission can be determined from general scattering theory, as $T_{1/2} = \hbar \ln 2/\Gamma$, where the quantity Γ is the decay width. For decay from an initial state which is the band head based on a K_i Nilsson level, to a daughter nucleus in a J_d state, the partial decay width, that corresponds to the contribution to decay from a component of the wave function with angular momentum and spin l_p, j_p of the emitted proton, is given by [43],

$$\Gamma^{J_d}_{l_p j_p} = \frac{\hbar^2 k}{\mu} \frac{2(2J_d+1) < J_d, 0, j_p, K_i | K_i, K_i >^2}{(2K_i+1)} |N^{K_i}_{l_p j_p}|^2 u^2_{K_i}, \quad (1)$$

while the total width for the decay in a specific state is a sum of partial widths of Eq. (1), restricted by angular momentum and parity conservation, i.e.,

$$\Gamma^{J_d} = \sum_{j_p=\max(|J_d-K_T|,K_p)}^{J_d+K_T} \Gamma^{J_d}_{l_p j_p}. \quad (2)$$

The quantity $N^{K_i}_{l_p j_p}$ is the asymptotic normalization with respect to the Coulomb outgoing wave function, of the $l_p j_p$ component of the single particle wave function of the decaying state, given by the solution of the Dirac coupled channel equation. Since the residual interaction is mainly due to pairing, the spectroscopic factor is simply the probability u^2_K that the single particle level K is empty in the daughter nucleus, evaluated in the BCS approach with a constant gap.

This means that we use BCS occupation probabilities for the calculation of the densities

$$v^2_K = \frac{1}{2}\left[1 - \frac{(\varepsilon_K - \lambda)}{\sqrt{(\varepsilon_K - \lambda)^2 + \Delta^2}}\right] \quad (3)$$

with the empirical value $\Delta = 12/A^{1/2}$ for the gap parameter [44].

If decay occurs to the ground state, since we are dealing with an odd–even nucleus $J_d = 0$only component of the s.p. wave function that contributes to the width, is the one with the same angular momentum as the ground state of the parent nucleus, that is, $j_p = J_i = K_i$.

Due to energy considerations, proton decay should proceed mainly to the ground state of the daughter nucleus. However, in rotational nuclei the first excited state could be very low in energy and a sizeable branching ratio could be expected, known as fine structure.

The branching ratio between the decay to the ground and first excited 2^+ states can be obtained from the ratio $\Gamma^{J=2}/(\Gamma^{J=2} + \Gamma^{J=0})$ of the total widths defined in Eq. (2).

3. Results and discussion

As an example, we discuss decay from ^{131}Eu, a highly deformed proton emitter where fine structure in the radioactive decay from the ground state was identified [45,46]. The experiment shows the ground-state peak at 932(7) keV, $t_{1/2} = 17.8(19)$ ms, and a second proton peak with energy 811(7) keV, $t_{1/2} = 23^{+10}_{-6}$ ms, interpreted as proton decay from the ground state of ^{131}Eu, to the first excited 2^+ state of the daughter nucleus ^{130}Sm, with a branching ratio of 0.24(5), and a total half-live $t_{1/2} = 20.2(2.2)$ ms.

The deformation of ^{130}Sm can be estimated from the well-known empirical relation [47], between the energy of the 2^+ state and the deformation, $E2^+ \approx 1225/(A^{7/3}\beta_2^2)$ MeV, followed by most even–even deformed nuclei. This relation suggests for ^{130}Sm a $\beta_2 \approx 0.34$ since the 2^+ state lies at 121(3) keV. If there is no change of deformation during the decay, ^{131}Eu, should have a similar deformation.

From the observation of the proton resonances of Fig. 1, the $3/2^+[411]$ state is close to the Fermi surface for a large quadrupole deformation, so it is the candidate to be the decaying state, similarly to what was predicted by the non-relativistic calculation [43].

The half-lives depend strongly on the energy, therefore, it is important that the resonance is at the experimental energy, which is the separation energy. Since this usually differs from the single particle energy coming from the RMF calculation, we have adopted a prescription commonly used in non-relativistic calculations, and changed the depth of the nuclear potential $V + S$ by a few percent in such a way to get a resonance at the experimental energy. Of course this change of the potential depth violates the self-consistency slightly. This is, however a very small effect.

The Coulomb potential was kept unchanged, since this is the potential felt by the proton outside the nucleus.

The half-life for decay from the various states close to the Fermi surface, obtained from the use Eq. (1), are shown in Fig. 2, in comparison with the experimental value. The half-life for the negative parity states are not shown, since one should take into account the Coriolis interaction, as they come from a state with very high angular momentum, the $h_{11/2}$. In this case the half-life would become much longer than the experimental one, so they cannot be good candidates to interpret the decay.

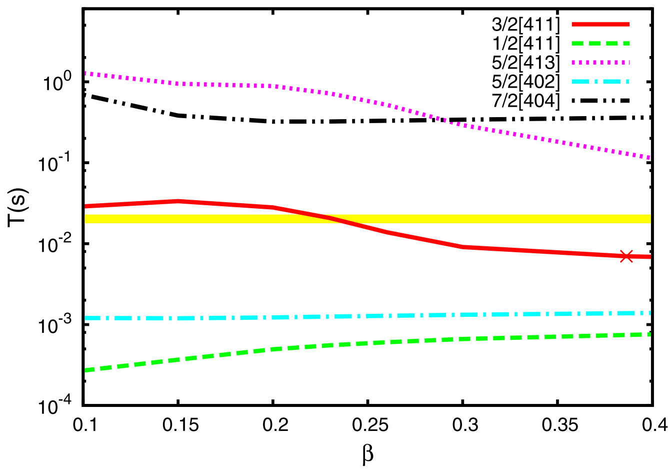

Fig. 2. Theoretical and experimental (yellow horizontal band) half-lives as a function of deformation for decay from the positive parity single particle levels, using the DD-PC1 field. The width of the experimental band corresponds to the error on the half-life. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

It can be seen that the $3/2^+$ state is the only one that has a half-life close to the experimental result, but this happens at a quadrupole deformation of order of 0.25, lower than the one expected for ^{131}Eu, and also smaller than the deformation obtained from the minimization of the energy functional, in the self-consistent calculation.

The half-life depends strongly on many quantities, like quantum numbers of the decaying state, but also on details of the interaction like for example the nuclear radius, and strength of the spin-orbit force. The latter could influence the relative energies of the levels, and therefore, change drastically the occupation probability of the levels, and the half-life. This is illustrated in Fig. 3, where it can be seen that the change of the half-life as a function of deformation observed in Fig. 2 is mainly due to the change of the BCS spectroscopic factor, implying that a small shift in the position of the Nilsson energies could bring to a better agreement with values expected for the deformation.

In contrast with the half-lives, the branching ratios are instead quite sensitive to details of the wave function components with different angular momentum, which are a probe of nuclear structure properties.

In the case of decay to the 2^+ state, different values for the angular momentum of the proton are allowed, as expressed by the various terms in Eq. (2). The dominant contribution corresponds to situations where the centrifugal barrier is low. If two channels have the same barrier, it is the component of the wave function with the largest normalization $N^{K_i}_{l_p j_p}$ that controls the value of the width. For $K_i = l_p + 1/2$, there is only one large term in the sum, the one with the same $l_p j_p$ as the decay to the 0^+, and the branching ratio depends only on the energy of the 2^+ state. This gives in our case a branching ratio for the levels 5/2[413], 5/2[402] practically constant, of the order of 0.02–0.03, since the centrifugal barrier of the $j_p = g_{7/2}$ and $g_{9/2}$ components is very high, and $j_p = d_{5/2}$ dominates the decay. A very small dependence on deformation is observed, since $N^{K_i}_{l_p j_p}$ cancels out in the ratio. As can be seen in Fig. 4, where the branching ratio for decay to the 2^+ is presented, this value is far from the experiment, and can be disregarded. The level 1/2[411] decays to the ground state with $l = 0$, but can only decay to the 2^+ if $l = 2$. Consequently, the decay to the excited state is hindered not only from the energy but also from the centrifugal barrier, so it will be even smaller.

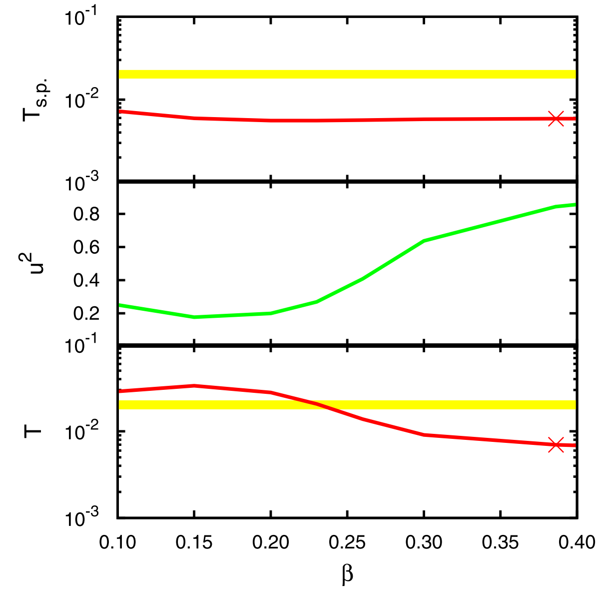

Fig. 3. Theoretical half-lives as a function of deformation for the $3/2^+$ state, without (first panel) and with (third panel) the BCS spectroscopic factor, compared with the experimental value, given by the yellow horizontal band. The dependence on deformation of u^2 is shown in the second panel. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

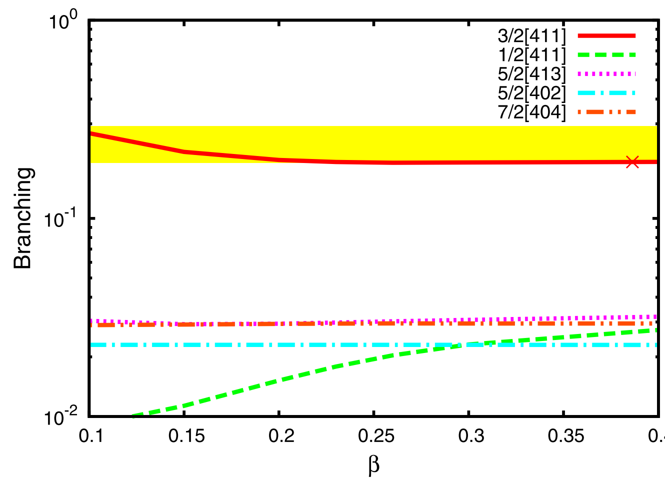

Fig. 4. Theoretical and experimental (yellow) branching ratio as a function of deformation for decay from different single particle levels, using the DD-PC1 field. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

The only possibility to expect a branching ratio close to the experiment is to have $K_i = l_p - 1/2$, since two channels with the same centrifugal barrier can contribute to decay to the 2^+, and a large branching ratio can be observed if $N^{K_i}_{l_i K_i}$ for decay to the ground state is much smaller than the other component. Therefore, Fig. 4 confirms without ambiguity that it is the $3/2^+$ state that can interpret the experimental value.

If one analyzes the various terms that enter in the calculation of the branching ratio, we can see that the spectroscopic factor u^2, present in the numerator and denominator, is the same and cancels out. In the sum over the various partial decay widths for decay from the $K = 3/2^+$ state, the component of the wave function for the state $d_{3/2}$ is very small, whereas the $d_{5/2}$ is quite large as displayed in Fig. 5. One is then testing the ratio between these two very different amplitudes, and it is the delicate balance between them that determines the value of the branching ratio.

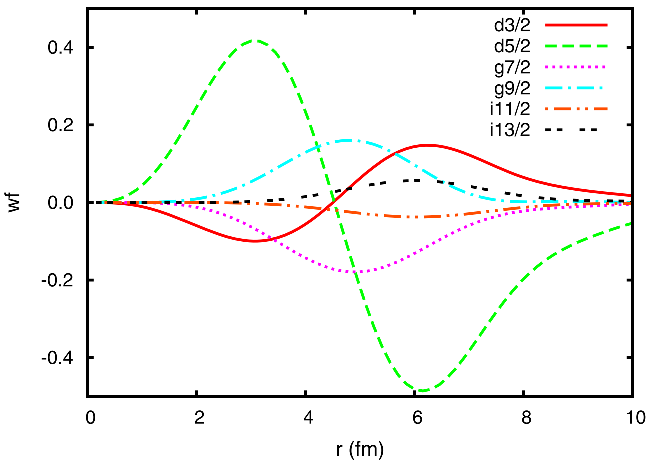

Fig. 5. Upper components of the Dirac wave function of the $3/2^+[411]$ state with different angular momentum.

The effect of the Coriolis coupling was not included in the calculation, since for the positive parity states of ^{131}Eu, it has been shown [48] that its contribution is negligible.

We have performed a similar study for the point coupling interaction PC-PK1, but found only minor differences in the behaviour of the half-lives, that do not change our conclusions. This does not mean, that the proton-decay does not depend on the underlying model, because, as discussed in a recent global investigation [36] these two point-coupling models provide for many physical observables rather similar results. Further investigation with other relativistic and non-relativistic density functionals are definitely necessary to clarify this point.

In conclusion, we have presented the first self-consistent calculation of proton radioactivity from deformed nuclei, that accounts for the experimental data, using density dependent and point coupling interactions derived from covariant density functional theory. The agreement with the experimental data provided by the DD-PC1 and PC-PK1 is perfect for the branching ratio, but for the half-life it would predict a deformation for ^{131}Eu smaller than what is expected. However, the half-lives depend strongly on details of the interaction, in contrast with the branching ratio which is more stable in relation to these quantities, and depends instead on the details of the components of the single particle wave functions. To be able to interpret correctly the branching ratio implies that the components of the Nilsson states are very well described, and include the correct nuclear structure features.

This an important new test for the Non-Linear Meson Exchange and Density Dependent Point Coupling interactions, derived from covariant relativistic density functional theory, at the limits of stability, since it comes from another perspective, the observation and interpretation of decay, in contrast to the standard tests provided by the interpretation of global properties, where these interactions perform well.

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