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Relativistic Hartree-Bogoliubov Description of the Deformed Ground-State Proton Emitters

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Ground-state properties of deformed proton-rich odd-Z nuclei in the region $59 \leq Z \leq 69$ are described in the framework of relativistic Hartree-Bogoliubov (RHB) theory. One-proton separation energies and ground-state quadrupole deformations that result from fully self-consistent microscopic calculations are compared with available experimental data. The model predicts the location of the proton drip-line, the properties of proton emitters beyond the drip-line, and provides information about the deformed single-particle orbitals occupied by the odd valence proton. [S0031-9007(99)09353-9]

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The decay by direct proton emission provides the opportunity to study the structure of systems beyond the drip-line. The phenomenon of ground-state proton radioactivity is determined by a delicate interplay between the Coulomb and centrifugal terms of the effective potential. While low-Z nuclei lying beyond the proton drip-line exist only as short lived resonances, the relatively high potential energy barrier enables the observation of ground-state proton emission from medium-heavy and heavy nuclei. At the drip-lines proton emission competes with β^+ decay; for heavy nuclei also fission or α decay can be favored. The proton drip-line has been fully mapped up to $Z = 21$, and possibly for odd-Z nuclei up to In [1]. No examples of ground-state proton emission have been discovered below $Z = 50$. Proton radioactivity has been studied from odd-Z nuclei in the two spherical regions from $51 \leq Z \leq 55$ and $69 \leq Z \leq 83$. The systematics of proton decay spectroscopic factors is consistent with half-lives calculated in the spherical WKB or distorted-wave Born approximation (DWBA). Recently reported proton decay rates [2] indicate that the missing region of light rare-earth nuclei contains strongly deformed nuclei at the drip-lines. The lifetimes of deformed proton emitters provide direct information on the last occupied Nilsson configuration, and therefore on the shape of the nucleus. Modern models for proton decay rates from deformed nuclei have only recently been developed [3]. However, even the most realistic calculations are not based on a fully microscopic and self-consistent description of proton unstable nuclei. In particular, such a description should also include important pairing correlations.

The model that we use for the description of ground-state properties of proton emitters is formulated in the framework of relativistic Hartree-Bogoliubov (RHB) theory. Models of quantum hadrodynamics that are based on the relativistic mean-field approximation have been successfully applied in the description of a variety of nuclear structure phenomena in spherical and deformed β-stable nuclei [4] and, more recently, in studies of exotic nuclei far from the valley of β stability. RHB presents a relativistic extension of the Hartree-Fock-Bogoliubov theory. It was derived in Refs. [5,6] in an attempt to develop a unified framework in which relativistic mean-field and pairing correlations could be described simultaneously. Such a unified and self-consistent formulation is especially important in applications to drip-line nuclei, in which the separation energy of the last nucleons can become extremely small, the Fermi level is found close to the particle continuum, and the lowest particle-hole or particle-particle modes are embedded in the continuum. The RHB model with finite range pairing interactions has been used to describe halo phenomena in light nuclei [7], the neutron drip-line in light nuclei [8], the reduction of the spin-orbit potential in drip-line nuclei [9], ground-state properties of Ni and Sn isotopes [10], and the deformations and shape coexistence phenomena that result from the suppression of the spherical $N = 28$ shell gap in neutron-rich nuclei [11]. In particular, in Ref. [12] we have applied the RHB model to describe properties of proton-rich spherical even-even nuclei $14 \leq Z \leq 28$ and $N = 18$, 20, and 22. It has been shown that the model correctly predicts the location of the proton drip-line. The isospin dependence of the effective spin-orbit potential has been studied.

In the relativistic Hartree-Bogoliubov model, the ground state of a nucleus $|\Phi\rangle$ is represented by the product of independent single-quasiparticle states. These states are eigenvectors of the generalized single-nucleon Hamiltonian which contains two average potentials: the self-consistent mean-field $\hat{\Gamma}$, which encloses all the long range particle-hole (ph) correlations, and a pairing field $\hat{\Delta}$, which sums up the particle-particle (pp) correlations. The single-quasiparticle equations result from the variation of the energy functional with respect to the Hermitian density matrix ρ and the antisymmetric pairing tensor κ. In the Hartree approximation for the self-consistent mean field, the relativistic Hartree-Bogoliubov equations read

$$\begin{pmatrix} \hat{h}_D - m - \lambda & \hat{\Delta} \\ -\hat{\Delta}^* & -\hat{h}_D + m + \lambda \end{pmatrix} \begin{pmatrix} U_k(\mathbf{r}) \\ V_k(\mathbf{r}) \end{pmatrix} = E_k \begin{pmatrix} U_k(\mathbf{r}) \\ V_k(\mathbf{r}) \end{pmatrix}. \tag{1}$$

where $\hat{h}_D$ is the single-nucleon Dirac Hamiltonian [4] and m is the nucleon mass

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

The chemical potential λ has to be determined by the particle-number subsidiary condition in order that the expectation value of the particle-number operator in the ground state equals the number of nucleons. The column vectors denote the quasiparticle spinors, and E_k are the quasiparticle energies. The Dirac Hamiltonian contains the mean-field potentials of the isoscalar scalar σ meson, the isoscalar vector ω meson, the isovector vector ρ meson, as well as the electrostatic potential. The RHB equations have to be solved self-consistently with potentials determined in the mean-field approximation from solutions of Klein-Gordon equations. The equation for the σ meson contains the nonlinear σ self-interaction terms. Because of charge conservation, only the third component of the isovector ρ meson contributes. The source terms for the Klein-Gordon equations are calculated in the *no-sea* approximation. In the present version of the model we do not perform angular momentum or particle-number projection.

The pairing field $\hat{\Delta}$ in (1) is an integral operator with the kernel

$$\Delta_{ab}(\mathbf{r},\mathbf{r}') = \frac{1}{2}\sum_{c,d} V_{abcd}(\mathbf{r},\mathbf{r}')\boldsymbol{\kappa}_{cd}(\mathbf{r},\mathbf{r}'), \quad (3)$$

where a, b, c, and d denote quantum numbers that specify the Dirac indices of the spinors, $V_{abcd}(\mathbf{r},\mathbf{r}')$ are matrix elements of a general relativistic two-body pairing interaction, and the pairing tensor is defined as

$$\boldsymbol{\kappa}_{cd}(\mathbf{r},\mathbf{r}') = \sum_{E_k>0} U^*_{ck}(\mathbf{r})V_{dk}(\mathbf{r}'). \quad (4)$$

In most of the applications of the RHB model we have used a phenomenological nonrelativistic interaction in the pairing channel: the pairing part of the Gogny force

$$V^{pp}(1,2) = \sum_{i=1,2} e^{-[(\mathbf{r}_1-\mathbf{r}_2)/\mu_i]^2} \times (W_i + B_iP^\sigma - H_iP^\tau - M_iP^\sigma P^\tau), \quad (5)$$

with the set D1S [13] for the parameters μ_i, W_i, B_i, H_i, and M_i $(i = 1,2)$. This force has been very carefully adjusted to the pairing properties of finite nuclei all over the periodic table. In particular, the basic advantage of the Gogny force is the finite range, which automatically guarantees a proper cutoff in momentum space.

The eigensolutions of Eq. (1) form a set of orthogonal and normalized single-quasiparticle states. The corresponding eigenvalues are the single-quasiparticle energies. The self-consistent iteration procedure is performed in the basis of quasiparticle states. A simple blocking procedure 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 quasiparticle eigenspectrum is then transformed into the canonical basis of single-particle states, in which the RHB ground state takes the Bardeen-Cooper-Schrieffer form. The transformation determines the energies and occupation probabilities of the canonical states.

The input parameters are the coupling constants and masses for the effective mean-field Lagrangian and the effective interaction in the pairing channel. As in most applications of the RHB model, we use the NL3 effective interaction [14] for the relativistic mean field (RMF) Lagrangian. Properties calculated with NL3 indicate that this is probably the best RMF effective interaction so far, for nuclei both at and away from the line of β stability. For the pairing field we employ the pairing part of the Gogny interaction, with the parameter set D1S [13].

In Fig. 1 we display the one-proton separation energies

$$S_p(Z,N) = B(Z,N) - B(Z-1,N) \quad (6)$$

for the odd-Z nuclei $59 \le Z \le 69$, as a function of the number of neutrons. The model predicts the drip-line nuclei: ^{124}Pr, ^{129}Pm, ^{134}Eu, ^{139}Tb, ^{146}Ho, and ^{152}Tm. In heavy proton drip-line nuclei the potential energy barrier, which results from the superposition of the Coulomb and centrifugal potentials, is relatively high. For the proton decay to occur the odd valence proton must penetrate the potential barrier, and this process competes with β^+ decay. Since the logarithm of the half-life for proton decay is inversely proportional to the energy of the odd

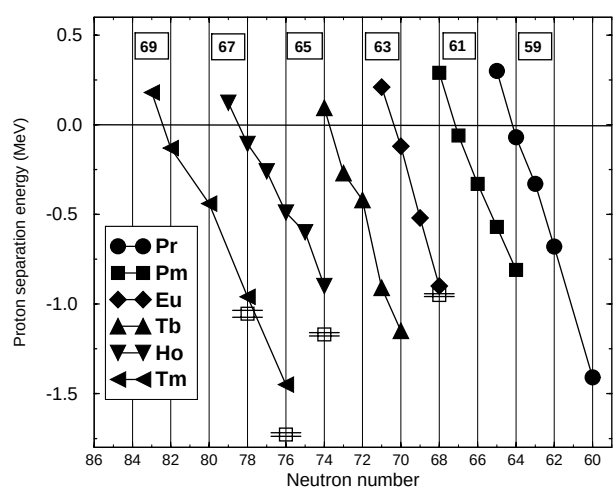

FIG. 1. Calculated one-proton separation energies for odd-Z nuclei $59 \le Z \le 69$ at and beyond the drip-line. Results of self-consistent RHB calculations are compared with experimental transition energies for ground-state proton emission in ^{131}Eu, ^{141}Ho [2], ^{145}Tm [15], and ^{147}Tm [16]. Empty squares denote the negative values of the transition energies E_p, and reported experimental errors are indicated by the space between horizontal lines.

proton, in many nuclei the decay will not be observed immediately after the drip-line. Proton radioactivity is expected to dominate over β^+ decay only when the energy of the odd proton becomes relatively high. This is also a crucial point for the relativistic description of proton emitters, since the precise values of the separation energies depend on the isovector properties of the spin-orbit interaction.

The calculated separation energies should be compared with recently reported experimental data on proton radioactivity from ^{131}Eu, ^{141}Ho [2], ^{145}Tm [15], and ^{147}Tm [16]. The ^{131}Eu transition has an energy $E_p = 0.950(8)$ MeV and a half-life 26(6) ms, consistent with decay from either a $3/2^+[411]$ or $5/2^+[413]$ Nilsson orbital. For ^{141}Ho the transition energy is $E_p = 1.169(8)$ MeV, and the half-life 4.2(4) ms is assigned to the decay of the $7/2^-[523]$ orbital. The calculated proton separation energy, both for ^{131}Eu and ^{141}Ho, is of -0.9 MeV. In the RHB calculation for ^{131}Eu the odd proton occupies the $5/2^+[413]$ orbital, while the ground state of ^{141}Ho corresponds to the $7/2^-[523]$ proton orbital. This orbital is also occupied by the odd proton in the calculated ground states of ^{145}Tm and ^{147}Tm. For the proton separation energies, we obtain -1.46 MeV in ^{145}Tm and -0.96 MeV in ^{147}Tm. These are compared with the experimental values for transition energies: $E_p = 1.728(10)$ MeV in ^{145}Tm, and $E_p = 1.054(19)$ MeV in ^{147}Tm. When compared with spherical WKB or DWBA calculations [17], the experimental half-lives for the two Tm isotopes are consistent with spectroscopic factors for decays from the $h_{11/2}$ proton orbital. Although our predicted ground-state configuration $7/2^-[523]$ indeed originates from the spherical $h_{11/2}$ orbital, we find that the two nuclei are deformed. ^{145}Tm has a prolate quadrupole deformation $\beta_2 = 0.23$, and ^{147}Tm is oblate in the ground state with $\beta_2 = -0.19$. Calculations also predict possible proton emitters ^{136}Tb and ^{135}Tb with separation energies -0.90 MeV and -1.15 MeV, respectively. In both isotopes the predicted ground-state proton configuration is $3/2^+[411]$.

The calculated mass quadrupole deformation parameters for the odd-Z nuclei $59 \leq Z \leq 69$ at and beyond the drip line are shown in Fig. 2. The Pr, Pm, Eu, and Tb isotopes are strongly prolate deformed ($\beta_2 \approx 0.30$–0.35). By increasing the number of neutrons, Ho and Tm display a transition from prolate to oblate shapes. The absolute values of β_2 decrease as we approach the spherical solutions at $N = 82$. The quadrupole deformations calculated in the RHB model with the NL3 effective interaction are found in excellent agreement with the predictions of the macroscopic-microscopic mass model [18].

The structure of proton levels, including the corresponding spectroscopic factors, can be analyzed in the canonical basis which results from the fully microscopic and self-consistent RHB calculations. In a very recent work [19], we performed such an analysis for the proton-rich odd-Z nuclei in the region $53 \leq Z \leq 69$. In particular for the Eu isotopes, in Fig. 4 of Ref. [19], the proton single-particle energies in the canonical basis have been plotted as functions of the neutron number. For the proton emitter ^{131}Eu the calculations predict that the ground state corresponds to the odd valence proton in the $5/2^+[413]$ orbital. However, since the orbital $5/2^-[532]$ is found at almost the same energy, it is not possible to conclude unambiguously which state is occupied by the valence proton. The calculation of proton decay rates from these orbitals would perhaps provide more conclusive information on the last occupied Nilsson configuration.

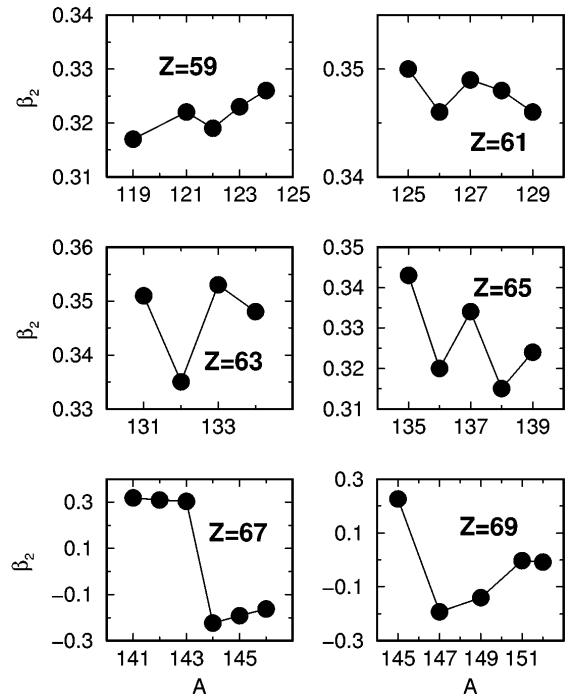

FIG. 2. Self-consistent ground-state quadrupole deformations for the odd-Z nuclei $59 \leq Z \leq 69$, at and beyond the proton drip-line.

In conclusion, this study presents a detailed analysis of deformed proton emitters $59 \leq Z \leq 69$ in the framework of the relativistic Hartree-Bogoliubov theory. We have investigated the location of the proton drip-line, the separation energies for proton emitters beyond the drip-line, and ground-state quadrupole deformations. 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. The RHB results for proton separation energies are found to be in very good agreement with recent experimental data on direct proton decay of ^{131}Eu, ^{141}Ho, and ^{147}Tm. The theoretical value is not as good for ^{145}Tm; the calculated and experimental proton energies differ by more than 200 keV. Predictions for the deformed single-particle orbitals occupied by the valence odd protons are consistent with experimental half-lives for proton transitions. The model

also predicts possible proton emitters ^{136}Tb and ^{135}Tb. It should be emphasized that the theoretical framework is based on the mean-field plus pairing approximation. Correlations beyond the mean-field level, in particular the effects of fluctuations, may modify some RHB results. In specific nuclei, for example, correlations might alter the effective mass and the resulting prediction for the last occupied Nilsson configuration. Nevertheless, the present analysis has shown that the RHB with finite range pairing provides a fully self-consistent microscopic model which can be used to map the entire proton drip-line for medium-heavy and heavy nuclei $51 \leq Z \leq 83$.

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