Ab Initio Description of p-Shell Hypernuclei

Roland Wirth,^{1,*} Daniel Gazda,^{2,3} Petr Navrátil,⁴ Angelo Calci,¹ Joachim Langhammer,¹ and Robert Roth^{1,†}

¹Institut für Kernphysik, Technische Universität Darmstadt, Schlossgartenstraße 2, 64289 Darmstadt, Germany

²ECT^{*}, Villa Tambosi, 38123 Villazzano, Trento, Italy

³Nuclear Physics Institute, 25068 Řež, Czech Republic

⁴TRIUMF, 4004 Wesbrook Mall, Vancouver, British Columbia V6T 2A3, Canada

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We present the first *ab initio* calculations for *p*-shell single- Λ hypernuclei. For the solution of the manybaryon problem, we develop two variants of the no-core shell model with explicit Λ and Σ^+ , Σ^0 , $\Sigma^$ hyperons including Λ - Σ conversion, optionally supplemented by a similarity renormalization group transformation to accelerate model-space convergence. In addition to state-of-the-art chiral two- and threenucleon interactions, we use leading-order chiral hyperon-nucleon interactions and a recent mesonexchange hyperon-nucleon interaction. We validate the approach for *s*-shell hypernuclei and apply it to *p*-shell hypernuclei, in particular to ${}^{7}_{\Lambda}$ Li, ${}^{9}_{\Lambda}$ Be, and ${}^{13}_{\Lambda}$ C. We show that the chiral hyperon-nucleon interactions provide ground-state and excitation energies that generally agree with experiment within the cutoff dependence. At the same time we demonstrate that hypernuclear spectroscopy provides tight constraints on the hyperon-nucleon interactions.

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Over the past decades, the structure of hypernuclei has been the focus of a number of experimental programs worldwide, providing a wealth of high-precision data on excitation spectra as well as binding energies [1-6]. These experimental efforts continue and are intensified, e.g., in several present and future experiments at international facilities like J-PARC, JLab, and FAIR. Hypernuclear structure theory has a rich history of phenomenological models that have accompanied and driven the experiments, most notably the shell model for p-and sd-shell hypernuclei [7,8], cluster models [9-12], various mean-field models [13–16], and recent Monte Carlo calculations with simplified phenomenological interactions [17,18]. Ab initio calculations based on realistic nucleonic and hyperonic interactions were limited to systems of up to four nucleons so far [19–22]. Nevertheless, these calculations established a direct link between experimental observables and the underlying interactions and helped to elucidate the role of hyperons in matter. Advancing ab initio methods beyond their current limits is highly desirable. It would allow us to exploit the wealth of accurate experimental data, e.g., on *p*-shell hypernuclei, for constraining and improving the underlying interactions and to make predictions for yet unobserved phenomena.

There are two main aspects that hindered *ab initio* calculations for *p*-shell hypernuclei in the past. First, a prerequisite is accurate *ab initio* calculations of the non-strange parent nucleus. The approach has to be able to provide converged results for the parent nucleus and the nucleonic Hamiltonian has to yield a good description of the experimental nuclear spectra. In the past few years, *ab initio* methods using two-nucleon (NN) and

three-nucleon (3N) interactions constructed in chiral effective field theory (EFT) succeeded in providing a quantitative description of ground states and spectra of nuclei in the p shell and beyond [23,24]. This is facilitated by a multitude of developments on computational many-body methods that give access to an unprecedented range of nuclei [25–30].

Second, the hyperon-nucleon (YN) interaction is ill constrained due to the scarce scattering data in the YN sector. Different models for the YN interaction, such as the widely used Nijmegen soft-core and extended soft-core models of the Nijmegen group [31,32], quark models [33], and the Jülich meson exchange models [34], already yield different results at the level of cross sections, rendering a meaningful ab initio description of hypernuclei difficult. In a new development, chiral EFT has been employed to derive YN interactions within the same conceptual framework as the nucleonic interactions. Leading-order (LO) and, very recently, next-to-leading-order (NLO) chiral YN interactions were developed by Polinder et al. [35] and Haidenbauer et al. [36], respectively, succeeding their earlier meson-exchange interactions like the Jülich'04 model [34]. An exciting option for constraining YN interactions directly from QCD emerges from recent lattice QCD calculations [37,38], e.g., for YN phase shifts. In combination with the advances in ab initio many-body methods, this opens unique opportunities to learn about the structure of hypernuclei from first principles. By confronting accurate calculations with precise hypernuclear data, one can characterize and constrain the YN interaction, which is still the main source of uncertainty, and assess the relevance of three-baryon interactions for hypernuclear structure. Quantitative knowledge of the two-and threebaryon interactions is vital to understand not only hypernuclear structure but also the role of hyperons in dense baryonic matter in connection with the structure of neutron stars [39–41].

In this Letter, we present the first *ab initio* calculations for *p*-shell single- Λ hypernuclei. We employ two versions of the no-core shell model (NCSM) for the solution of the many-body problem [42,43], the Jacobi NCSM (J-NCSM) and the importance-truncated NCSM (IT-NCSM). We include nucleons, the Λ , and all Σ hyperons as explicit degrees of freedom, thus accounting for the full Λ - Σ coupled-channel problem. In both approaches we employ the same NN and 3N interactions derived in chiral EFT. We use the chiral NN interaction at N³LO by Entem and Machleidt [44] and the local form of the chiral 3N interaction at N²LO [45] with low-energy constants determined from A = 3 binding energies and triton half-life [46], both for 500 MeV/c cutoff momentum. In the YN sector we employ the Jülich'04 interaction [34] as a representative for the meson-exchange models and the LO chiral YN interaction [35] with cutoff momenta of 600 and 700 MeV/c to probe the cutoff dependence. The hypernuclear Hamiltonian is transformed via a similarity renormalization group (SRG) evolution to accelerate the convergence of the NCSM-type many-body calculations.

Many-body method.—The NCSM provides an extremely versatile framework for the formulation of an ab initio method for hypernuclei. We have developed two independent but equivalent variants: (i) The J-NCSM using a harmonic-oscillator (HO) basis in relative Jacobi coordinates [47], which enables an explicit center-of-mass separation and allows for calculations up to large numbers of HO excitation quanta, defining the basis-truncation parameter N_{max} , for three- and four-baryon systems. (ii) The IT-NCSM using a basis of Slater determinants of HO single-particle states with an optional importance truncation of the N_{max} model space [24,48], which allows us to treat hypernuclei throughout the whole p shell and beyond. Both approaches include nucleons and the Λ and $\Sigma^+, \Sigma^0, \Sigma^-$ hyperons explicitly with their physical rest masses [49]. The many-baryon model spaces are constrained by the total baryon number A, the electric charge Q, and the strangeness S; thus, the full coupled-channel problem—including Λ - Σ conversion and explicit Σ baryons-is solved. Furthermore, all Coulomb interactions, as well as the charge symmetry breaking terms of the NN and YN interaction, are included.

Similarity renormalization group.—In order to accelerate the convergence of the NCSM calculations with modelspace size, we optionally employ an SRG transformation of the Hamiltonian [24,50–52], which has been very successful in the context of *ab initio* nuclear structure calculations [23–25]. This specific unitary transformation is based on the flow equation $dH_{\alpha}/d\alpha = [\eta_{\alpha}, H_{\alpha}]$, using the dynamic generator $\eta_{\alpha} = m_N^2[T_{\text{int}}, H_{\alpha}]$, with the intrinsic kinetic energy T_{int} , the evolved Hamiltonian H_{α} , and the flow parameter α . The flow equation is solved numerically in a momentum or HO basis. We use an explicit particle representation, again accounting for all possible channel couplings resulting from tensor-type interactions, the antisymmetric spin-orbit terms, and the Λ - Σ conversion, as well as for the different rest masses. Furthermore, we introduce different flow parameters α_N and α_Y for channels involving only nucleons and channels involving a hyperon, respectively. For purely nucleonic channels we perform the evolution in two- and three-particle space, giving access to the SRG-evolved NN and 3N interactions, which is state of the art for nuclear structure calculations [24].

For channels involving hyperons, we are presently limited to evolutions in two-body space; thus, hyperonnucleon-nucleon (YNN) interactions formally induced by the SRG transformation cannot be included directly. However, a variation of the flow parameters α_N and α_Y probes the effect of induced YNN interactions—this is completely analogous to the use of the flow parameter as a diagnostic tool for induced 3N and 4N interactions in nucleonic systems [23,24]. We find that the SRG evolution of YN channels generates large induced YNN interactions, whereas the evolution in NN channels only yields a weak flow-parameter dependence. Therefore, we restrict ourselves to $\alpha_Y = 0$ fm⁴ in the following. We will discuss the origin of the strong induced YNN interactions, as well as their physical impact, in a separate publication.

Validation for s-shell hypernuclei.-In a first step we validate the two NCSM implementations for the s-shell hypernuclei ${}^{3}_{\Lambda}$ H and ${}^{4}_{\Lambda}$ H, ${}^{4}_{\Lambda}$ He, where exact few-body calculations using the same YN interactions are available. Figure 1 shows the N_{max} -dependence of the ground-state energies obtained in the J-NCSM and the IT-NCSM for the LO chiral YN interaction, with cutoff 600 MeV/c, compared to results from Faddeev calculations [21]. For ${}^{3}_{\Lambda}$ H we observe an extremely slow convergence related to the weak binding. However, the large N_{max} spaces accessible with the J-NCSM, in combination with recent EFT-motivated extrapolation schemes for weakly bound states [see Eq. (44) of Ref. [53], using between 5 and 10 data points for the largest $N_{\rm max}$ to extract nominal value and uncertainty], yield a ground-state energy of -2.33(1) MeV using the bare Hamiltonian in excellent agreement with the result of Ref. [21]. There is a tiny difference of the extrapolated energies for $\alpha_N = 0$ and 0.08 fm⁴ of about 50 keV, hinting at a small effect of induced YNN terms resulting from the SRG evolution of the nucleonic channels. For ${}^{4}_{\Lambda}$ He and ${}^{4}_{\Lambda}$ H the $N_{\rm max}$ convergence is much better, even with the bare Hamiltonian including chiral NN, 3N, and YN interactions, as shown in Fig. 1(b). The energies for the 0^+ ground state obtained from an exponential extrapolation using between 3 and 6 data points for the largest N_{max} are -11.1(1) and -10.3(1) MeV for ${}^{4}_{\Lambda}$ H and ${}^{4}_{\Lambda}$ He, respectively,



FIG. 1 (color online). Ground-state energy of *s*-shell hypernuclei obtained with the LO chiral YN interaction with cutoff 600 MeV/*c*. Solid symbols represent J-NCSM results, crosses show IT-NCSM results. Panel (a) shows the ground-state energies of ${}^{3}_{\Lambda}$ H for $\hbar\Omega = 20$ MeV, $\alpha_Y = 0$ fm⁴ and $\alpha_N = 0$ fm⁴ (square) and $\alpha_N = 0.08$ fm⁴ (circle), with EFT-motivated extrapolations (colored bands) compared to the experimental value (gray band) and the result of a Faddeev calculation [21] (black line, see inset). Panels (b) and (c) show results for the 0⁺ ground states (square) and 1⁺ first excited states (circle) of ${}^{4}_{\Lambda}$ H and ${}^{4}_{\Lambda}$ He, respectively, using $\alpha_Y = \alpha_N = 0$ fm⁴ and $\hbar\Omega = 28$ MeV. The upper plots show absolute energies, the lower plots excitation energies. The colored bands give the result of an exponential extrapolation of the ground-state energy and the solid lines represent results of previous few-body calculations [21].

corresponding to Λ separation energies of 2.6(1) MeV for both nuclei, consistent with Ref. [21]. The excitation energies of the 1⁺ excited states, as shown in the lower plots, also agree very well with previous few-body calculations and with experiment. Both NCSM approaches agree at the level of 1–5 keV in all model spaces accessible to both, thus validating the implementations.

Application to p-shell hypernuclei.—The IT-NCSM enables ab initio calculations for all single- Λ hypernuclei throughout the p shell. Here we focus on a representative subset, where precise experimental data on the spectroscopy is available. We discuss ${}^{7}_{\Lambda}$ Li as one of the best studied p-shell hypernuclei in both experiment and phenomenological models, ${}^{9}_{\Lambda}$ Be for which the first spin doublet is degenerate posing a fine-tuning problem for the interaction, and ${}^{13}_{\Lambda}$ C representing the upper p shell. In comparison to the well studied s shell, hypernuclei in the p shell probe higher relative partial waves of the YN interaction and thus enhance spin-orbit and tensor effects. Based on these calculations we assess the performance of present YN interactions, in particular, the Jülich'04 and the LO chiral YN interactions for cutoff momenta 600 and 700 MeV/c.

We start with the discussion of ${}^{7}_{\Lambda}$ Li in Fig. 2. Panel (a) shows the absolute energies and the excitation energies of the nonstrange parent nucleus ⁶Li obtained for the chiral NN + 3N interaction with an SRG evolution to $\alpha_N = 0.08 \text{ fm}^4$. Note that the converged energies are practically independent of α_N in the lower *p* shell [23,24]. The good agreement of absolute and excitation energies with experiment resulting from the chiral NN + 3N Hamiltonian and the good convergence of the IT-NCSM are evident and are a prerequisite for accurate hypernuclear calculations.

When adding a hyperon to the nonstrange parent nucleus, in a simple picture, the weak attractive YN interaction leads to a lowering of the ground-state energy and to a splitting of each J > 0 level into a doublet with angular momenta J + 1/2 and J - 1/2. The energy splitting is directly controlled by and sensitive to the YN interaction. Both effects are evident in the IT-NCSM results for ${}^{7}_{\Lambda}$ Li in panels (b) and (c) of Fig. 2. Moreover, the differences between the YN interactions are evident. For the Jülich'04 interaction employed in Fig. 2(c), the ground-state energy is in reasonable agreement with experiment, but the level ordering is wrong. The splitting of the spin doublet is significantly too large and has the wrong sign,



FIG. 2 (color online). Absolute and excitation energies of the first four states of ${}^7_{\Lambda}$ Li for the LO chiral (b) and the Jülich'04 YN interaction (c) compared to the nonstrange parent nucleus 6 Li (a). For the LO chiral YN interaction in panel (b) we use the two cutoff values 600 MeV/*c* (full bars) and 700 MeV/*c* (dashed bars). Experimental data from Refs. [1,2,54]. All calculations use $\alpha_N = 0.08 \text{ fm}^4$, $\alpha_Y = 0.0 \text{ fm}^4$, and $\hbar\Omega = 20 \text{ MeV}$.

leading to a systematically reversed level ordering. This deficiency is already visible for the excited states of the A = 4 hypernuclei [21].

The LO chiral YN interactions employed in Fig. 2(b) provide a consistently better description of the spectra. The ground-state energies obtained for cutoffs 600 and 700 MeV/c are slightly below and above experiment, respectively. The excitation energies exhibit a weaker cutoff dependence, with the cutoff 600 MeV/c yielding slightly lower excitation energies. If we interpret this dependence on the YN cutoff as an estimator for the effects of higher-order terms in the chiral expansion, then we can state that the LO chiral YN interaction gives ground-state and excitation energies that agree with experiment within the truncation uncertainties.

The IT-NCSM also gives access to spectroscopic observables such as transition strengths. As an example we consider the B(E2) strength for the $5/2^+ \rightarrow 1/2^+$ transition in ${}^7_{\Lambda}$ Li, which has been experimentally determined to $B(\text{E2}) = 3.6^{+0.5}_{-0.5}(\text{stat})^{+0.5}_{-0.4}(\text{syst})e^2 \text{ fm}^4$ [55]. For the LO chiral YN interaction with cutoff 600 MeV/c, we obtain B(E2) = 2.3(1) and $2.4(1)e^2 \text{fm}^4$ for $N_{\text{max}} = 10$ and 12, respectively, using $\hbar\Omega = 20$ MeV. The numbers in brackets indicate the uncertainties of the threshold extrapolation [24]. Obviously, convergence of this long-range observable is problematic and a systematic study exploiting the frequency dependence to perform extrapolations is needed. A simpler example is the B(M1) strength for the spin-flip transition $3/2^+ \rightarrow 1/2^+$. We obtain $B(M1) = 0.31(1) \ \mu_N^2$ for $N_{\text{max}} = 10$ and 12, indicating good convergence. This is in excellent agreement with a preliminary experimental value reported in [56].

As a second case we discuss the spectrum of ${}^{9}_{\Lambda}$ Be, as depicted in Fig. 3. The nucleonic parent nucleus ⁸Be is unbound with respect to decay into two α particles, but the IT-NCSM still provides a good description of the groundand excited-state energies in a bound-state approximation. The addition of the hyperon binds the ${}^{9}_{\Lambda}$ Be hypernucleus. Again, the LO chiral YN interactions for cutoff 600 and 700 MeV/c yield different ground-state energies that bracket the experimental value. A peculiarity of ${}^{9}_{\Lambda}$ Be is that the spin doublet resulting from the 2^+ state in ⁸Be is practically degenerate, with the higher-J state being at slightly lower excitation energy experimentally, contrary to the other light hypernuclei. The LO chiral YN interactions reproduce the excitation energy of the doublet and the near degeneracy within threshold extrapolation and convergence uncertainties. In contrast, the Jülich'04 interaction gives a significant splitting of the spin doublet, in contradiction to experiment.

As a final example from the upper *p* shell, we discuss ${}^{13}_{\Lambda}C$ in Fig. 4. The SRG-evolved chiral NN + 3N interaction at $\alpha_N = 0.08$ fm⁴ gives a ground-state energy of the nucleonic parent ${}^{12}C$ about 6 MeV below experiment. This overbinding is related to the emergence of SRG-induced



FIG. 3 (color online). Same as Fig. 2, but for ${}^{9}_{\Lambda}$ Be and 8 Be.

4*N* interactions in the upper *p* shell that are not included in the present calculations (see Refs. [23,24]). The absolute energies of ${}^{13}_{\Lambda}$ C inherit this overbinding; however, taking this into account, the chiral LO interactions are consistent with the experimental ground-state energies within the cutoff uncertainty. Also the excited spin doublet appears at a slightly too low excitation energy since the 2⁺ excited state in 12 C is already too low. The splitting of the spin



FIG. 4 (color online). Same as Fig. 2, but for ${}^{13}_{\Lambda}C$ and ${}^{12}C$. Note the change of scale in the lower panels.

doublet is predicted by the LO chiral YN interactions to be 650 to 700 keV for the largest model spaces. Again, the Jülich'04 YN interaction predicts the opposite level ordering for the doublet. Note that the $5/2^+$ state was not yet observed experimentally, but cluster-model calculations [11] put it below the $3/2^+$ state, in contrast to the LO chiral YN interaction. We also calculated the lowest doublet of unnatural parity states, shown in the lower panels of Fig. 4, which are dominated by a hyperon in a *p* orbit. Neither the chiral nor the Jülich'04 YN interaction can reproduce the near degeneracy of the $1/2^-$ and $3/2^-$ states observed experimentally. This hints at deficiencies in higher partial waves, which are strongly affected by subleading contributions to the chiral YN interactions.

Conclusions.-We have performed the first ab initio calculations for single- Λ p-shell hypernuclei using NCSM approaches with explicit hyperons. After a validation for s-shell hypernuclei, we have studied selected p-shell hypernuclei using Jülich'04 and the LO chiral YN interactions. Within the expected cutoff dependence, the LO chiral YN interactions reproduce the experimental data up to the mid p shell, whereas the Jülich'04 YN interaction systematically gives wrong orderings and splittings of the spin-doublet states. For ${}^{13}_{\Lambda}C$ the situation is unclear, as the 5/2⁺ state is not known experimentally. Neither of the YN interactions describes the first negative-parity doublet correctly, which hints at deficiencies in the higher relative partial waves. This illustrates the potential of systematic *ab initio* studies of *p*-shell hypernuclei for improving our understanding of the YN interaction. In this context, the inclusion and validation of the chiral YN interactions at NLO is highly desirable. At the same time, the impact of SRG-induced and initial chiral YNN interactions needs to be investigated.

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^{*}roland.wirth@physik.tu-darmstadt.de

[†]robert.roth@physik.tu-darmstadt.de

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