Shell Effects in Nuclei near the Neutron-Drip Line

M. M. Sharma,[1] G. A. Lalazissis,[2] W. Hillebrandt,[1] and P. Ring[2]
[1]*Max Planck Institut für Astrophysik, Karl-Schwarzschildstrasse 1, D-85740 Garching, Germany*
[2]*Physik Department, Technische Universität München, D-85747 Garching, Germany*
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Shell effects in nuclei close to the neutron-drip lines have been investigated. It has been demonstrated in the relativistic mean-field theory that nuclei very far from stability manifest the shell effects strongly. This behavior is in accord with the predictions of nuclear masses in the finite-range droplet model including shell corrections. The shell effects predicted in the existing Skyrme mean-field theory in comparison are significantly weaker than those of the other approaches.

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Very neutron-rich nuclei and, in particular, those near the neutron-drip lines and near closed shells, play an important role in nuclear astrophysics. Their properties such as binding energies, neutron separation energies, deformation parameters, etc., strongly affect the way neutron-rich stable isotopes are formed in nature by the so-called r process. Conversely, a precise knowledge of such properties will help to determine the astrophysical conditions of their formation [1]. A second example is the equation of state of neutron stars, where in the crust neutron-rich nuclei persist in coexistence with a gas of free neutrons and in the core the isospin dependence of the nucleon-nucleon interaction determines the stiffness of the equation of state and, consequently, their maximum mass, moment of inertia, etc. [2, 3].

The shell effects in nuclei manifest themselves in the form of magic numbers. These depend principally on the spin-orbit coupling and seem to have been understood along the valley of β stability. Theoretically, the description of nuclei is provided by the density-dependent Skyrme mean field [4], which has been employed for two decades, and by the relativistic mean-field (RMF) theory [5, 6], a framework which has been successful for finite nuclei. Whereas in the former ground state properties of nuclei close to the magic numbers can be described successfully, the properties of nuclei away from stability still remain a problem. In the RMF theory, on the other hand, the binding energies, charge radii, and neutron-skin thickness of nuclei with closed shells as well as of those far away from stability can be reproduced well [7]. Approaches based upon semiempirical mass formulas [8] with a large number of parameters also strive to provide descriptions of nuclei close to and far off the stability line. Although many of these mass formulas give similar fits along the line of stability, their predictions vary considerably for short-lived nuclei and especially near the drip line.

In this Letter, we examine in the RMF theory the behavior of the shell effects in nuclei near neutron drip. We show that for the first time a microscopic model describes the properties of nuclei very far off stability, such that the results are in striking conformity with predictions of the empirical finite-range droplet model [9]. We also show that they differ considerably from those provided by the Skyrme mean-field approach.

We have considered the chain of heavy Zr isotopes to demonstrate the shell effects. Nuclei from $A = 110$ to $A = 136$ with even neutron number have been included. This range is well outside the valley of β stability and encompasses also the neutron-drip line. The shell closure occurs at $A = 122$ ($N = 82$). This nucleus lies close to the neutron-drip line. In the nuclei heavier than this, shell effects due to the next higher shell might come into play.

Calculations have been performed with the relativistic Hartee approach taking deformed configuration into account. The force NL-SH (Ref. [7]), which has been shown to describe the properties of nuclei at and away from the stability line very well, has been used. The correct asymmetry energy of NL-SH allows its judicious application to nuclei with large neutron excesses. For open-shell nuclei, pairing has been added in the BCS formalism with constant pairing gaps.

Figure 1 shows the ground-state binding energies of Zr isotopes obtained with NL-SH. With each successive addition of a pair of neutrons, the nuclear binding energy increases monotonously from $A = 110$ to $A = 122$ where the shell closure occurs. Further addition of neutrons to the magic core puts the extra neutrons in the higher shell. Evidently, these neutrons provide barely any extra binding to the nucleus and the binding energy in this region stagnates. This depicts an onset of the neutron drip where the outer neutrons become loosely bound. The kink in the binding energy curve at $A = 122$ signifies the strong shell effects that are encountered when further neutrons are added to this nucleus. Calculations assuming spherical configurations for all Zr isotopes do yield a curve very close and similar in shape to the deformed case and the shell effects are thus retained also in the spherical case.

In Fig. 1 we also give a comparison with the finite-range droplet model (FRDM) [9]. The agreement of

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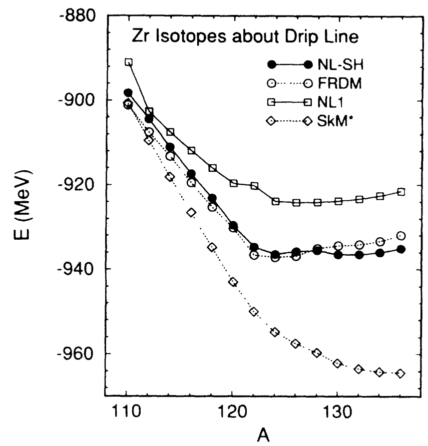

FIG. 1. The binding energy of Zr isotopes obtained from the deformed relativistic Hartree calculations with the force [7] NL-SH with constant pairing gaps obtained from $\Delta_{n(p)} = 12/\sqrt{N(Z)}$. Results for NL1 [6] are also shown. The smooth curve shows the binding energy from Skyrme interaction SkM* [10] using spherical configuration. A comparison has also been made with the predictions of the finite-range droplet model (FRDM) [9].

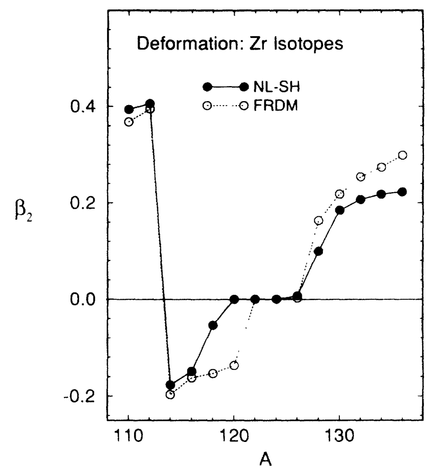

FIG. 2. The quadrupole deformation β_2 obtained from NL-SH. The values from predictions of FRDM are also shown. The overall agreement of NL-SH with FRDM, including the shape transition from prolate to oblate at $A = 112$, is noteworthy.

our results with those of the FRDM is striking. From $A = 110$ to $A = 128$ the deviations are at most 1–2 MeV. The shell effects in both the RMF theory and the FRDM are amazingly similar. Even beyond $A = 130$ there are only minor differences between the two and the binding energies differ by about 2–3 MeV. The agreement between the RMF theory and the FRDM on the general trend in the stagnation in the binding energies of nuclei close to the drip lines is excellent.

For comparison we include in Fig. 1 the binding energies calculated within the spherical Skyrme Hartree-Fock and BCS approximation using the interaction SkM* [10]. The SkM* energies deviate strongly from FRDM and NL-SH as the neutron number increases. The lack of shell effects at $N = 82$ in the Skyrme approach is evident from the smooth variation in energy about $A = 122$. This seems to be a typical feature of Skyrme forces, which has also been observed in Ref. [11] in several chains of isotopes crossing shell closure.

Finally, we also give in Fig. 1 the results for the force NL1 [6]. The binding energies for NL1 differ from NL-SH and FRDM by up to 15 MeV. This is due to very large asymmetry energy of 44 MeV of the force NL1, which also leads to neutron skin thickness [12] larger than the empirical values. The kink at $A = 122$ also present in NL1, however, points again to shell effects similar to NL-SH. Such kinks thus seem to be a characteristic of the RMF theory in contrast to the Skyrme ansatz.

Deformation properties of nuclei have been obtained from the RMF theory. The quadrupole deformation β_2 from NL-SH is shown in Fig. 2. The values obtained from the FRDM are also shown for comparison. Both the RMF theory and the FRDM agree remarkably well on the shape transition from prolate to oblate at $A = 114$. The β_2 values from the RMF theory are in general close to those from the FRDM. The fact that nuclei above $A = 126$ again assume prolate shape in the FRDM is well reproduced by NL-SH. Only above $A = 116$ is the shape transition from oblate to spherical in approaching the closed shell more gradual in the RMF theory than in the FRDM. The agreement in the deformation properties of nuclei near the drip line predicted by both the RMF theory and the FRDM is astonishing.

In order to understand why the binding energies beyond the closed neutron shell stagnate, we show in Fig. 3 single-particle energies of levels below and above the Fermi energy for spherical configuration of nuclei for both (a) NL-SH and (b) SkM*. The noteworthy aspect in this figure is the change in the Fermi surface as a function of neutron number, as shown by the dotted curves. Both the approaches show a sudden change in the Fermi surface as the next shell is being filled. The change in the Fermi surface after $A = 124$ for NL-SH is very gradual and as the neutron number increases, it is connected very gradually to the continuum. In this process the nuclei still take up more neutrons without contributing to the total binding energy. This also is the reason that the drip line is approached considerably earlier than with SkM* and that already above $A = 124$ neutrons get unbound. This picture contrasts with the one of SkM*, where the Fermi energy reaches the continuum limit only for very heavy isotopes, leading to an increase in the binding energy with the addition of further neutrons to the next shell. The drip line is encountered suddenly at about $A = 134$ and therefore the coupling to the continuum arises rather suddenly. The drip nucleus being close to

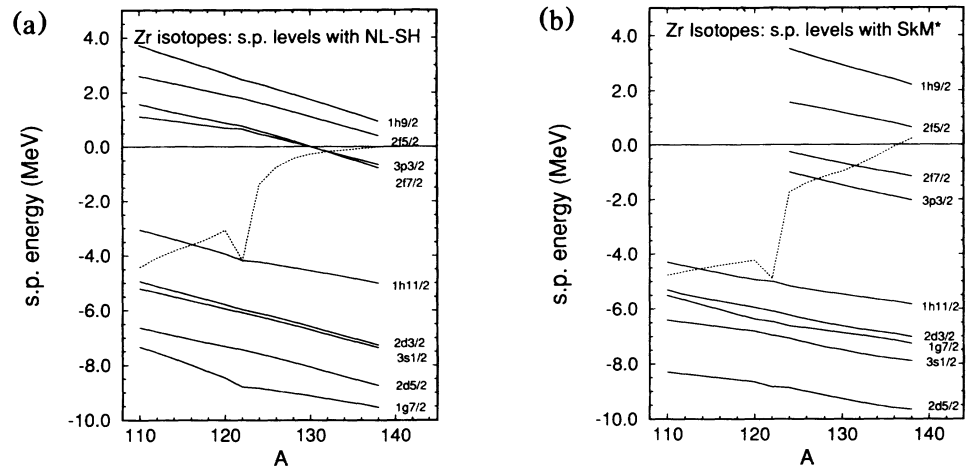

FIG. 3. The single-particle levels for (a) the RMF theory and (b) the Skyrme ansatz. The Fermi energy in both cases is shown by the dotted curve.

$A = 134$ is consistent with the predictions of Ref. [11], where with the Skyrme force SkP shell effects were found to be very weak for extremely neutron-rich nuclei.

Shell effects in the RMF theory and the Skyrme approaches have recently been a matter of discussion for stable nuclei also. Experimentally, isotope shifts in nuclei near shell closure have always been found to show a kink [13]. Such kinks can be construed as being a manifestation of shell effects. Microscopic calculations have until recently not been successful in describing such kinks. The Skyrme mean-field approach [14] including various other correlations has failed to reproduce such empirical effects. Only very recently has the RMF theory succeeded [15] in describing these kinks in charge radii differences. The kinks in the binding energies in Fig. 1 in the RMF theory and the FRDM reflect shell effects which may be of similar nature as in the charge radii. However, here the issue concerns the shell effects at the drip line which is truly far away from the stability.

Shell effects at drip lines have also been looked into in Ref. [16] using the Skyrme HFB and the RMF theory. Contrary to clear differences found in our work between the Skyrme and the RMF approaches, Ref. [16] points to a quenching of shell effects in both theories, a conclusion which is clearly in contradiction with ours. Variations in pairing and single-particle properties with mass number along an isobaric chain about $A = 100$ have been shown [16] to be similar both for the Skyrme and the RMF theory, a situation very different from our Fig. 3, although the weakening of shell effects near the drip line with the Skyrme interaction SkP (Ref. [16]) is consistent with that of Ref. [11]. Using the same interaction, this result obviously is inconsistent with the shell effects exhibited by our results in the RMF theory. The spin-orbit splitting of some levels in both approaches is considerably different (Fig. 3). We suspect that the differences between our conclusions and those of Ref. [16] in part stem from the selection of isobaric chains in Ref. [16], which does not include any shell closure, and therefore, the shell effects do not manifest themselves clearly. Indeed, in the middle of a shell both approaches provide similar results as shown in Ref. [16].

We have compared some of the quantities that may lead to the differences in the shell effects in the two approaches. The sum of single-particle energies in the two approaches, both for the protons and neutrons, do not show any compelling difference as do the interaction energies as a function of mass (the details will be provided elsewhere). The differences between the two, however, become evident when we examine the single-particle structure and the corresponding spin-orbit splittings. The orbits $1g_{7/2}$ and $1h_{11/2}$ seem to play a dominant role in defining the shell effects in the two approaches, whence the differences appear. First, the spin-orbit splittings $1h_{9/2}$-$1h_{11/2}$ and $1g_{7/2}$-$1g_{9/2}$ are systematically larger in the Skyrme approach than in the RMF theory by 30% and 20%, respectively, as can be seen partly from Fig. 3. The splitting $2d_{3/2}$-$2d_{5/2}$ for SkM* is about 2 times larger than the one for NL-SH. The large spin-orbit splitting in the Skyrme theory reduces the gap between the $1h_{11/2}$ and the next unoccupied level and therefore tends to smoothen the shell effects in nuclei. Second, the slightly different sequence of single-particle levels arising from differences in the spin-orbit splitting leads to different filling of the orbitals. As the mass number increases from $A = 110$ to $A = 122$, the preferred subshell to be filled in the RMF theory is $1g_{7/2}$, which lies deeper than in SkM*, whereas in the Skyrme theory $1h_{11/2}$ is being filled at the expense of $1g_{7/2}$. The different occupations of levels give rise to different Fermi energies which in turn modify the shell effects.

The differences in the spin-orbit properties of the two approaches can be traced back partly to the density dependence of the spin-orbit term. In the Skyrme ansatz, it takes the form

$$\frac{3}{4}W_0\left(\frac{1}{r}\frac{d}{dr}\rho\right)\boldsymbol{\sigma}\cdot\mathbf{L}, \tag{1}$$

where W_0 is the spin-orbit strength. A nonrelativistic reduction of the relativistic Hamiltonian, on the other hand, gives rise to an approximate spin-orbit term

$$\frac{1}{m^{*2}}\left(\frac{1}{r}\frac{d}{dr}\rho\right)\boldsymbol{\sigma}\cdot\mathbf{L}. \tag{2}$$

It can be seen clearly that the coefficient of the spin-orbit term in the RMF theory possesses a density dependence which goes as $1/m^{*2}$ in contrast to W_0 in the Skyrme theory, which is indepedent of ρ. This density dependence in the RMF theory arises as a natural consequence of the Lorentz structure of the interaction, where the saturation mechanism is different from that of the Skyrme forces. A detailed study on these aspects is in progress.

The consequence of the above Fermi surface in the RMF theory is evidently a large tail in the density of the neutrons; i.e., further addition of neutrons to the $A = 122$ core leads to an extension of neutrons in the space. Thus, in the vicinity of the drip line, nuclei with a "giant halo" are being created. To illustrate the existence of neutron halos, here we give rms neutron radii and diffuseness of two isotopes ^{122}Zr and ^{130}Zr. The rms radii for these nuclei are 5.01 and 5.44 fm with the diffuseness being 2.45 and 2.90 fm, respectively. The larger values of both the rms radius and diffuseness for ^{130}Zr as compared to ^{122}Zr provide an indication of neutron halo in ^{130}Zr. This behavior is exhibited by all Zr nuclei near the drip line. A detailed discussion on neutron halo in nuclei near the neutron-drip line will be given elsewhere [17].

In conclusion, we have shown that in the RMF theory the shell effects at the neutron-drip line are significantly stronger than those in the Skyrme mean-field theory. For the RMF theory, this view is supported by the phenomenological finite-range droplet model, the overall predictions of which are reproduced very well by the RMF theory. Striking differences have been found in the spin-orbit properties of the RMF theory as compared to the Skyrme ansatz. As a consequence we predict large neutron halos in nuclei near the drip line. From our analysis we expect, furthermore, strong shell effects also for other elements and magic neutron numbers in the r process path, in contrast to what was found in Ref. [16]. This would be in accord with the fact that strong r process abundance peaks are observed at $A \simeq 80$, 130, and 195, which require shell effects for $N = 50$, 82, and 126, respectively, and neutron separation energies around 2 or 3 MeV [1].

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