Transitional Lu and spherical Ta ground-state proton emitters in the relativistic Hartree-Bogoliubov model

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(Received 7 July 1999; published 1 October 1999)

Properties of transitional Lu and spherical Ta ground-state proton emitters are calculated with the relativistic Hartree-Bogoliubov model. The NL3 effective interaction is used in the mean-field Lagrangian, and pairing correlations are described by the pairing part of the finite range Gogny interaction DIS. Proton separation energies, ground-state quadrupole deformations, single-particle orbitals occupied by the odd valence proton, and the corresponding spectroscopic factors are compared with recent experimental data, and with results of the macroscopic-microscopic mass model. [S0556-2813(99)51011-X]

PACS number(s): 21.60.Jz, 21.10.Dr, 23.50.+z, 27.60+j

The structure and decay modes of nuclei beyond the proton drip line represent one of the most active areas of experimental and theoretical studies of exotic nuclei with extreme isospin values. In the last few years many new data on ground-state and isomeric proton radioactivity have been reported. In particular, detailed studies of odd-Z ground-state proton emitters in the regions $51 \leq Z \leq 55$ and $69 \leq Z \leq 83$ have shown that the systematics of spectroscopic factors is consistent with half-lives calculated in the spherical WKB or distorted-wave Born (DWBA) approximations [1,2]. More recent data [3,4] indicate that the missing region of light rare-earth nuclei contains strongly deformed systems at the drip line.

In the theoretical description of ground-state and isomeric proton radioactivity, two essentially complementary approaches have been reported. One possibility is to start from a spherical or deformed phenomenological single-particle potential, a Woods-Saxon potential, for instance, and to adjust the parameters of the potential well in order to reproduce the experimental one-proton separation energy. The width of the single-particle resonance is then determined by the probability of tunneling through the Coulomb and centrifugal barriers. Since the probability strongly depends on the valence proton energy and on its angular momentum, the calculated half-lives provide direct information about the spherical or deformed orbital occupied by the odd proton. For a spherical proton emitter it is relatively simple to calculate half-lives in the WKB or DWBA approximations [2]. On the other hand, it is much more difficult to quantitatively describe the process of three-dimensional quantum mechanical tunneling for deformed proton emitters. Modern reliable models for calculating proton emission rates from deformed nuclei have been developed only recently [4,5]. A shortcoming of this approach is that it does not predict proton separation energies, i.e., the models do not predict which nuclei are likely to be proton emitters. In fact, if they are used to calculate decay rates for proton emission from excited states, the depth of the central potential has to be adjusted for each proton orbital separately. In addition, the models of Refs. [2,4,5] do not provide any information about the spectroscopic factors of the proton orbitals. Instead, experimental spectroscopic factors are defined as ratios of calculated and measured half-lives, and the deviation from unity is attributed to nuclear structure effects.

In Refs. [6–8] we have used the relativistic Hartree-Bogoliubov (RHB) theory to calculate properties of protons and odd-rich spherical even-even nuclei with $14 \leq Z \leq 28$, and to describe odd-Z deformed ground-state proton emitters in the region $53 \leq Z \leq 69$. RHB presents a relativistic extension of the Hartree-Fock-Bogoliubov theory, and it provides a unified framework for the description of relativistic mean-field and pairing correlations. Such a unified and self-consistent formulation is especially important in applications to drip-line nuclei. The RHB framework has been used to study the location of the proton drip line, the ground-state quadrupole deformations and one-proton separation energies at and beyond the drip line, the deformed single particle orbitals occupied by the odd valence proton, and the corresponding spectroscopic factors. The results of fully self-consistent calculations have been compared with experimental data on ground-state proton emitters. However, since it is very difficult to use the self-consistent ground-state wave functions in the calculation of proton emission rates, one could say that the RHB model provides information that is complementary to that obtained with the models of Refs. [2,4,5]. It should be noted that in the relativistic framework the strength and the shape of the spin-orbit term are determined self-consistently. This is essential for a correct description of spin-orbit splittings in regions of nuclei far from stability, where the extrapolation of effective strength parameters becomes questionable. The motivation for the present work is the very recent data on proton emission from the closed neutron shell nucleus $^{155}$Ta [9], and the proposed experiment to search for direct proton emission from $^{140}$Lu [10]. The analysis of ground-state proton radioactivity in the Lu and Ta isotopes completes our study of deformed and transitional proton emitters in the region $53 \leq Z \leq 73$.

A very detailed description of the relativistic Hartree-Bogoliubov theory can be found, for instance, in Ref. [7]. In the following we only outline the essential features of the model that will be used to describe nuclei at the proton drip line. The ground state of a nucleus is represented by the Slater determinant of independent single-quasiparticle states, which are obtained as solutions of the relativistic Hartree-Bogoliubov equations...
\[
\begin{pmatrix}
\hat{h}_D - m - \lambda & \Delta \\
-\Delta^* & -\hat{h}_D + m + \lambda
\end{pmatrix}
\begin{pmatrix}
U_k(\mathbf{r}) \\
V_k(\mathbf{r})
\end{pmatrix} = E_k \begin{pmatrix}
U_k(\mathbf{r}) \\
V_k(\mathbf{r})
\end{pmatrix}.
\]
(1)

The column vectors denote the quasiparticle spinors, and \(E_k\) are the quasiparticle energies. In the Hartree approximation for the self-consistent mean field, the single-nucleon Dirac Hamiltonian reads

\[
\hat{h}_D = -i \alpha \cdot \nabla + \beta(m + g_\sigma \sigma(\mathbf{r})) + g_\omega \tau_3 \omega^0(\mathbf{r}) + g_\rho \rho^0(\mathbf{r}) + e \frac{(1 - \tau_3)}{2} A^0(\mathbf{r}).
\]
(2)

It describes the motion of independent Dirac nucleons in the mean-field potentials: the isoscalar scalar \(\sigma\)-meson potential, the isoscalar vector \(\omega\) meson, and the isovector vector \(\rho\)-meson potential. The photon field \(A\) accounts for the electromagnetic interaction. The meson potentials are determined self-consistently by the solutions of the corresponding Klein-Gordon equations. The source terms for these equations are calculated in the \(\text{no-sea}\) approximation. Because of charge conservation, only the third component of the isovector \(\rho\) meson contributes. For an even-even system, due to time reversal invariance, the spatial vector components \(\omega, \rho_1, \text{and } A\) of the vector meson fields vanish. In nuclei with odd numbers of protons or neutrons, time reversal symmetry is broken. The odd particle induces polarization currents and the time-odd components in the meson fields. These components play an essential role in the description of magnetic moments and of moments of inertia in rotating nuclei. However, their effect on deformations and binding energies is very small and can be neglected to a good approximation. As in our previous studies of nuclei at the proton drip lines, we choose the NL3 set of meson masses and meson-nucleon coupling constants [11] for the effective interaction in the particle-hole channel: \(m = 939\) MeV, \(m_\sigma = 508.194\) MeV, \(m_\omega = 782.501\) MeV, \(m_\rho = 763.0\) MeV, \(g_\sigma = 10.217, \ g_\rho = -10.431 \text{ fm}^{-1}, \ g_3 = -28.885, \ g_\omega = 12.868, \text{ and } g_\rho = 4.474.\)

The pairing field \(\Delta\) is defined as

\[
\Delta_{ab}(\mathbf{r}, \mathbf{r}') = \frac{1}{2} \sum_{c,d} V_{abcd}(\mathbf{r}, \mathbf{r}') \kappa_{cd}(\mathbf{r}, \mathbf{r}'),
\]
(3)

where \(V_{abcd}(\mathbf{r}, \mathbf{r}')\) are matrix elements of a two-body pairing interaction, and \(\kappa_{cd}(\mathbf{r}, \mathbf{r}')\) is the pairing tensor. The pairing part of the phenomenological Gogny force

\[
V^{BP}(1,2) = \sum_{i=1,2} e^{-\mu_i r_i} \langle \sigma_1 - \sigma_2 | P_1 - P_2 | M_1 P_1 P_2 M_1 P_2 \rangle,
\]
(4)

with the set D1S [12] for the parameters \(\mu_i, W_i, B_i, H_i, \text{and } M_i\) (\(i = 1,2\)), is used to describe pairing correlations.

The RHB single-quasiparticle equations (1) are solved self-consistently. The iteration procedure is performed in the quasiparticle basis. The chemical potential \(\lambda\) has to be determined by the particle number subsidiary condition so that the expectation value of the particle number operator in the ground state equals the number of nucleons. A simple blocking prescription is used in the calculation of odd-proton and/or odd-neutron systems. The blocking calculations are performed without breaking the time-reversal symmetry. The resulting eigenspectrum is transformed into the canonical basis of single-particle states, in which the RHB ground state takes the BCS form. The transformation determines the energies and occupation probabilities of the canonical states.

The one-proton separation energies

\[
S_p(Z,N) = B(Z,N) - B(Z-1,N)
\]
(5)

for the Lu and Ta isotopes are displayed in Fig. 1, as a function of the number of neutrons. The predicted drip-line nuclei are \(^{154}\text{Lu}\) and \(^{159}\text{Ta}\). In the process of proton emission the valence particle tunnels through the Coulomb and centrifugal barriers, and the decay probability depends strongly on the energy of the proton and on its angular momentum. In rare-earth nuclei the decay of the ground-state by direct proton emission competes with \(\beta^+\) decay; for heavy nuclei fission or \(\alpha\) decay can also be favored. In general, ground-state proton emission is not observed immediately after the drip line. For small values of the proton separation energies, the width is dominated by the \(\beta^+\) decay. On the other hand, large separation energies result in extremely short proton-emission half-lives, which are difficult to observe experimentally. For a typical rare-earth nucleus, the separation energy window, in which ground-state proton decay can be directly observed, is about \(0.8-1.7\) MeV [2]. In Fig. 1 we have compared the calculated separation energies with experimental transition energies for ground-state proton emission in \(^{150}\text{Lu}\), \(^{151}\text{Lu}\) [13], \(^{155}\text{Ta}\) [9], \(^{156}\text{Ta}\) [14], and \(^{157}\text{Ta}\) [15]. The filled diamonds denote the negative values of the transition energies \(E_p\).
TABLE I. Lu ground-state proton emitters. The results of the RHB calculation for the one-proton separation energies $S_p$, quadrupole deformations $\beta_2$, and the deformed single-particle orbitals occupied by the odd valence proton, are compared with predictions of the macroscopic-microscopic mass model, and with the experimental transition energies. All energies are in units of MeV; the RHB spectroscopic factors are displayed in the sixth column.

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<tbody>
<tr>
<td>$^{149}$Lu</td>
<td>78</td>
<td>-1.77</td>
<td>-0.158</td>
<td>7/2[-523]</td>
<td>0.60</td>
<td>5/2$^-$</td>
<td>-1.51</td>
<td>-0.175</td>
</tr>
<tr>
<td>$^{150}$Lu</td>
<td>79</td>
<td>-1.31</td>
<td>-0.153</td>
<td>7/2[-523]</td>
<td>0.61</td>
<td>5/2$^-$</td>
<td>-1.00</td>
<td>-0.158</td>
</tr>
<tr>
<td>$^{151}$Lu</td>
<td>80</td>
<td>-1.24</td>
<td>-0.151</td>
<td>7/2[-523]</td>
<td>0.58</td>
<td>7/2$^-$</td>
<td>-0.99</td>
<td>-0.150</td>
</tr>
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</table>

In the detailed analysis of odd-$Z$ proton emitters ($53\leq Z \leq 69$) [7] it has been shown that, while the proton-rich isotopes of La, Pr, Pm, Eu, and Tb are all strongly prolate deformed ($\beta_2 \approx 0.30-0.35$), Ho and Tm isotopes at the proton drip line display a transition from prolate to oblate shapes. Spherical shapes are expected as the nuclei with unbound protons approach the $N=82$ neutron shell. The Lu proton emitters are found in the transitional region between oblate and spherical shapes. This is illustrated in Fig. 2, where we plot the binding energy curve for $^{151}$Lu as a function of the quadrupole deformation parameter. The binding energies result from self-consistent RHB/NL3 calculations performed by imposing a quadratic constraint on the quadrupole moment. A very shallow minimum is found at $\beta \approx -0.15$, but otherwise the potential is rather flat with a shoulder at $\beta = 0$. In Fig. 3 we compare the ground-state quadrupole deformations of the proton-rich Lu isotopes with those of Ho and Tm [8]. For $N=80$ all three chains of isotopes display oblate deformations; starting with $N=81$, a sharp transition to the spherical shape is observed.

The proton-rich Ta isotopes are spherical. In Fig. 1 we compare the calculated one-proton separation energies with experimental transition energies for $^{155}$Ta [9], $^{156}$Ta [14], and $^{157}$Ta [15]. The predictions for the spherical orbitals occupied by the odd proton and the corresponding spectroscopic factors are displayed in Table II. Results of the FRDM calculation [17] have also been included in the comparison. As in the case of the Lu ground-state proton emitters, an excellent agreement between RHB separation energies and experimental data on transition energies for proton emission is observed. In particular, our calculation reproduces the very recent data on proton emission from the...
TABLE II. Spherical Ta ground-state proton emitters. RHB results for the proton separation energies, the single-particle orbitals occupied by the odd proton, and the corresponding spectroscopic factors are compared with the predictions of the finite-range droplet mass model (FRDM) and with experimental data.

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<tr>
<td>155Ta</td>
<td>$S_p$</td>
<td>$J^*$</td>
<td>$h$</td>
</tr>
<tr>
<td></td>
<td>-1.677</td>
<td>11/2$^-$</td>
<td>9/2$^-$</td>
</tr>
<tr>
<td></td>
<td>spectr. factor</td>
<td>0.60</td>
<td>0.58(20)</td>
</tr>
<tr>
<td>156Ta</td>
<td>$S_p$</td>
<td>$J^*$</td>
<td>$h$</td>
</tr>
<tr>
<td></td>
<td>-1.129</td>
<td>3/2$^+$</td>
<td>3/2$^-$</td>
</tr>
<tr>
<td></td>
<td>spectr. factor</td>
<td>0.51</td>
<td></td>
</tr>
<tr>
<td>157Ta</td>
<td>$S_p$</td>
<td>$J^*$</td>
<td>$h$</td>
</tr>
<tr>
<td></td>
<td>-1.040</td>
<td>11/2$^-$</td>
<td>9/2$^-$</td>
</tr>
<tr>
<td></td>
<td>spectr. factor</td>
<td>0.42</td>
<td>0.56(24)</td>
</tr>
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The significant decrease in proton binding for $^{155}$Ta, as compared to $^{155,156}$Ta, has been associated to the $N=82$ closure. In comparison, the FRDM results are found to be in rather poor agreement with experimental data. Except for $^{155}$Ta, the spherical orbitals predicted to be occupied by the odd proton agree with the experimental assignments, and the theoretical spectroscopic factor of the $h_{11/2}$ orbital in $^{155}$Ta is very close to the experimental value. For $^{157}$Ta, the RHB model predicts ground-state proton emission from the $h_{11/2}$ orbital. The experimental assignment for the ground-state configuration is $s_{1/2}$, but an alpha decaying state is identified in $^{155}$Ta at an excitation energy of only 22(5) keV and assigned to an $h_{11/2}$ isomer [15]. We have also calculated the one-proton separation energy for $^{156}$Ta: $S_p = -1.250$ MeV; the orbital is $h_{11/2}$ and the spectroscopic factor is 0.79. This is to be compared with the experimental transition energy $E_p = 1.103(12)$ MeV [19], assigned to the $h_{11/2}$ orbital with the experimental spectroscopic factor 0.92(4) [1].

In conclusion, the relativistic Hartree-Bogoliubov model has been applied in the description of ground-state properties of transitional Lu and spherical Ta proton emitters. The NL3 effective interaction has been used for the mean-field Lagrangian, and pairing correlations have been described by the pairing part of the finite range Gogny interaction D1S. We would like to emphasize that this particular combination of effective forces has been used in most of our recent applications of the RHB model, not only for spherical and deformed $β$-stable nuclei, but also for nuclear systems with large isospin values on both sides of the valley of $β$ stability. The model parameters therefore have not been adjusted to the specific properties of nuclei studied in this work, or to the properties of deformed proton emitters discussed in Refs. [7,8]. The self-consistent calculation reproduces in detail the observed transition energies for ground-state proton emission in $^{150}$Lu, $^{155}$Lu [13], $^{155}$Ta [9], $^{156}$Ta [14], and $^{157}$Ta [15], as well as the assignments for the orbitals occupied by the valence odd proton and the corresponding spectroscopic factors. The model also predicts the one-proton separation energy of $-1.77$ MeV for the possible proton emitter $^{149}$Lu. Oblate ground-state deformations are predicted for all Lu proton emitters, while spherical shapes are calculated for the Ta isotopes at and beyond the proton drip line. With the excellent agreement observed between the RHB results and the very recent data on proton emission from the closed neutron shell nucleus $^{152}$Ta [9], we complete our study of ground-state properties of deformed and transitional proton emitters [7,8].

[10] J.C. Batchelder et al. (private communication).