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New Horizons in Ab Initio Nuclear Structure Theory

Robert Roth, Joachim Langhammer, Sven Binder, Angelo Calci
Institut für Kernphysik, Technische Universität Darmstadt, 64289 Darmstadt, Germany

Abstract.
Nuclear interactions derived within chiral effective field theory enable nuclear structure and reaction calculations solidly rooted in QCD. Using chiral two- and three-body interactions in ab initio studies of a variety of nuclear observables is, both, promising and challenging. Particularly the inclusion of chiral 3N interactions into exact and approximate many-body calculations is demanding and computationally expensive. We present recent key developments that facilitate ab initio calculations of ground and low-lying excited states of p- and sd-shell nuclei with full 3N interactions in the Importance-Truncated No-Core Shell Model using consistent Similarity Renormalization Group transformations of the NN+3N Hamiltonian. The treatment of 3N interactions without approximations allows for first studies of the dependence of nuclear-structure observables on the details of chiral interactions. Moreover, we present results for heavy nuclei obtained in Coupled Cluster calculations using a normal-ordered two-body approximation of the 3N interaction.

1. Introduction

Chiral effective field theory (EFT) provides the most systematic approach to QCD-based Hamiltonians for nuclear structure calculations today. Starting from nucleons and pions as relevant degrees of freedom and the symmetries of low-energy QCD, chiral EFT provides nuclear two-, three- and higher-body interactions in a consistent way. A remaining challenge is to incorporate these QCD-based Hamiltonians in ab initio nuclear structure and reaction calculations, in order to make precise predictions and compare to experiment to provide feedback for the improvement of chiral EFT.

The most advanced nuclear Hamiltonian from chiral EFT available in terms of matrix elements at the moment consists of a high-precision two-body (NN) interaction at N^3LO [1, 2] along with a chiral three-body (3N) force at N^2LO [3, 4]. Computations are underway to provide matrix elements of the 3N force consistently at order N^3LO [5, 6]. Of course, the direct inclusion of these Hamiltonians into nuclear structure calculations is desirable, however this would require huge, computationally intractable model spaces to account for the strong short-range correlations induced by the bare interaction. One possibility to tame these correlations is to transform the Hamiltonian by means of a unitary transformation in the framework of the so called Similarity Renormalization Group (SRG) [7, 8]. As a result, the transformed Hamiltonians exhibit a improved convergence behavior and facilitate the subsequent many-body calculations. The SRG transformation can be carried out consistently, i.e. without refitting the low-energy constants afterwards. Moreover, it does not depend on the investigated nuclei or the many-body method and model space. In summary, we obtain a universal transformed Hamiltonian and observables with favorable convergence behavior useful for a variety of many-body methods.

In the following we present nuclear structure calculations including the transformed NN+3N interactions for two different many-body methods. One of them is the No-Core Shell Model (NCSM) [9] and its extension the Importance-Truncated No-Core Shell Model (IT-NCSM) [10, 11]. These ab initio methods are applicable for nuclei up to the lower-sd shell and yield ground states as well as low-lying excited states including all relevant observables with exact inclusion of full NN+3N interactions. Since the inclusion of 3N forces is computationally demanding, we have developed new approaches for handling the 3N matrix elements. Together with the importance truncation, this technique permits ab initio calculations for heavier nuclei in much larger model spaces than before.

Beyond the sd shell we use a different many-body method, the Coupled Cluster approach, which is the method of choice especially if one is interested in ground-states of nuclei near closed shells. Instead of the inclusion of the full 3N interaction, we employ the so called Normal-Ordered Two-Body approximation of the 3N interaction. We have benchmarked this approximation extensively and found it to be very accurate, while it reduces the computational cost tremendously. In combination with the coupled cluster approach we can compute nuclear properties including 3N interaction effects even for heavy nuclei.

2. Similarity Renormalization Group with 3N Interactions

The Similarity Renormalization Group (SRG) is one of the most flexible and still simple methods to unitarily evolve the Hamiltonian into band-diagonal form with respect to a chosen uncorrelated many-body basis. The unitary transformation of the Hamiltonian is governed by the so-called flow equation

$$\frac{\mathrm{d}}{\mathrm{d}\alpha} H_\alpha = [\eta_\alpha, H_\alpha] \,, \qquad \eta_\alpha = (2\mu)^2 [T_{\mathrm{int}}, H_\alpha] = -\eta_\alpha^\dagger \,, \tag{1}$$

with η_α as generator of the transformation. Note that this generator itself depends on the continuous flow parameter α. In order to obtain the transformed Hamiltonian (or other consistently transformed observables, e.g. multipole operators or radii), one has to solve a first-order differential equation, which is a rather simple task. The flexibility of the SRG is rooted in the fact that one is completely free in choosing an appropriate generator of the transformation as long as it is antihermitian. In the following we restrict ourselves to the definition of the generator as commutator of the intrinsic kinetic energy T_{int} with the transformed Hamiltonian, which is common in context of nuclear physics, see for example [12]. However, other choices of the generator are possible and under discussion.

We solve the operator equation (1) by converting it into matrix-element representation with respect to a n-body basis. Technically, this results in a system of coupled ordinary differential equations for the matrix elements of the transformed Hamiltonian H_α, which can be solved using standard Runge-Kutta methods. The effect of the SRG transformation on the matrix elements of the NN+3N interaction in the harmonic oscillator Jacobi basis is depicted in Fig. 1. In the left-hand panel we show the initial interaction, i.e. $\alpha = 0\,\mathrm{fm}^4$. The matrix consists of matrix elements with large absolute values even in far off-diagonal regions. The right-hand panel shows the SRG transformed matrix for flow parameter $\alpha = 0.16\,\mathrm{fm}^4$. Clearly, the SRG yields the desired prediagonalization of the matrix, i.e. a decoupling of the high- and low-energy degrees of freedom.

The introduction of the n-body states projects the Fock-space operator equation on the n-body space, i.e. flow-induced operator contributions beyond the n-body level are discarded. Currently, we can account for all many-body contributions up to the three-body level, i.e. we are able to include all two- and three-body terms of the evolved Hamiltonian. In consequence, we can define three different SRG-evolved Hamiltonians which we will distinguish in the discussion of our many-body calculations later on: *(i) NN-only*: we start with an initial NN interaction

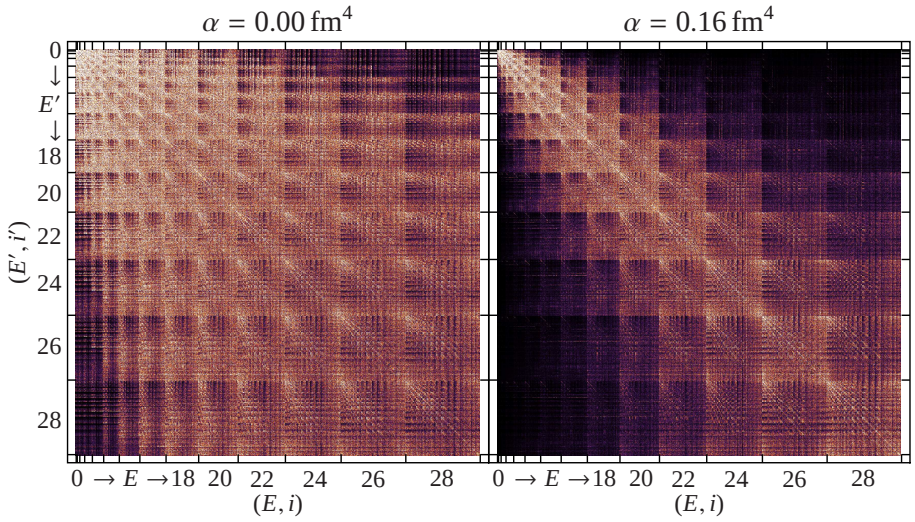

Figure 1. Effect of the SRG evolution on the matrix elements of the NN+3N-full interaction in a three-body harmonic oscillator Jacobi basis. Plotted are the absolute values of the matrix elements, where light colors represent large values and dark colors represent values near zero.

and keep the two-body terms only; *(ii) NN+3N-induced*: we start with an initial NN interaction and keep two- and induced three-body terms; *(iii) NN+3N-full*: we start with an initial NN+3N interaction and keep the two- and all three-body terms.

However, we have to omit all four- and higher-order many-body forces, which are induced during the unitary flow. This truncation formally violates the unitary character of the SRG. To assess the relevance of these neglected contributions we can investigate the dependence of the eigenvalues of the Hamiltonian (or any other observable) on a variation of the SRG flow parameter α. If omitted many-body forces are important, we will detect it after exact many-body calculations by an α-dependence of the energy eigenvalues.

3. Importance Truncated No-Core Shell Model

As a first example we discuss the application of consistently SRG-transformed chiral NN+3N interactions in nuclear-structure calculations for nuclei throughout the p- and lower-sd-shell. To solve the eigenvalue problem of the Hamiltonian, we use the Importance Truncated No-Core Shell Model (IT-NCSM), which was developed in our group [10, 11]. The underlying idea is that a significant part of the NCSM Slater-determinant basis is not required for a proper description of most of the low-lying spectrum of the nuclear Hamiltonian, which is what we are interested in. With help of an *a priori* importance measure, one can quantify the importance of each individual Slater determinant. All states with importance measure below a specific threshold are discarded, and consequently the dimension of the matrix eigenvalue problem is reduced. Nevertheless, after a sequence of IT calculations for a set of threshold values we are able to recover the full NCSM results with an *a posteriori* extrapolation of the desired observables to vanishing threshold [11]. Therefore, we can compute via the IT-NCSM all observables which can be calculated in the NCSM framework. Furthermore, we developed a new handling of the 3N matrix elements, essentially by storing J,T-coupled matrix elements and taking advantage of an efficient on-the-fly decoupling of these matrix elements. It turned out that this new scheme is the key for the inclusion of 3N forces in huge model spaces in particular for nuclei in the upper p-shell and beyond [13].

In Figure 2 we show ground-state energies obtained from IT-NCSM calculations for ^{12}C

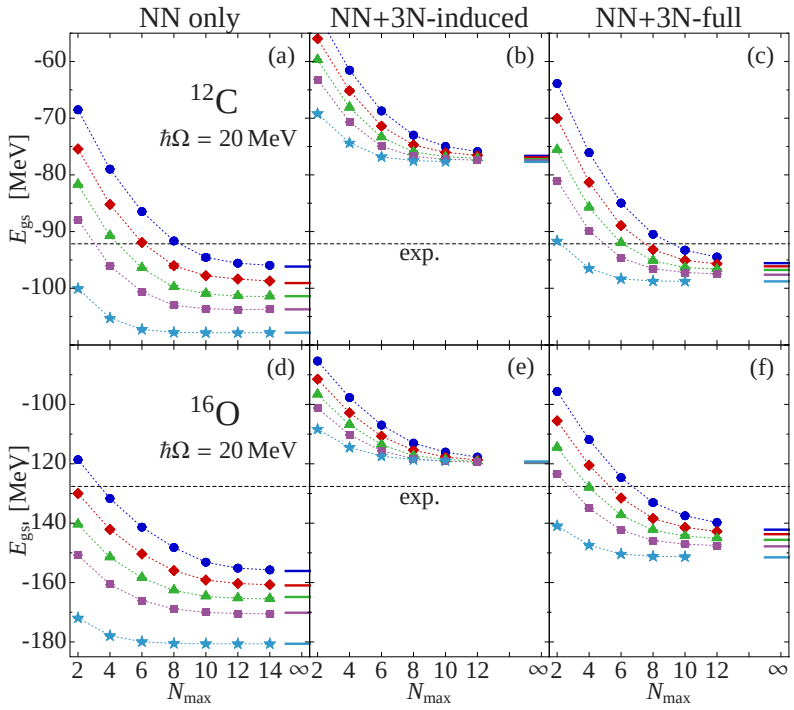

Figure 2. IT-NCSM ground-state energies for ^{12}C and ^{16}O as function of $N_{\max}$ for the three types of Hamiltonians (see column headings) for a set of flow parameters: $\alpha = 0.04\,\mathrm{fm}^4$ (●), $0.05\,\mathrm{fm}^4$ (◆), $0.0625\,\mathrm{fm}^4$ (▲), $0.08\,\mathrm{fm}^4$ (■), and $0.16\,\mathrm{fm}^4$ (★). Taken from Ref. [14].

and ^{16}O for a set of flow parameters α as function of the model space size $N_{\max}$. Due to the importance truncation and the new handling of 3N matrix elements we are able to reach $N_{\max} = 12$ model spaces, which is sufficient to obtain converged ground-state energies for the soft interactions. The left panel shows our results using the NN-only Hamiltonian, i.e. without any 3N force, which show a strong dependence on the SRG flow parameter. This behavior hints at relevant, omitted induced 3N forces. If we include them consistently using the NN+3N-induced Hamiltonian as shown in the middle panel, the α-dependence vanishes. This means the induced higher-order many-body forces coming from the initial two-body force are irrelevant. The resulting ground-state energies are shifted towards less binding and can be seen as the true answer starting from an initial two-body force. The right panel shows the results from the NN+3N-full Hamiltonian, i.e. including the initial 3N force, with a re-emergence of the α-dependence of the ground-state energies. Thus, omitted 4N contributions that are induced during the SRG transformation with the initial 3N interaction have sizeable effects on the ground-state energies of nuclei beyond the lower p-shell [14, 15].

The impact of induced 4N interactions depend on the observables — it is much weaker e.g. for excitation energies. We show in Figure 3 the spectrum of ^{12}C computed with the three different Hamiltonians for two different SRG parameters. Once the spectra are converged with respect to model space size, they do not show a relevant dependence on α. Therefore, benchmarks of the chiral NN+3N forces against experiment are possible through spectroscopic studies in the upper p- and sd-shell, even without the inclusion of SRG-induced 4N forces. Two examples are shown in Figure 4, where we compare the spectrum of ^{12}C obtained with the standard NN+3N-full Hamiltonian to spectra obtained with modified 3N interactions: in the middle panel we use a new set of low-energy constants c_1, c_3 and c_4, which we get by shifting their original values. These

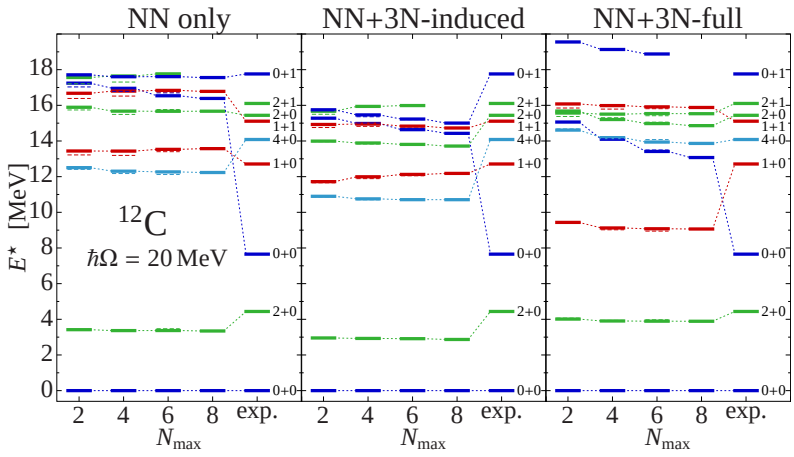

Figure 3. Excitation spectrum for the lowest positive-parity states (labelled $J\pi T$) in ^{12}C for the NN-only, the NN+3N-induced, and the NN+3N-full Hamiltonian with $\alpha = 0.08\,\mathrm{fm}^4$. The thin dashed bars (mostly hidden) show results for $\alpha = 0.0625\,\mathrm{fm}^4$. Taken from Ref. [14].

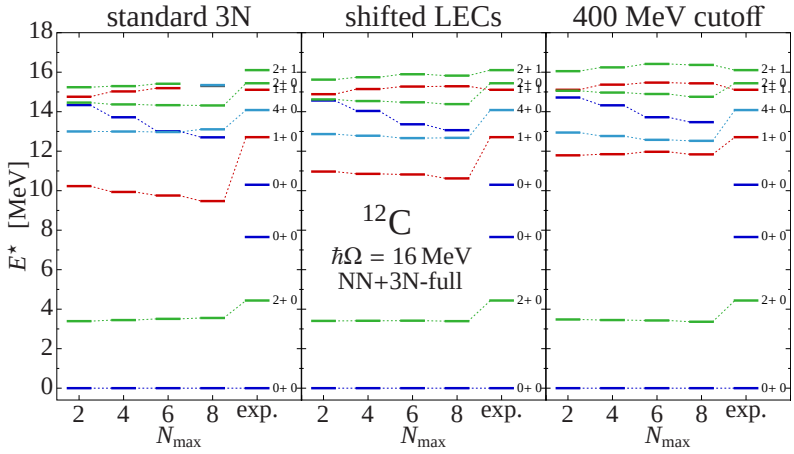

Figure 4. Excitation spectrum for the lowest positive-parity states (labelled $J\pi T$) in ^{12}C using NN+3N-full Hamiltonians with different chiral 3N interactions at $\alpha = 0.08\,\mathrm{fm}^4$. In the left panel using the standard initial 3N interaction, in the middle with shifted low-energy constants c_i for the initial 3N interaction and in the right panel using a modified 3N interaction with cutoff 400 MeV.

shifts are motivated and specified in Ref. [16]. We observe only minor changes in the excitation energies of most of the states, except for the first 1^+ state. In the right panel we show the ^{12}C spectrum resulting from an initial 3N interaction with reduced cutoff $\Lambda = 400\,\mathrm{MeV}$. Again the first 1^+ state is most sensitive to this cutoff variation. Note that we refit the low-energy constant c_E to the ^{4}He binding energy. These studies motivate a more detailed sensitivity analysis of nuclear spectra in this mass range, e.g. with respect to the low-energy constants and the cutoff of the initial 3N force [17].

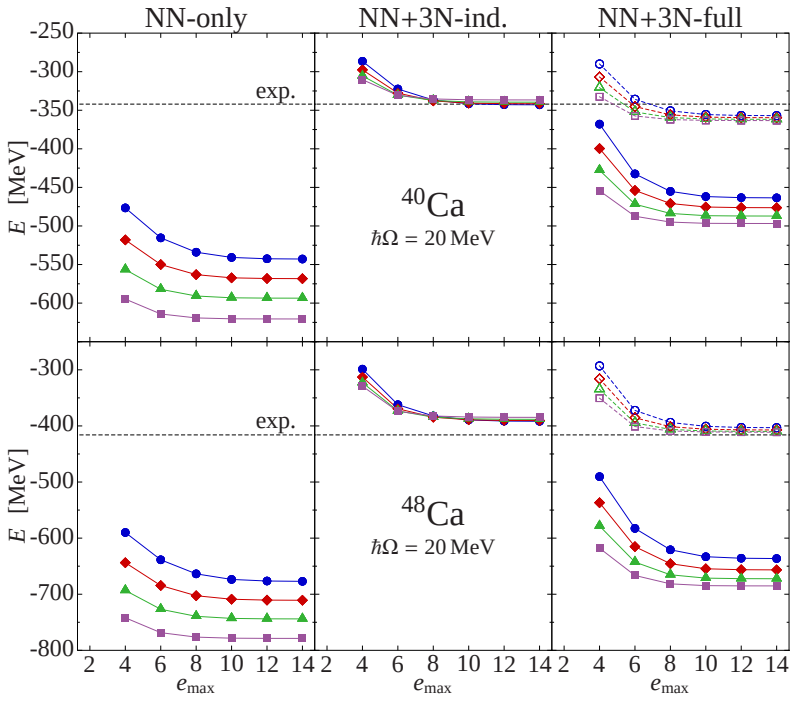

Figure 5. CCSD ground-state energies for ^{40}Ca and ^{48}Ca computed for the three types of Hamiltonians using the NO2B approximation for a set of flow parameters: $\alpha = 0.04\,\mathrm{fm}^4$ (●), $0.05\,\mathrm{fm}^4$ (◆), $0.0625\,\mathrm{fm}^4$ (▲), and $0.08\,\mathrm{fm}^4$ (■). Filled symbols for the NN+3N-full Hamiltonian are for the standard chiral 3N interaction with cutoff 500 MeV, the open symbols for a modified 3N interaction with cutoff 400 MeV. Taken from Ref. [15].

4. Coupled Cluster Theory

Beyond nuclei of the sd-shell our method of choice for studies of the SRG-evolved chiral NN+3N interactions is Coupled Cluster Theory, which is a standard technique in quantum chemistry. For our nuclear studies we employ the Coupled Cluster Singles and Doubles (CCSD) approximation [18], which eventually can be improved using the non-iterative ΛCCSD(T) correction for the energy [20, **?**]. We include the 3N interactions using the so-called Normal-Ordered Two-Body (NO2B) approximation. We benchmarked this approximation extensively by comparing it to results obtained using the exact 3N force and found remarkably good agreement at the order of 1% for ground-state energies [15]. Computationally, the benefit of this NO2B approximation is that we have to handle two-body terms only, which decreases the computational cost significantly.

Exemplarily, we show in Figure 5 ground-state energies for ^{40}Ca and ^{48}Ca obtained from CCSD calculations, for the first time including effects of chiral 3N forces. The flow-parameter dependence of the energies computed with the NN+3N-full Hamiltonian confirms the relevance of induced 4N forces for heavier nuclei. Moreover, the open symbols correspond to calculations using the initial 3N force with lowered cutoff of 400 MeV leading to a much weaker α dependence. This offers the possibility to test chiral NN+3N Hamiltonians in ab initio calculations throughout the nuclear chart using the NO2B approximation alongside with CCSD.

5. Conclusions

We have discussed our recent progress regarding the consistent SRG-transformation of NN+3N Hamiltonians, the handling of matrix-elements of 3N forces, and their use in IT-NCSM and CCSD approaches for ab initio studies with chiral NN+3N interactions. This paves the way for extensive studies of the spectroscopy of p- and sd-shell nuclei and their sensitivity to details of the chiral forces, e.g. low-energy constants or cutoffs. Furthermore, ab initio predictions of binding energies including the effects of 3N forces are now possible even for medium mass nuclei, which is crucial in particular in the region of drip lines. In parallel we are working on the implementation of 3N forces into the formalism of the NCSM combined with the Resonating Group Method, which enables ab initio predictions of scattering and reactions of light nuclei. Together, these advances establish new horizons in ab initio nuclear structure and reaction theory and lead into an era of precise QCD-based low-energy nuclear theory.

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References

[1] Entem D R and Machleidt R 2003 *Phys. Rev. C* **68** 041001(R)
[2] Epelbaum E, Glöckle W and Meißner U G 2005 *Nucl. Phys. A* **747** 362
[3] Epelbaum E, Nogga A, Glöckle W, Kamada H, Meißner U G and Witala H 2002 *Phys. Rev. C* **66** 064001
[4] Navratil P 2007 *Few Body Syst.* **41** 117
[5] Bernard V, Epelbaum E, Krebs H and Meißner U G 2008 *Phys. Rev. C* **77** 064004
[6] Bernard V, Epelbaum E, Krebs H and Meissner U G 2011 *Phys. Rev. C* **84** 054001
[7] Roth R, Neff T and Feldmeier H 2010 *Prog. Part. Nucl. Phys.* **65** 50
[8] Bogner S K, Furnstahl R J and Schwenk A 2010 *Prog. Part. Nucl. Phys.* **65** 94
[9] Navrátil P, Quaglioni S, Stetcu I and Barrett B 2009 *J. Phys. G: Nucl. Part. Phys.* **36** 083101
[10] Roth R and Navrátil P 2007 *Phys. Rev. Lett.* **99** 092501
[11] Roth R 2009 *Phys. Rev. C* **79** 064324
[12] Bogner S K, Furnstahl R J and Perry R J 2007 *Phys. Rev. C* **75** 061001(R)
[13] Roth R, Calci A, Langhammer J and Binder S, in prep.
[14] Roth R, Langhammer J, Calci A, Binder S and Navrátil P 2011 *Phys. Rev. Lett.* **107** 072501
[15] Roth R, Binder S, Vobig K, Calci A, Langhammer J and Navrátil P 2012 *Phys. Rev. Lett.* **109** 052501
[16] Skibiński R, Golak J, Topolnicki K, Witała H, Epelbaum E, Glöckle W, Krebs H, Nogga A and Kamada H 2011 *Phys. Rev. C* **84** 054005
[17] Roth R, Langhammer J, Calci A and Binder S, in prep.
[18] Hagen G, Papenbrock T, Dean D J and Hjorth-Jensen M 2010 *Phys. Rev. C* **82** 034330
[19] Taube A G and Bartlett R J 2008 *J. Chem. Phys.* **128** 044110
[20] Taube A G and Bartlett R J 2008 *J. Chem. Phys.* **128** 044111