Nuclear energy density functionals constrained by low-energy QCD

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Relativistic nuclear energy density functionals are formulated and developed, guided by two important features that establish connections with chiral dynamics and the symmetry breaking pattern of low-energy QCD: a) strong scalar and vector fields related to in-medium changes of QCD vacuum condensates; b) the long- and intermediate-range interactions generated by one-and two-pion exchange, derived from in-medium chiral perturbation theory.

1. INTRODUCTION

The successes of modern nuclear structure models in predicting many new phenomena in regions of exotic nuclei far from stability, and the recent applications of chiral effective field theory to nucleon-nucleon scattering and the few-body problem, have highlighted one of the fundamental problems in theoretical nuclear physics: the relationship between low-energy, non-perturbative QCD and the rich structure of nuclear many-body systems.

The most complete and accurate description of structure phenomena in heavy nuclei is currently provided by self-consistent non-relativistic and relativistic mean-field models [1,2]. The self-consistent mean-field approach to nuclear structure represents an approximate implementation of Kohn-Sham density functional theory. DFT provides a description of the nuclear many-body problem in terms of an energy density functional $E[\rho]$. Mean-field models approximate the exact energy functional which includes all higher-order correlations. A major goal of nuclear structure theory is to build an energy density functional which is universal, in the sense that the same functional is used for all nuclei, with the same set of parameters. This framework should then provide a reliable microscopic description of infinite nuclear and neutron matter, ground-state properties of bound nuclei, rotational spectra, low-energy vibrations and large-amplitude adiabatic properties [3].

In order to formulate a microscopic density functional, one must be able to go beyond the mean-field approximation and systematically calculate the exchange-correlation part, $E_{xc}[\rho]$, of the energy functional, starting from the relevant active degrees of freedom at low energy. The *exact E_{xc}* includes all many-body effects. Thus the usefulness of DFT crucially depends on our ability to construct accurate approximations to the exact exchange-correlation energy. The natural microscopic framework is chiral effective field theory. It is based on the separation of scales between long-range pion-nucleon dynamics, described explicitly, and short-distance interactions not resolved in detail at low energies.

An extensive program, synthesizing effective field theory methods and density functional

theory, has recently been introduced [4–6]. It is based on the following conjectures: (i) the nuclear ground state is characterized by strong scalar and vector mean fields which have their origin in the in-medium changes of the scalar quark condensate (the chiral condensate) and of the quark density, (ii) nuclear binding and saturation arise primarily from chiral (pionic) fluctuations (reminiscent of van der Waals forces) in combination with Pauli blocking effects and three-nucleon (3N) interactions, superimposed on the condensate background fields and calculated according to the rules of in-medium chiral perturbation theory (ChPT).

The starting point is the description of nuclear matter based on the chiral effective Lagrangian with pions and nucleons, recently improved by including explicit $\Delta(1232)$ degrees of freedom [7]. The relevant "small" scales are the Fermi momentum k_f, the pion mass m_π and the $\Delta - N$ mass difference $\Delta \equiv M_\Delta - M_N \simeq 2.1 m_\pi$, all of which are well separated from the characteristic scale of spontaneous chiral symmetry breaking, $4\pi f_\pi \simeq 1.16$ GeV with the pion decay constant $f_\pi = 92.4$ MeV. The calculations have been performed to three-loop order in the energy density. They incorporate the one-pion exchange Fock term, iterated one-pion exchange and irreducible two-pion exchange, including one or two intermediate Δ's. The resulting nuclear matter equation of state is given as an expansion in powers of the Fermi momentum k_f. The expansion coefficients are functions of k_f/m_π and Δ/m_π, the dimensionless ratios of the relevant small scales. Regularization dependent contributions to the energy density are absorbed in contact interactions, with constants representing unresolved short-distance dynamics.

This framework is translated into a covariant point-coupling model for finite nuclei, with density-dependent interaction vertices. The chiral nuclear matter energy density functional is mapped onto the exchange-correlation energy density functional, including gradient corrections. This model has been employed in the description of ground-state properties of a broad range of spherical and deformed nuclei. The results have been analyzed in comparison with data on binding energies, charge radii, neutron radii and deformation parameters for several isotopic chains, and found at the similar level of quantitative agreement with data as those obtained with the best phenomenological self-consistent mean-field models.

2. THE NUCLEAR ENERGY DENSITY FUNCTIONAL

In the DFT framework [8,9] the free energy functional is commonly decomposed into three separate terms:

$$F_{HK}[\rho] = E_{kin}[\rho] + E_H[\rho] + E_{xc}[\rho] \,, \tag{1}$$

where E_{kin} is the kinetic energy of the non-interacting N-particle system, E_H is a Hartree energy, and E_{xc} denotes the exchange-correlation energy which, by definition, contains everything else. The practical usefulness of the Kohn-Sham scheme depends entirely on whether accurate approximations for E_{xc} can be found. The local ground-state density is constructed using so-called auxiliary orbitals, $\rho(\mathbf{r}) = \sum_{k=1}^{N} |\psi_{KS}^k(\mathbf{r})|^2$, which are unique functionals of the density $\rho(\mathbf{r})$, i.e. the KS scheme defines a self-consistency problem.

The conjectures on which the present approach to the nuclear energy density functional is based, with contact to low-energy QCD, can be adapted as follows: (i) The

large scalar and vector mean fields (with opposite signs) that have their origin in the in-medium changes of the chiral condensate and of the quark density, determine the Hartree energy functional $E_H[\rho]$. (ii) The chiral (pionic) fluctuations including one- and two-pion exchange with single and double virtual $\Delta(1232)$-isobar excitations plus Pauli blocking effects, determine the exchange-correlation energy functional $E_{xc}[\rho]$.

The density distribution and the energy of the nuclear ground state are obtained from self-consistent solutions of the relativistic generalizations of the linear single-nucleon Kohn-Sham equations. In order to derive those equations it is useful to construct a point-coupling model with density dependent interaction terms, designed such as to reproduce the detailed density dependence of the nucleon self-energies resulting from $E_H[\rho] + E_{xc}[\rho]$. A successful framework that meets these requirements for a two component system of protons and neutrons starts from a relativistic Lagrangian which includes isoscalar-scalar (S), isoscalar-vector (V), isovector-scalar (TS) and isovector-vector (TV) effective four-fermion interaction vertices with density-dependent coupling strengths:

$$\mathcal{L} = \mathcal{L}_{\text{free}} + \mathcal{L}_{\text{int}}^{(1)} + \mathcal{L}_{\text{int}}^{(2)} + \mathcal{L}_{\text{coul}}. \tag{2}$$

The four terms read:

$$\mathcal{L}_{\text{free}} = \bar{\psi}(i\gamma_\mu \partial^\mu - M_N)\psi , \tag{3}$$

$$\mathcal{L}_{\text{int}}^{(1)} = -\frac{1}{2} G_S(\hat{\rho})(\bar{\psi}\psi)(\bar{\psi}\psi) - \frac{1}{2} G_V(\hat{\rho})(\bar{\psi}\gamma_\mu\psi)(\bar{\psi}\gamma^\mu\psi)$$
$$- \frac{1}{2} G_{TS}(\hat{\rho})(\bar{\psi}\vec{\tau}\psi)\cdot(\bar{\psi}\vec{\tau}\psi) - \frac{1}{2} G_{TV}(\hat{\rho})(\bar{\psi}\vec{\tau}\gamma_\mu\psi)\cdot(\bar{\psi}\vec{\tau}\gamma^\mu\psi) , \tag{4}$$

$$\mathcal{L}_{\text{int}}^{(2)} = -\frac{1}{2} D_S \partial_\nu(\bar{\psi}\psi)\partial^\nu(\bar{\psi}\psi) , \tag{5}$$

$$\mathcal{L}_{\text{em}} = eA^\mu\bar{\psi}\frac{1+\tau_3}{2}\gamma_\mu\psi - \frac{1}{4}F_{\mu\nu}F^{\mu\nu} , \tag{6}$$

where ψ is the Dirac field of the nucleon with its two isospin components (p and n). Vectors in isospin space are denoted by arrows. In addition to the free nucleon Lagrangian $\mathcal{L}_{\text{free}}$ and the interaction terms contained in $\mathcal{L}_{\text{int}}^{(1)}$, when applied to finite nuclei, the model must include the coupling $\mathcal{L}_{\text{em}}$ of the protons to the electromagnetic field A^μ with $F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu$, and a derivative (surface) term $\mathcal{L}_{\text{int}}^{(2)}$. One could, of course, construct additional derivative terms in $\mathcal{L}_{\text{int}}^{(2)}$, further generalized to include density dependent strength parameters. However, there appears to be no need in practical applications to go beyond the simplest ansatz (5) with a constant D_S. The classical variational principle applied to the Lagrangian (2) leads to the self-consistent single-nucleon Dirac equations, the relativistic analogue of the (non-relativistic) Kohn-Sham equations. The nuclear dynamics produced by chiral (pionic) fluctuations in the medium is now encoded in the density dependence of the interaction vertices.

The couplings $G_i(\hat{\rho})$ ($i = S, V, TS, TV$) are decomposed as follows:

$$G_i(\hat{\rho}) = G_i^{(0)} + G_i^{(\pi)}(\hat{\rho}) \quad (\text{for } i = S, V)$$
$$\text{and} \quad G_i(\hat{\rho}) = G_i^{(\pi)}(\hat{\rho}) \quad\quad\quad (\text{for } i = TS, TV) , \tag{7}$$

into density-independent parts $G_i^{(0)}$ which arise from strong isoscalar scalar and vector background fields, and density-dependent parts $G_i^{(\pi)}(\hat{\rho})$ generated by (regularized) one-

and two-pion exchange dynamics. It is assumed that only pionic processes contribute to the isovector channels.

The relativistic density functional describing the ground-state energy of the system can be re-written as a sum of four distinct terms:

$$E_0[\hat{\rho}] = E_{\text{free}}[\hat{\rho}] + E_{\text{H}}[\hat{\rho}] + E_{\text{coul}}[\hat{\rho}] + E_{\pi}[\hat{\rho}] \, , \tag{8}$$

with

$$E_{\text{free}}[\hat{\rho}] = \int d^3r \, \langle \phi_0 | \bar{\psi} [-i\boldsymbol{\gamma} \cdot \boldsymbol{\nabla} + M_N] \psi | \phi_0 \rangle \, , \tag{9}$$

$$E_{\text{H}}[\hat{\rho}] = \frac{1}{2} \int d^3r \, \{ \langle \phi_0 | G_S^{(0)} (\bar{\psi}\psi)^2 | \phi_0 \rangle + \langle \phi_0 | G_V^{(0)} (\bar{\psi}\gamma_\mu\psi)^2 | \phi_0 \rangle \} \, , \tag{10}$$

$$\begin{aligned} E_{\pi}[\hat{\rho}] = \frac{1}{2} \int d^3r \, \Big\{ & \langle \phi_0 | G_S^{(\pi)}(\hat{\rho}) (\bar{\psi}\psi)^2 | \phi_0 \rangle + \langle \phi_0 | G_V^{(\pi)}(\hat{\rho}) (\bar{\psi}\gamma_\mu\psi)^2 | \phi_0 \rangle \\ & + \langle \phi_0 | G_{TS}^{(\pi)}(\hat{\rho}) (\bar{\psi}\vec{\tau}\psi)^2 | \phi_0 \rangle + \langle \phi_0 | G_{TV}^{(\pi)}(\hat{\rho}) (\bar{\psi}\gamma_\mu\vec{\tau}\psi)^2 | \phi_0 \rangle \\ & - \langle \phi_0 | D_S^{(\pi)} [\boldsymbol{\nabla}(\bar{\psi}\psi)]^2 | \phi_0 \rangle \Big\} \, , \end{aligned} \tag{11}$$

$$E_{coul}[\hat{\rho}] = \frac{1}{2} \int d^3r \, \langle \phi_0 | A^\mu e \bar{\psi} \frac{1 + \tau_3}{2} \gamma_\mu \psi | \phi_0 \rangle \quad , \tag{12}$$

where $|\phi_0\rangle$ denotes the nuclear ground state. Here E_{free} is the energy of the free (relativistic) nucleons including their rest mass. E_{H} is a Hartree-type contribution representing strong scalar and vector mean fields, later to be connected with the leading terms of the corresponding nucleon self-energies deduced from in-medium QCD sum rules. Furthermore, E_{π} is the part of the energy generated by chiral $\pi N \Delta$-dynamics, including a derivative (surface) term, with all pieces explicitly derived in [7].

3. LINKING THE ENERGY FUNCTIONAL TO THE LOW-ENERGY SECTOR OF QCD.

The QCD ground state (or "vacuum") is characterized by strong condensates of quark-antiquark pairs and gluons, an entirely non-perturbative phenomenon. The quark condensate $\langle \bar{q}q \rangle$, i.e. the ground state expectation value of the scalar quark density, plays a particularly important role as an order parameter of spontaneously broken chiral symmetry. At a renormalization scale of about 1 GeV (with up and down quark masses $m_u + m_d \simeq 12$ MeV) the value of the chiral vacuum condensate is $\langle \bar{q}q \rangle_0 \simeq -(240 \text{ MeV})^3 \simeq -1.8 \text{ fm}^{-3}$.

In-medium QCD sum rules relate the leading changes of the scalar quark condensate and of the quark density at finite baryon density, with the scalar and vector self-energies of a nucleon in the nuclear medium. To first order in the scalar and baryon densities, these self-energies can be expressed as follows [10,11]:

$$\Sigma_S^{(0)} = -\frac{\sigma_N M_N}{m_\pi^2 f_\pi^2} \rho_S \qquad \text{and} \qquad \Sigma_V^{(0)} = \frac{4(m_u + m_d) M_N}{m_\pi^2 f_\pi^2} \rho \, , \tag{13}$$

where $\sigma_N = \langle N | m_q \bar{q}q | N \rangle$ is the nucleon sigma term ($\simeq 50$ MeV), m_π is the pion mass (138 MeV), and $f_\pi = 92.4$ MeV is the pion decay constant. The resulting $\Sigma_S^{(0)}$ and $\Sigma_V^{(0)}$ are individually of the order of $300 - 400$ MeV in magnitude. Their ratio

$$\frac{\Sigma_S^{(0)}}{\Sigma_V^{(0)}} = -\frac{\sigma_N}{4(m_u + m_d)} \frac{\rho_S}{\rho} \tag{14}$$

is close to -1, suggesting a large cancellation of scalar and vector potentials in the single-nucleon Dirac equation, a feature characteristic of relativistic mean-field phenomenology.

Comparing the expressions for the isoscalar vector and scalar potentials of the single-nucleon Dirac equations, with the Eq. (13) for the condensate background self-energies, respectively, the following estimates hold for the couplings of the nucleon to the background fields (the Hartree terms in the energy functional):

$$G_S^{(0)} = -\frac{\sigma_N M_N}{m_\pi^2 f_\pi^2} \qquad \text{and} \qquad G_V^{(0)} = \frac{4(m_u + m_d)M_N}{m_\pi^2 f_\pi^2} \ , \tag{15}$$

which implies $G_S^{(0)} \simeq -G_V^{(0)} \simeq -10.6$ fm^2 for typical values $\sigma_N \simeq 48$ MeV and $m_u + m_d \simeq$ 12 MeV. In the actual applications to finite nuclei, $G_{S,V}^{(0)}$ will have to be fine-tuned.

The many-body effects represented by the exchange-correlation density functional are approximated by chiral $\pi N\Delta$-dynamics, including Pauli blocking effects. In the simplest DFT approach, the exchange-correlation energy for a finite system is determined in the local density approximation (LDA) from the exchange-correlation functional of the corresponding infinite homogeneous system, replacing the constant density ρ by the local density $\rho(\mathbf{r})$ of the actual inhomogeneous system. In our case the exchange-correlation terms of the nuclear density functional are determined within LDA by equating the corresponding self-energies in the single-nucleon Dirac equation, with those arising from the in-medium chiral perturbation theory calculation of $\pi N\Delta$-dynamics in homogeneous isospin symmetric and asymmetric nuclear matter.

The density-dependent couplings $G_i^{(\pi)}$ are expressed as polynomials in fractional powers of the baryon density:

$$G_i^{(\pi)}(\rho) = c_{i1} + c_{i2}\rho^{\frac{1}{3}} + c_{i3}\rho^{\frac{2}{3}} + c_{i4}\rho \dots \ (i = S, V, TS, TV) \ . \tag{16}$$

The coefficient $D_S^{(\pi)}$ of the derivative term in the equivalent point-coupling model can be determined from ChPT calculations for inhomogeneous nuclear matter. The inclusion of derivative terms in the model Lagrangian and the determination of its strength parameters from ChPT actually goes beyond the local density approximation. The term Eq. (5) represents a second-order gradient correction to the LDA, i.e. the next-to-leading term in the gradient expansion of the exchange-correlation energy calculated by in-medium chiral perturbation theory.

While bulk properties of infinite nuclear matter are useful for orientation, the large amount of nuclear observables provides a far more accurate data base that permits a fine tuning of the parameters. The total number of adjustable parameters of the point-coupling model is seven, and they are fixed simultaneously to properties of nuclear matter, and to binding energies, charge radii and differences between neutron and proton radii of spherical nuclei, starting from the estimates for the couplings of the condensate background fields (Hartree term), and the constants in the expressions for the self-energies arising from chiral $\pi N\Delta$-dynamics (exchange-correlation term). The resulting optimal parameter set (FKVW) [6] is remarkably close to the anticipated QCD sum rule and ChPT values, with the exception of the two constants associated with three-body correlations, for which the fit to nuclear data systematically requires an attractive shift as compared to the ChPT calculation [7].

4. NUCLEAR GROUND-STATE PROPERTIES

The effective FKVW interaction has been tested in self-consistent calculations of ground-state observables for spherical and deformed medium-heavy and heavy nuclei. The calculations, including open-shell nuclei, are performed in the framework of the relativistic Hartree-Bogoliubov (RHB) model, a relativistic extension of the conventional Hartree-Fock-Bogoliubov method, that provides a basis for a consistent microscopic description of ground-state properties of medium-heavy and heavy nuclei, low-energy excited states, small-amplitude vibrations, and reliable extrapolations toward the drip lines [2]. In the particle-hole channel the new microscopic FKVW interaction [6] is employed, in comparison with one of the most successful effective meson-exchange phenomenological relativistic mean-field interactions: DD-ME1 [12]. Pairing effects in nuclei are restricted to a narrow window of a few MeV around the Fermi level. Their scale is well separated from the scale of binding energies which are in the range of several hundred to thousand MeV, and thus pairing can be treated as a non-relativistic phenomenon. In most applications of the RHB model the pairing part of the well known and successful Gogny force [13] has been employed in the particle-particle channel, and the same interaction is used in the illustrative examples included in this section.
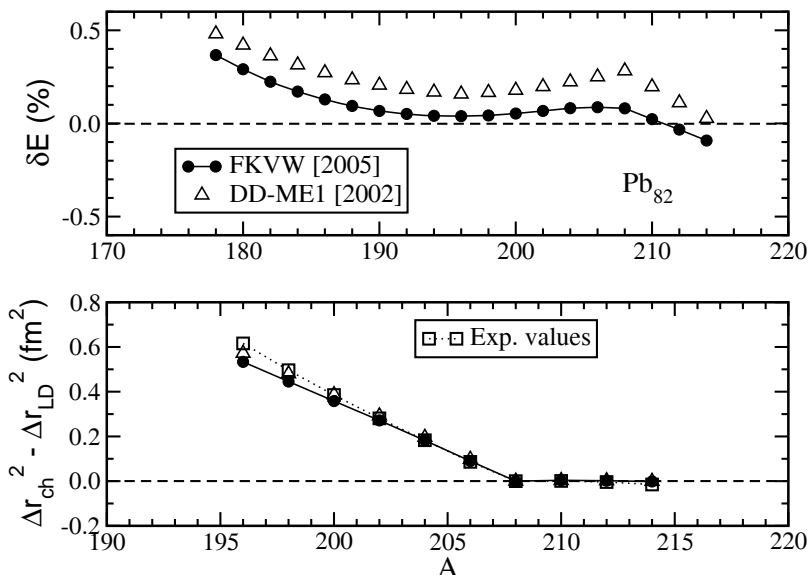

Figure 1. The deviations (in percent) of the calculated binding energies from the experimental values (upper panel), and the calculated charge isotope shifts in comparison with data, for the chain of even-A Pb isotopes. The charge isotope shifts are defined: $\Delta r_{ch}^2 = r_{ch}^2(A) - r_{ch}^2(^{208}Pb)$ and $\Delta r_{LD}^2 = r_{LD}^2(A) - r_{LD}^2(^{208}Pb)$, where the liquid-drop estimate is $r_{LD}^2(A) = \frac{3}{5}r_0^2 A^{2/3}$.

The isotopic dependence of the deviations (in percent) between the calculated binding energies and the experimental values for even-A Pb nuclei, is plotted in the upper panel of Fig. 1. It is interesting to note that, although DD-ME1 and FKVW represent different physical models, they display a similar mass dependence of the calculated binding energies for the Pb isotopic chain. On a quantitative level the FKVW interaction produces better results, with the absolute deviations of the calculated masses below 0.1 % for $A \geq 190$. In lighter Pb isotopes one expects that the observed shape coexistence phenomena will have a pronounced effect on the measured masses. Because of the intrinsic isospin dependence of the effective single-nucleon spin-orbit potential, relativistic mean-field models naturally reproduce the anomalous charge isotope shifts. The well known example of the anomalous kink in the charge isotope shifts of Pb isotopes is illustrated in the lower panel of Fig. 1. The results of RHB calculations with the DD-ME1 and FKVW effective interactions are shown in comparison with experimental values. Both interactions reproduce in detail the A-dependence of the isotope shifts and the kink at ^{208}Pb.
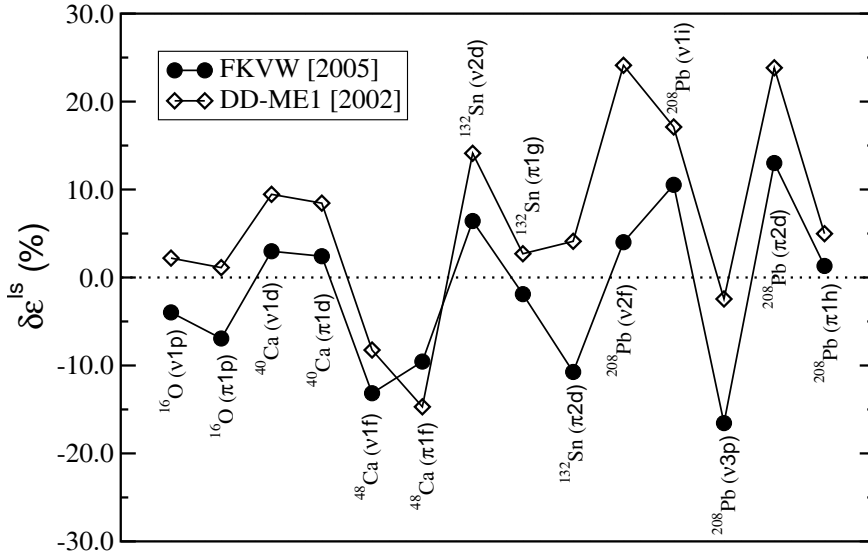

Figure 2. The deviations (in percent) between the theoretical and experimental values of the energy spacings between spin-orbit partner-states in doubly closed-shell nuclei.

One of the principal advantages of using the relativistic framework lies in the fact that the effective single-nucleon spin-orbit potential arises naturally from the Dirac equation. The single-nucleon potential does not introduce any adjustable parameter for the spin-orbit interaction. In the FKVW model, in particular, the large effective spin-orbit potential in finite nuclei is generated by the strong scalar and vector condensate back-

ground fields of about equal magnitude and opposite sign, induced by changes of the QCD vacuum in the presence of baryonic matter [5]. Fig. 2 displays the deviations (in percent) between the calculated and experimental values of the energy spacings between spin-orbit partner-states in a series of doubly closed-shell nuclei. The theoretical spin-orbit splittings have been calculated with the FKVW and DD-ME1 interactions. For the phenomenological DD-ME1 interaction the large scalar and vector nucleon self-energies which generate the spin-orbit potential, arise from the exchange of "sigma" and "omega" bosons with adjustable strength parameters. One notices that, even though the values calculated with DD-ME1 are already in very good agreement with experimental data, a further improvement is obtained with the FKVW interaction. This remarkable agreement indicates that the initial estimates for the condensate background couplings have been more realistic than anticipated, considering the uncertainties of lowest-order in-medium QCD sum rules.
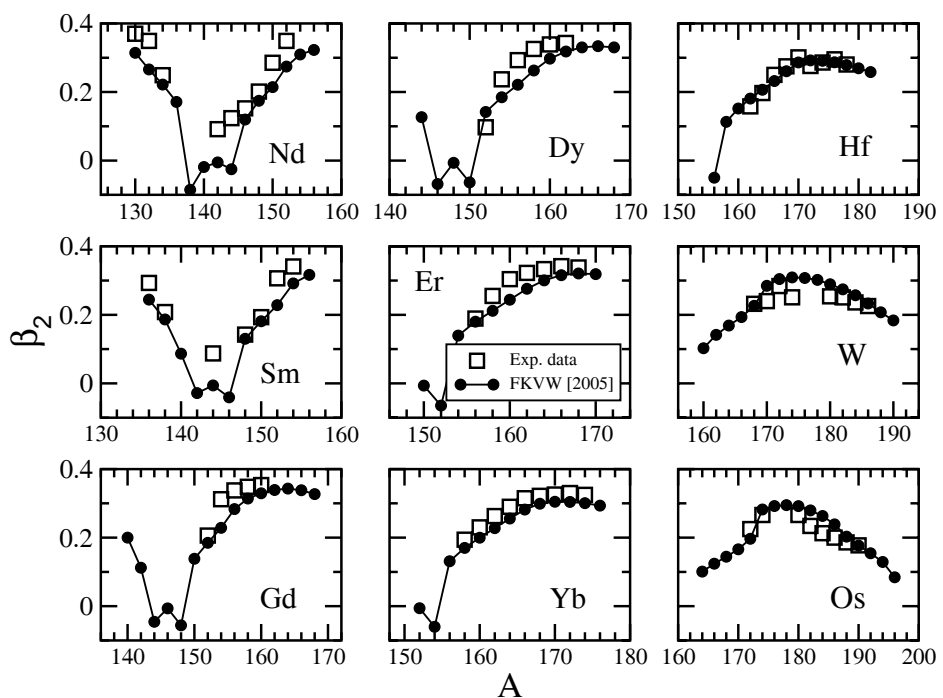

Figure 3. Comparison between the RHB model (FKVW interaction plus Gogny pairing) predictions for the ground-state quadrupole deformation parameters of the Nd, Sm, Gd, Dy, Er, Yb, Hf, W, and Os isotopes, and experimental values.

Deformed nuclei with $N > Z$ present further important tests for nuclear structure models. Ground-state properties, in particular, are sensitive to the isovector channel of

the effective interaction, to the spin-orbit term of the effective single-nucleon potentials and to the effective mass. The nuclear density functional constrained by low-energy QCD has been tested in the region $60 \leq Z \leq 80$. Predictions of the RHB calculations for the total binding energies, charge radii and ground-states quadrupole deformations of even-Z isotopic chains have been compared with available data. With the FKVW effective interaction in the particle-hole channel, and pairing correlations described by the finite range Gogny D1S interaction, very good agreement with experimental values has been found not only for the binding energies and charge radii over the entire region of deformed nuclei, but excellent results have also been obtained for the ground-state quadrupole deformations.

The level of agreement with data is illustrated in Fig. 3 where, for the chains of Nd, Sm, Gd, Dy, Er, Yb, Hf, W, and Os isotopes, the calculated ground-state quadrupole deformation parameters β_2, proportional to the expectation value of the quadrupole operator $\langle \phi_0 | 3z^2 - r^2 | \phi_0 \rangle$, are displayed in comparison with the empirical data extracted from $B(E2)$ transitions. One notices that the RHB results reproduce not only the global trend of the data but also the saturation of quadrupole deformations for heavier isotopes.

5. SUMMARY AND CONCLUSIONS

A relativistic nuclear energy density functional has been introduced with connections to two closely linked features of QCD in the low-energy limit: a) in-medium changes of vacuum condensates; b) spontaneous chiral symmetry breaking.

The leading changes of the chiral (quark) condensate and quark density in the presence of baryonic matter are sources of strong (attractive) scalar and (repulsive) vector fields experienced by nucleons in the nucleus. These fields produce Hartree potentials of about 0.35 GeV in magnitude at nuclear matter saturation density, in accordance with QCD sum rules. While these scalar and vector potentials cancel approximately in their contribution to the energy, they are at the origin of the large spin-orbit splitting in nuclei.

The spontaneously broken chiral symmetry in QCD introduces pions as Goldstone bosons with well-defined (derivative) couplings to baryons plus symmetry breaking corrections. In the present approach the exchange-correlation part of the energy density functional is deduced from the long- and intermediate-range interactions generated by one- and two-pion exchange processes. They have been computed using in-medium chiral perturbation theory with explicit inclusion of $\Delta(1232)$ degrees of freedom which turn out to be important. Regularization dependent contributions to the energy density, calculated at three-loop level, are absorbed in contact interactions with constants representing unresolved short-distance dynamics.

This framework is translated into a point-coupling model with density-dependent interaction vertices. This is done for the practical purpose of deriving and solving self-consistent Dirac equations (relativistic analogues of Kohn-Sham equations) in order to determine the nucleon densities which enter the energy functional. The construction of the density functional involves an expansion of nucleon self-energies in powers of the Fermi momentum up to and including terms of order k_f^6, or equivalently, $O(\rho^2)$ in the proton and neutron densities. The exchange-correlation energy functional in nuclear matter, determined by in-medium chiral perturbation theory, is used in Kohn-Sham calculations of

finite nuclei by employing a second-order gradient correction to the local density approximation. Up to this order the present model has seven parameters, four of which are related to contact (counter) terms that appear in the chiral perturbation theory treatment of nuclear matter. One parameter fixes a surface (derivative) term and two more represent the strengths of scalar and vector Hartree fields.

In the "best fit" set which reproduces a large amount of data on nuclear ground state properties, five of those seven parameters turn out to be surprisingly close to estimates and predictions from in-medium QCD sum rules and ChPT calculations for nuclear matter. The model works extremely well when confronted with a large number of high-precision nuclear data over a broad range of spherical and deformed nuclei. Even though the quality of the results is on the level of the best phenomenological (non-relativistic and relativistic) self-consistent mean-field models, obviously the goal is to further improve the accuracy of the calculated nuclear ground-state energies and density distributions all over the periodic table.

Chiral effective field theory provides a consistent microscopic framework in which both the isoscalar and isovector channels of a universal nuclear energy density functional can be formulated. The present approach to nuclear DFT establishes a fundamental link between low-energy QCD and ground-state properties of finite nuclei. From a practical point of view, a fully microscopic basis of effective nuclear interactions is especially important for studies of nuclear structure in regions far from the valley of β-stability, where extrapolations of phenomenological (non-relativistic and relativistic) models lack predictive power.

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