

Relativistic Hartree+Bogoliubov description of the deformed $N=28$ region

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Ground-state properties of neutron-rich $N \approx 28$ nuclei are described in the framework of relativistic Hartree plus Bogoliubov (RH+B) theory. The model uses the NL3 effective interaction in the mean-field Lagrangian, and describes pairing correlations by the pairing part of the finite range Gogny interaction D1S. Two-neutron separation energies and ground-state quadrupole deformations that result from fully self-consistent RH+B solutions are compared with available experimental data. The model predicts a strong suppression of the spherical $N=28$ shell gap for neutron-rich nuclei: the $1f7/2 \rightarrow fp$ core breaking results in deformed ground states. Shape coexistence is expected for neutron-rich Si, S, and Ar isotopes. [S0556-2813(99)04407-6]

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I. RELATIVISTIC HARTREE+BOGOLIUBOV THEORY WITH FINITE RANGE PAIRING INTERACTION

Ground states of deformed exotic nuclei, unstable isotopes with extreme isospin values, display many interesting and unique properties. The description of observed phenomena, as well as the prediction of new and unexpected properties, present an exciting challenge for modern theoretical advances. For neutron-rich nuclei, a fascinating example of the modification of the effective single-nucleon potential is the observed suppression of shell effects, the disappearance of spherical magic numbers, and the resulting onset of deformation and shape coexistence. Fine examples are ^{32}Mg (extreme quadrupole deformation) and ^{44}S (shape coexistence). Iso-vector quadrupole deformations are expected at the neutron drip-lines, and possible low-energy collective isovector modes have been predicted. A very interesting phenomenon is a possible formation of deformed halo structures in weakly bound nuclei. In much heavier neutron-rich systems, the modification of shell structure could produce an enhancement of stability for superheavy elements $Z \geq 110$. Proton-rich nuclei present 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. Proton decay rates indicate that the region $57 \leq Z \leq 65$ contains strongly deformed nuclei at the drip-lines. The lifetimes of deformed proton emitters provide direct information on the shape of the nucleus.

While an impressive amount of experimental data on deformed exotic nuclei has been published recently, relatively few pertinent theoretical studies have been reported. For relatively light exotic nuclei, as for example ^{32}Mg , shell model predictions for the onset of deformation and shape coexistence have been remarkably successful. However for medium-heavy and heavy systems, the only viable approach at present are large scale self-consistent mean-field calculations (Hartree-Fock, Hartree-Fock-Bogoliubov, relativistic mean-field). The problem is of course that, in addition to the self-consistent mean-field potential, pairing correlations have

to be included in order to describe ground-state properties of open-shell nuclei. And while for strongly bound systems pairing can be included in the simple BCS scheme in the valence shell, exotic nuclei with extreme isospin values require a careful treatment of the asymptotic part of the nucleonic densities, and therefore a unified description of mean-field and pairing correlations. The nonrelativistic Hartree-Fock-Bogoliubov (HFB) and relativistic Hartree plus Bogoliubov (RH+B) models have been very successfully applied in the description of a variety of nuclear structure phenomena in spherical exotic nuclei on both sides of the valley of β -stability. For deformed exotic nuclei however, so far pairing has been only described in the BCS approximation. The BCS scheme presents only a poor approximation for nuclei with small separation energies, i.e., with the Fermi level close to the particle continuum. The inclusion of deformation in HFB or RH+B models with finite range pairing still presents considerable difficulties, and it has not been possible yet to obtain reliable results in coordinate space calculations. In the present work we report on the first application of the relativistic Hartree + Bogoliubov theory with finite range pairing interaction to the structure of deformed nuclei in the $N=28$ region of neutron-rich nuclei.

In the framework of 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 . The relativistic model was formulated in Ref. [1]. In the Hartree approximation for the self-consistent mean field, the relativistic Hartree-Bogoliubov (RHB) equations read

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

where m is the nucleon mass and \hat{h}_D is the single-nucleon Dirac Hamiltonian [2]

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

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 quasi-particle 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 sigma 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.

As in most relativistic mean-field calculations, we neglect Fock terms, i.e., we solve the relativistic Hartree-Bogoliubov, instead of Hartree-Fock-Bogoliubov equations (which have also been derived in Ref. [1]). Of course, the Fock term does not have to be small. In fact, relativistic Hartree-Fock calculations in spherical nuclei [3,4], have shown that the inclusion of Fock terms necessitates a complete readjustment of the effective interaction (meson-nucleon coupling constants). However, in an effective theory with parameters adjusted to experimental data, even on the Hartree level the Fock term is partially taken into account. This is a consequence of the short range of the meson exchange interactions. For zero-range forces the Fock term has the same form as the direct term, it differs only in a statistical factor. Therefore, a phenomenological Hartree model with renormalized parameters, includes a large part of the Fock term. In addition, there are general arguments based on boson- or $1/N$ -expansion techniques [5], which show that the Fock term could be of the same order as RPA corrections. It would not be justified, therefore, to take into account only the Fock term, and to neglect RPA corrections. It is clear, however, that the argument of short range does not apply to the pion, and that its contribution to the Fock term could lead to specific effects, which are not included in relativistic Hartree models (nor in nonrelativistic calculations with Skyrme forces). If such effects were observed, they would call for relativistic Hartree-Fock-Bogoliubov calculations. This would require a new adjustment of the parameters. At present there is definitely not enough experimental evidence that would support the explicit inclusion of the Fock term. On the other hand, the pion field is included in a phenomenological way already on the Hartree level, through the two-pion exchange processes represented by the scalar sigma

field. However, it is possible that radically improved, or even completely new theoretical models, will be required for a correct description of new physical phenomena in nuclei far from the valley of β -stability. This might be true not only for relativistic mean-field models, but also for the nonrelativistic models based on the Skyrme interaction.

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

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

where a,b,c,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

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

In the applications of this theory to spherical nuclei [6–12] we have used a phenomenological nonrelativistic interaction in the pairing channel, the pairing part of the Gogny force

$$\begin{aligned} V^{pp}(1,2) = & \sum_{i=1,2} e^{-((\mathbf{r}_1-\mathbf{r}_2)/\mu_i)^2} \\ & \times (W_i + B_i P^\sigma - H_i P^\tau - M_i P^\sigma P^\tau), \end{aligned} \quad (5)$$

with the set DIS [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 fact that it is a nonrelativistic interaction has negligible influence on the results of RHB calculations. Of course, in order to have a consistent formulation of the model, the matrix elements in the pairing channel V_{abcd} should be derived as a one-meson exchange interaction by eliminating the mesonic degrees of freedom in the model Lagrangian [1]. However, although recently results have been reported in applications to nuclear matter, a microscopic and fully relativistic pairing force, derived starting from the Lagrangian of quantum hadrodynamics, still cannot be applied to nuclei. Therefore also in the present calculations we use the effective Gogny interaction in the pairing channel. In order to distinguish the present calculations, where the pairing channel is treated in a non-relativistic way, we use here the notation Relativistic Hartree plus Bogoliubov (RH+B) and reserve the name RHB for future calculations, which will include fully relativistic forces in the pairing channel. We have to emphasize, however, that the name RHB has already been used in earlier publications [6–12], where the identically the same method was used as here.

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. The resulting quasiparticle eigenspec-

trum is then 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 self-consistent solution of the Dirac-Hartree+Bogoliubov integro-differential eigenvalue equations and Klein-Gordon equations for the meson fields determines the nuclear ground state. For systems with spherical symmetry, i.e., single closed-shell nuclei, the coupled system of equations has been solved using finite element methods in coordinate space [7–10], and by expansion in a basis of spherical harmonic oscillator [6,11,12]. For deformed nuclei the present version of the model does not include solutions in coordinate space. The Dirac-Hartree+Bogoliubov equations and the equations for the meson fields are solved by expanding the nucleon spinors $U_k(\mathbf{r})$ and $V_k(\mathbf{r})$, and the meson fields in terms of the eigenfunctions of a deformed axially symmetric oscillator potential [14]. In the present calculations the number of oscillator shells in the expansion is 12 for fermion wave functions, and 20 for the meson fields. Of course for nuclei at the drip lines, solutions in configurational representation might not provide an accurate description of properties that crucially depend on the spatial extension of nucleon densities, as for example nuclear radii. In the present study we are particularly interested in the deformed $N=28$ region: shell effects and shape coexistence phenomena. For a description of general trends coordinate space solutions are not essential, solutions in the oscillator basis should present a pertinent approximation.

II. DEFORMED $N=28$ REGION: SHELL EFFECTS AND SHAPE COEXISTENCE

The region of neutron-rich $N\approx 28$ nuclei presents many interesting phenomena: the average nucleonic potential is modified, shell effects are suppressed, large quadrupole deformations are observed as well as shape coexistence, isovector quadrupole deformations are predicted at drip-lines. The detailed knowledge of the microscopic structure of these nuclei is also essential for a correct description of the nucleosynthesis of the heavy Ca, Ti, and Cr isotopes. In the present application of the RH+B theory we study the structure of exotic neutron rich-nuclei with $12\leq Z\leq 20$, and in particular the light $N=28$ nuclei. We are interested in the influence of the spherical shell $N=28$ on the structure of nuclei below ^{48}Ca , in deformation effects that result from the $1f7/2\rightarrow fp$ core breaking, and in shape coexistence phenomena predicted for these γ -soft nuclei.

The structure of exotic neutron-rich nuclei with $N\approx 28$ has been extensively studied by Werner *et al.* [15,16] in the framework of the self-consistent mean-field theory: Skyrme Hartree-Fock model and relativistic mean-field approach. Skyrme-HF calculations were performed by discretizing the energy functional on a three-dimensional Cartesian spline collocation lattice. The Skyrme interaction SIII [17] was used. For the RMF model the Dirac equation for the baryons and the Klein-Gordon equations for the meson fields were solved using the basis expansion methods. The NL-SH parameter set [18] was used for the mean-field Lagrangian. In

both models the pairing correlations were included using the BCS formalism in the constant gap approximation with a strongly reduced pairing interaction. HF and RMF results were compared with the predictions of the finite-range drop-let (FRDM) and the extended Thomas-Fermi with Strutinsky integral (ETFISI) mass models, as well as with available experimental data. In particular, the onset of deformations around $N=28$, the stability of the heaviest Si, S, Ar and Ca isotopes, and the isovector deformations were investigated. Calculations confirmed strong deformation effects caused by the $1f7/2\rightarrow fp$ core breaking, especially in the RMF model. Almost all deformed nuclei were found to be γ -soft, with the deformation dependence of the single-particle spectrum favoring prolate shapes for $Z=16$ and oblate for $Z=18$. The results obtained with the two models, HF and RMF, were found to be similar, although also important differences were calculated. For example, the equilibrium shape of the $N=28$ nucleus ^{44}S . RMF calculations predict a well deformed prolate ground state with $\beta_2=0.31$ for this nucleus, while according to the HF model, ^{44}S is γ -soft with a small quadrupole deformation $\beta_2\approx 0.13$. The FRDM and ETFISI models predict spherical and oblate ($\beta_2=-0.26$) ground states, respectively. Another detailed analysis of the ground-state properties of nuclei in the light mass region $10\leq Z\leq 22$ in the framework of the RMF approach is reported in Ref. [19]. The calculations were also performed in an axially deformed configuration using the NL-SH effective interaction. Pairing was included in the BCS approximation, but a somewhat different prescription was used to calculate the neutron and proton pairing gaps in regions where nuclear masses were not known [20]. Nuclei at the stability line were considered, as well as those close to the proton and neutron drip lines. Results of calculations were compared with available empirical data and predictions of mass models. A very interesting result is the predicted ground-state deformation for ^{44}S : oblate ($\beta_2=-0.2$), with a highly prolate shape ($\beta_2=0.38$) about 30 keV above the ground state. This result is at variance with the calculations of Refs. [15,16], although in both cases the same effective interaction was used for the mean-field Lagrangian. The pairing gaps used in the two calculations however were different. Therefore it appears that, for nuclei which are very γ -soft, the pairing interaction determines the shape transition to the deformed intruder configurations.

Results of Skyrme-HF and RMF calculations clearly indicate that mean-field and pairing correlations should be described in a unified self-consistent framework: the nonrelativistic Hartree-Fock-Bogoliubov theory [21] or the relativistic Hartree + Bogoliubov model that was described in the previous section. Only fully self-consistent HFB or RH+B models correctly describe the virtual scattering of nucleonic pairs from bound states to the positive energy particle continuum [22]. The correct representation of pairing correlations is an essential ingredient for microscopic models of the structure of neutron-rich nuclei.

The input parameters for our model are the coupling constants and masses for the effective mean-field Lagrangian, and the effective interaction in the pairing channel. In the present calculation we use the NL3 effective interaction [23]

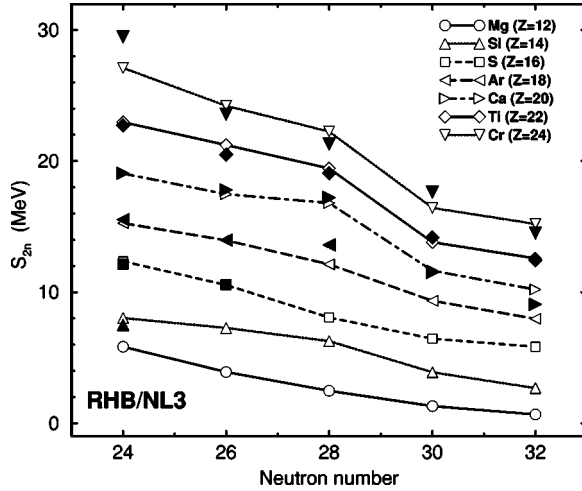


FIG. 1. Two-neutron separation energies in the $N \approx 28$ region calculated in the RH+B model and compared with experimental data (filled symbols) from the compilation of Audi and Wapstra.

for the RMF Lagrangian. We have used the NL3 force in most of the applications of RH+B theory to spherical nuclei: in the analysis of light neutron-rich nuclei in Refs. [7–9], in the study of ground-state properties of Ni and Sn isotopes [11], and in the description of proton-rich nuclei with $14 \leq Z \leq 28$ and $N = 18, 20, 22$. Properties calculated with NL3 indicate that this is probably the best RMF effective interaction so far, both for nuclei at and away from the line of β -stability. NL3 has also been used in calculations of binding energies and deformation parameters of rare-earth nuclei [24]. For the pairing field we employ the pairing part of the Gogny interaction, with the parameter set D1S [13].

In Fig. 1 the two-neutron separation energies are plotted

$$S_{2n}(Z, N) = B_n(Z, N) - B_n(Z, N-2) \quad (6)$$

for the even-even nuclei $12 \leq Z \leq 24$ and $24 \leq N \leq 32$. The values that correspond to the self-consistent RH+B ground-states (symbols connected by lines) are compared with experimental data and extrapolated values from Ref. [25] (filled symbols). Except for Mg and Si, the nuclei that we consider are not at the drip-lines. The theoretical values reproduce in detail the experimental separation energies, except for ^{48}Cr . In general we have found that RH+B model binding energies are in very good agreement with experimental data when one of the shells (proton or neutron) is closed, or when valence protons and neutrons occupy different major shells (i.e., below and above N and/or $Z = 20$). The differences are more pronounced when both protons and neutrons occupy the same major shell, and especially for the $N = Z$ nuclei. For these nuclei additional correlations should be taken into account, and in particular proton-neutron pairing could have a strong influence on the masses. Proton-neutron short-range correlations are not included in our model.

In Fig. 2 the calculated neutron radii are displayed. The model of course predicts an increase of the calculated radii with the number of neutrons. It is interesting however that Cr, Ti, Ca, Ar, and to a certain extent S isotopes, display very similar neutron radii in this region. Only for the two

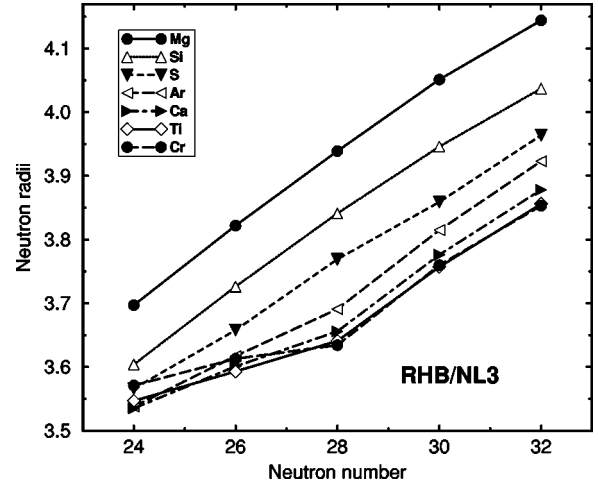


FIG. 2. Calculated neutron rms radii for the ground states of nuclei in the $N \approx 28$ region: $12 \leq Z \leq 24$ and $24 \leq N \leq 32$.

more exotic chains of Si and Mg isotopes, i.e., more neutron-rich, a substantial increase of the calculated radii is observed. Very important for our present investigation is the effect that the $N = 28$ spherical shell closure produces on the neutron radii of Cr, Ti and Ca isotopes. On the other hand, no effect of shell closure is observed for S, Si, and Mg. This is already an indication that the $N = 28$ shell effects are suppressed in neutron-rich nuclei.

The predicted mass quadrupole deformations for the ground states of $N = 28$ nuclei are shown in the upper panel of Fig. 3. We notice a staggering between prolate and oblate configurations, and this indicates that the potential is γ -soft. The absolute values of the deformation decrease as we approach the $Z = 20$ closed shell. Starting with Ca, the $N = 28$

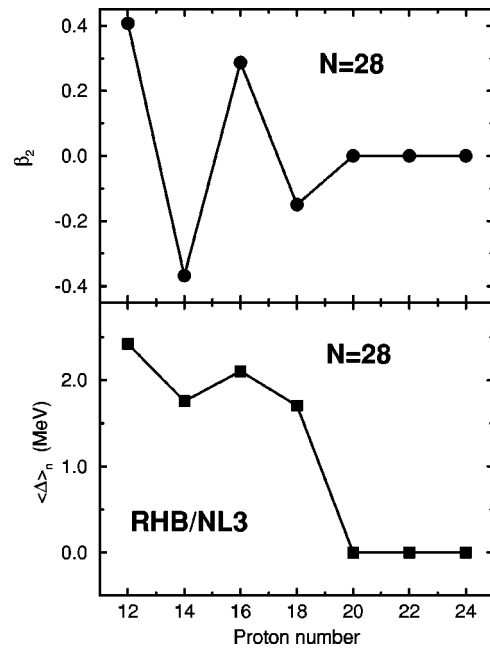


FIG. 3. Self-consistent RH+B quadrupole deformations for ground states of the $N = 28$ isotones (upper panel). Average neutron pairing gaps $\langle \Delta_N \rangle$ as function of proton number (lower panel).

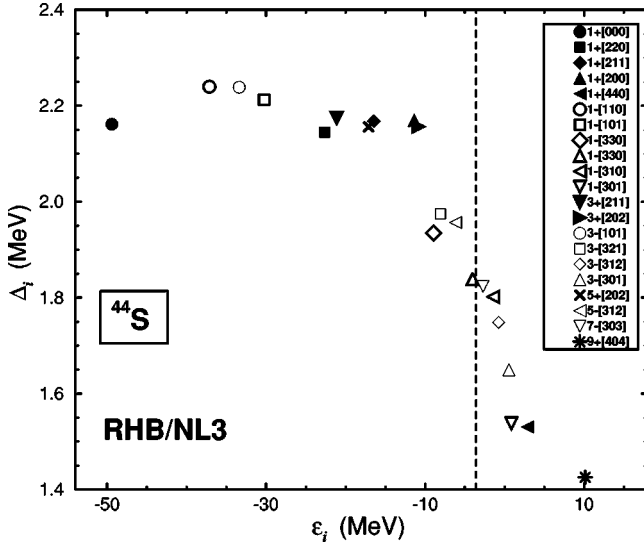


FIG. 4. Average values of the neutron canonical pairing gaps as function of canonical single-particle energies for states that correspond to the self-consistent ground state of ^{44}S . The NL3 parametrization has been used for the mean-field Lagrangian, and the parameter set D1S for the pairing interaction.

nuclei are spherical in the ground state. The calculated quadrupole deformations are in agreement with theoretical results reported by Werner *et al.* [15,16] (prolate for $Z=16$, oblate for $Z=18$), and with available experimental data: $|\beta_2| = 0.258(36)$ for ^{44}S [26,27], and $|\beta_2| = 0.176(17)$ for ^{46}Ar [28]. Experimental data [energies of 2_1^+ states and $B(E2; 0_{g.s.}^+ \rightarrow 2_1^+)$ values] do not determine the sign of deformation, i.e., do not differentiate between prolate and oblate shapes. In the lower panel of Fig. 3 we display the average values of the neutron pairing gaps for occupied canonical states

$$\langle \Delta_N \rangle = \frac{\sum_{[\Omega\pi]} \Delta_{[\Omega\pi]} v_{[\Omega\pi]}^2}{\sum_{[\Omega\pi]} v_{[\Omega\pi]}^2}, \quad (7)$$

where $v_{[\Omega\pi]}^2$ are the occupation probabilities, and $\Delta_{[\Omega\pi]}$ are the diagonal matrix elements of the pairing part of the RH+B single-nucleon Hamiltonian in the canonical basis. $\langle \Delta_N \rangle$ provides an excellent quantitative measure of pairing correlations. The calculated values of $\langle \Delta_N \rangle \approx 2$ MeV correspond to those found in open-shell Ni and Sn isotopes [11]. The spherical shell closure $N=28$ is strongly suppressed for nuclei with $Z \leq 18$, and only for $Z \geq 20$ neutron pairing correlations vanish. It is also interesting to notice how in the self-consistent RH+B model the calculated gaps reflect the staggering of ground-state quadrupole deformations.

For ^{44}S in Fig. 4 we plot the neutron canonical pairing gaps $\Delta_{[\Omega\pi]}$ as function of canonical single-particle energies. The gaps are displayed for canonical states that correspond to the self-consistent ground state. The dashed line denotes the position of the Fermi energy. The pairing gaps are more or less constant for deeply bound states and display a sharp

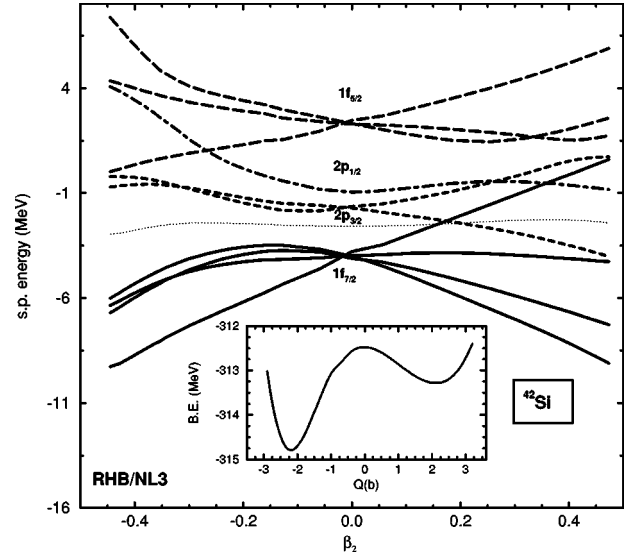


FIG. 5. The neutron single-particle levels for ^{42}Si as function of the quadrupole deformation. The energies in the canonical basis correspond to ground-state RH+B solutions with constrained quadrupole deformation. The dotted line denotes the neutron Fermi level. In the inset we display the corresponding total binding energy curve.

decrease at the Fermi surface. This is related to the volume character of the Gogny interaction in the pairing channel. The values of the $\Delta_{[\Omega\pi]}$ are around 2.2 MeV in the volume, and the average value at the Fermi surface is around 1.8 MeV.

The results of Skyrme+HF and RMF calculations of Refs. [15,16] have shown that neutron-rich Si, S and Ar isotopes can be considered as γ -soft, with deformations depending on subtle interplay between the deformed gaps $Z=16$ and 18, and the spherical gap at $N=28$. Because of cross-shell excitations to the $2p_{3/2}$, $2p_{1/2}$, and $1f_{5/2}$ shells, the $N=28$ gap appears to be broken in most cases. In the RMF analysis of Ref. [19] a careful study of the phenomenon of shape coexistence was performed for nuclei in this region. It was shown that several Si and S isotopes exhibit shape coexistence: two minima with different deformations occur in the binding energy. The energy difference between the two minima is of the order of few hundred keV. For ^{44}S this difference was found to be only 30 keV. In the fully microscopic and self-consistent RH+B model, we have the possibility to analyze in detail the single-neutron levels and to study the formation of minima in the binding energy. In Figs. 5–7 we display the single-neutron levels in the canonical basis for the $N=28$ nuclei ^{42}Si , ^{44}S , and ^{46}Ar , respectively. The single-neutron eigenstates of the density matrix result from constrained RH+B calculations performed by imposing a quadratic constraint on the quadrupole moment. The canonical states are plotted as function of the quadrupole deformation, and the dotted curve denotes the position of the Fermi level. In the insert we plot the corresponding total binding energy curve as function of the quadrupole moment. For ^{42}Si the binding energy displays a deep oblate minimum ($\beta_2 \approx -0.4$). The second, prolate minimum is found at an

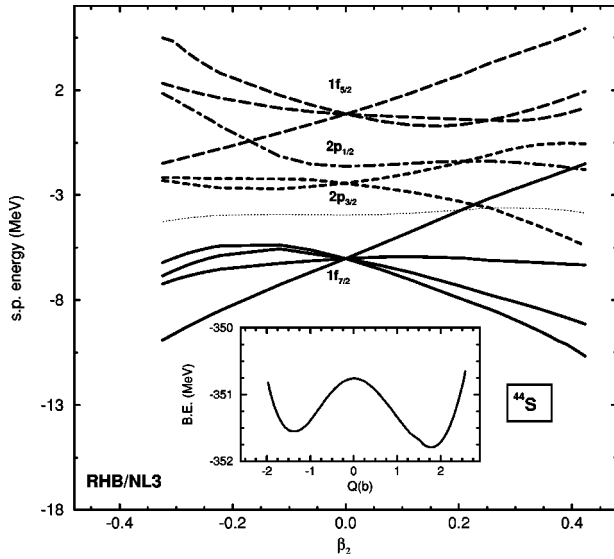


FIG. 6. The same as in Fig. 5, but for ^{44}S .

excitation energy of ≈ 1.5 MeV. Shape coexistence is more pronounced for ^{44}S . The ground state is prolate deformed, the calculated deformation in excellent agreement with experimental data [26,27]. The oblate minimum is found only ≈ 200 keV above the ground state. Finally, for the nucleus ^{46}Ar we find a very flat energy surface on the oblate side. The deformation of the ground-state oblate minimum agrees with experimental data [28], the spherical state is only few keV higher. It is also interesting to observe how the spherical gap between the $1f_{7/2}$ orbital and the $2p_{3/2}$, $2p_{1/2}$ orbitals varies with proton number. While the gap is really strongly reduced for ^{42}Si and ^{44}S , in the $Z=18$ isotone ^{46}Ar the spherical gap is ≈ 4 MeV. Of course from ^{48}Ca the $N=28$ nuclei become spherical. Therefore the single-neutron canonical states in Figs. 5–7 clearly display the disappearance of the spherical $N=28$ shell closure for neutron-rich nuclei below $Z=18$.

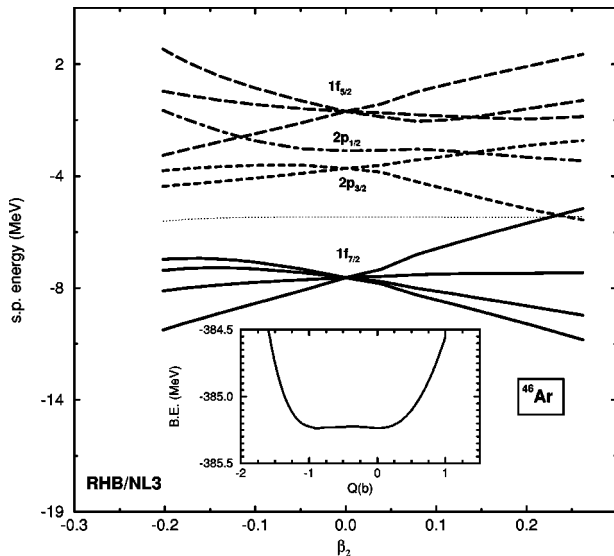


FIG. 7. The same as in Fig. 5, but for ^{46}Ar .

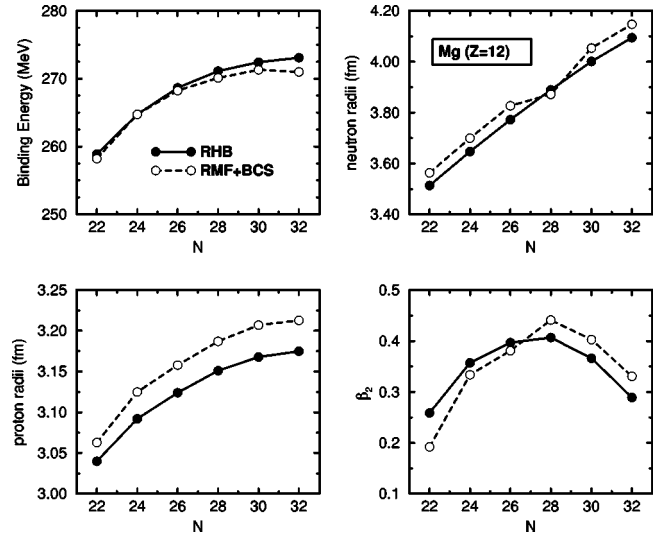


FIG. 8. Comparison of ground-state properties of neutron-rich Mg isotopes, calculated with the relativistic Hartree+Bogoliubov model (NL3 plus D1S Gogny in the pairing channel) and with the relativistic mean-field plus BCS model (NL3 plus constant-gap approximation in the pairing channel). Total binding energies, neutron and proton rms radii, and ground-state quadrupole deformations are compared.

In order to illustrate the importance of the correct description of pairing correlations, in Figs. 8–11 we compare results of fully self-consistent RH+B calculations with those obtained by a simplified RMF+BCS approach that was also used in Refs. [15,16,19]. Binding energies, neutron and proton rms radii, and ground-state quadrupole deformations are compared for chains of Mg, Si, S, and Ar isotopes. In both models the NL3 effective interaction has been used for the mean-field Lagrangian. The D1S Gogny interaction in the pairing channel of the RH+B calculation, the constant gap approximation in the BCS scheme. Since for many of these nuclei the experimental odd-even mass differences are not known, the proton and neutron gaps are calculated following the prescription of Möller and Nix [20]

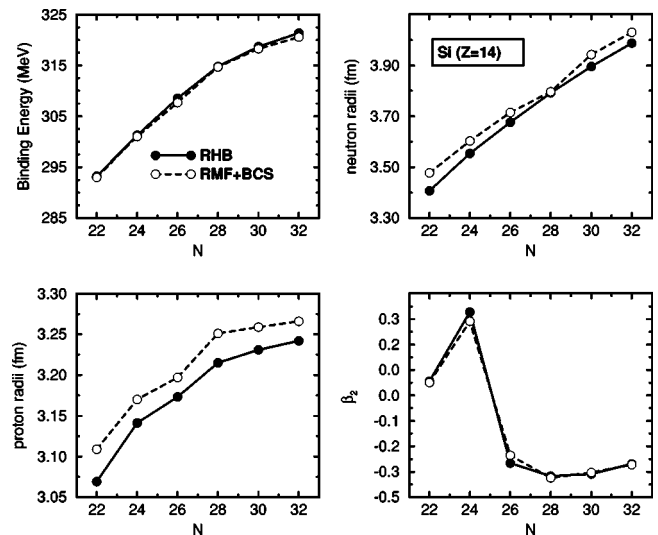


FIG. 9. The same as in Fig. 8, but for the Si isotopes.

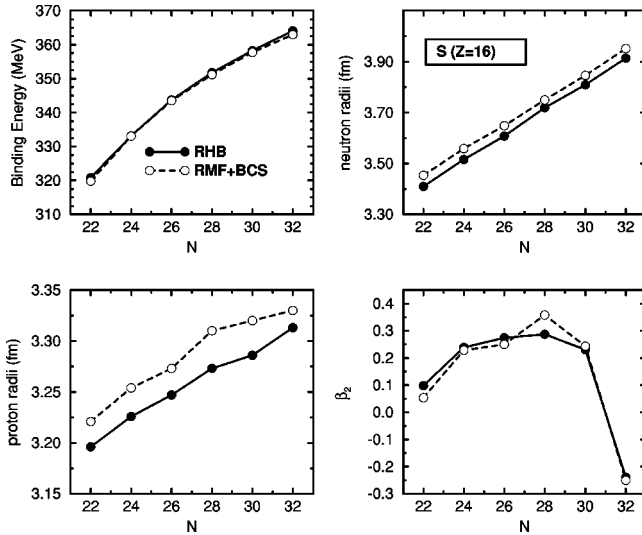


FIG. 10. The same as in Fig. 8, but for the S isotopes.

$$\Delta_n = \frac{4.8}{N^{1/3}}, \quad \Delta_p = \frac{4.8}{Z^{1/3}}. \quad (8)$$

From Figs. 8–11 we notice that, although the calculated binding energies are almost identical with a possible exception for Mg at the drip-line, the other quantities display significant differences. RMF+BCS systematically predicts larger rms radii, especially for protons. For neutron radii RMF+BCS calculations produce interesting kinks at $N=28$ for Mg, Si, and Ar, which suggest shell closure. In the case of Ar isotopes, a strong shift is also calculated for the proton rms radius at $N=28$. These discontinuities are not found in RH+B results, which display a uniform increase of radii with neutron number. The two models predict similar ground-state quadrupole deformations, except for the very γ -soft Ar isotopes. For $^{42,44}\text{Ar}$ the differences are rather pronounced, the ground states of ^{44}Ar is prolate in RMF+BCS, slightly oblate in RH+B calculations.

In conclusion, in the present work we have performed a detailed analysis of the deformed $N=28$ region of neutron-rich nuclei in the framework of the relativistic Hartree + Bogoliubov theory with finite range pairing interaction. This is the first application of the RH+B model to the structure of deformed nuclei. In particular, we have investigated the suppression of the spherical $N=28$ shell gap for neutron-rich nuclei, and the related phenomenon of shape coexistence. 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 interac-

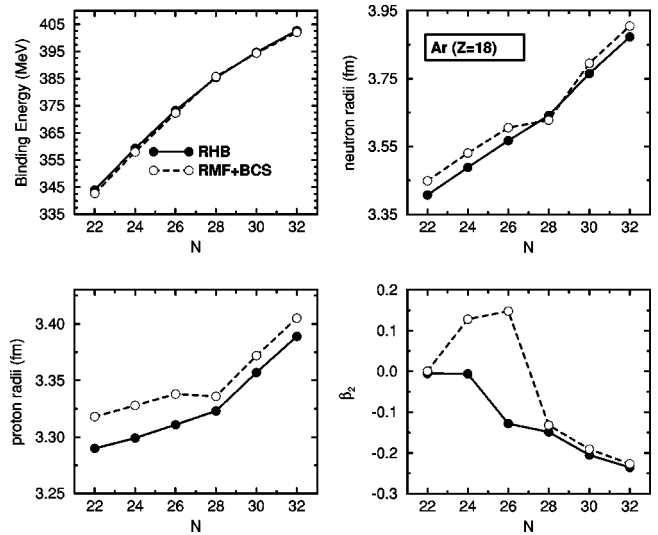


FIG. 11. The same as in Fig. 8, but for the Ar isotopes.

tion D1S. Two-neutron separation energies, rms radii, and ground-state quadrupole deformations have been compared with available experimental data and results of previous Skyrme Hartree-Fock and relativistic mean-field + BCS calculations. We have shown that the present version of the RH+B model produces results in excellent agreement with experimental data, both for binding energies and quadrupole deformations. Our results confirm the strong deformations caused by $1f_{7/2} \rightarrow fp$ neutron excitations. Constrained RH+B calculations have been used to construct the binding energy curves as function of quadrupole deformation. Pronounced shape coexistence is found to be a characteristic of neutron-rich nuclei in this region. $N \approx 28$ nuclei become extremely γ -soft just before the closure of the $Z=20$ shell. For $Z \leq 16$ single neutron spectra in the canonical basis of RH+B display a strong reduction of the gap between the $1f_{7/2}$ orbital and the $2p_{3/2}$, $2p_{1/2}$ levels. The suppression of the spherical $N=28$ shell closure favors deformed ground states. The importance of the full RH+B description of pairing correlations has been illustrated by a comparison with ground-state properties of Mg, Si, S, and Ar isotopes calculated in the RMF+BCS scheme with constant gap approximation.

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