# Momentum-space evolution of chiral three-nucleon forces

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# Momentum space evolution of chiral three-nucleon forces

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A framework to evolve three-nucleon (3N) forces in a plane-wave basis with the Similarity Renormalization Group (SRG) is presented and applied to consistent interactions derived from chiral effective field theory at next-to-next-to-leading order ($N^2LO$). We demonstrate the unitarity of the SRG transformation, show the decoupling of low and high momenta, and present the first investigation of universality in chiral 3N forces at low resolution scales. The momentum-space-evolved 3N forces are consistent and can be directly combined with the standard SRG-evolved two-nucleon (NN) interactions for ab-initio calculations of nuclear structure and reactions.

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The interplay of chiral effective field theory (EFT) and Renormalization Group (RG) methods offers new opportunities for efficient and simplified microscopic calculations of many-body systems based on systematically derived nuclear forces [1, 2]. Recent applications range from calculations of finite nuclei [3–7] to infinite nucleonic systems [8, 9] to astrophysical applications [10]. A key challenge in all of these cases is the control of many-body forces. In this letter we present a new tool to address this challenge, the RG evolution of 3N forces in a plane-wave basis (see Fig. 1), which we use to explore universality in the evolved chiral 3N forces (see Fig. 4).

The SRG provides a framework to construct unitary transformations that consistently renormalize all operators, including many-body forces, while preserving low-energy observables [11, 12]. Wegner's formulation of the SRG is a continuous series of unitary transformations of the Hamiltonian $H = T_{\rm rel} + V$ as a function of the flow parameter $s$:

$$\frac{dH_s}{ds} = [\eta_s, H_s] \ . \tag{1}$$

Here $\eta_s$ specifies the unitary transformation, $T_{\rm rel}$ denotes the relative kinetic energy and $V$ all the interparticle interactions. In the following we make the common choice $\eta_s = [T_{\rm rel}, H_s]$, which generates transformations that lead to a decoupling of low and high momenta in NN interactions as they are evolved to lower resolution scales [13]. Such an evolution leads to much less correlated wave functions at low resolution and the nuclear many-body problem becomes more perturbative.

In recent RG-based calculations, two different strategies have been used to handle the 3N forces. Starting from nuclear NN and 3N forces, derived and fitted in chiral EFT, it is possible to systematically evolve the full Hamiltonian. So far, this has been achieved by representing Eq. (1) using a discrete harmonic oscillator basis [14]. Results for light nuclei based on such evolved interactions are promising [3]. For heavier nuclei however, significant

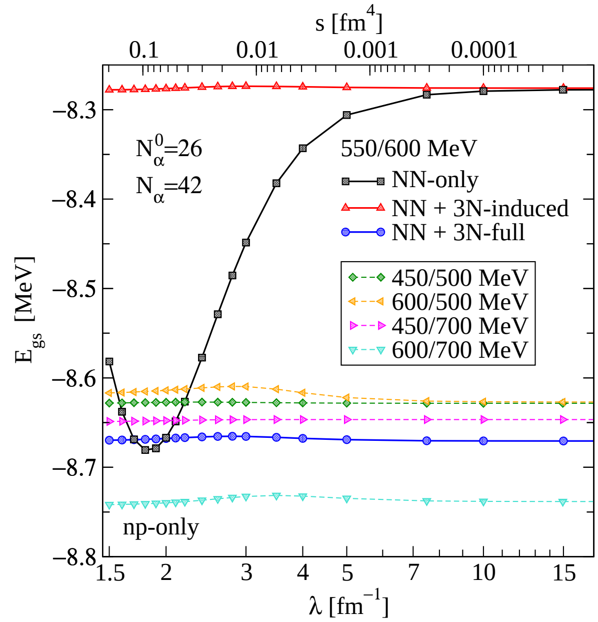


FIG. 1. (Color online) Ground state energy of $^3$H as a function of the flow parameter $\lambda = s^{-1/4}$ for different chiral interactions at $N^2LO$, which are labeled by the value of the cutoffs $\Lambda/\tilde{\Lambda}$ (see Ref. [19]). The solid lines show the results for $\Lambda/\tilde{\Lambda} = 550/600$ MeV separately for NN-only, NN+3N-induced and NN+3N-full (see Ref. [14]). The dashed lines show the NN+3N-full results for the other given values of $\Lambda/\tilde{\Lambda}$. Only *np* NN interactions have been used.

scale dependencies have been found [4, 15], which suggest that infinite matter will not be realistic. These could be indications of significant induced 4N forces or of an insufficient evolution of 3N forces due to basis truncations.

An alternative strategy has been used for calculations of infinite nuclear systems [9] (and elsewhere [5, 6]). Instead of fitting the 3N forces at the chiral EFT cutoff scale, only the NN interactions have been evolved with RG methods and then the short-range parameters of the $N^2LO$ 3N forces have been determined from fits to few-body systems at the low-momentum scale. This procedure assumes that the long-range part of the 3N forces remains invariant under the RG transformations and that

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the N$^2$LO operator structure is a sufficiently complete operator basis that induced contributions can be absorbed to good approximation. The results from this procedure are found to be in agreement with nuclear phenomenology within the theoretical uncertainties [8, 9]. However, these results do not imply that induced 3N forces have the same structure as chiral N$^2$LO 3N interactions.

A complementary evolution of nuclear many-body forces using the SRG in a momentum plane-wave basis would allow us to reconcile the seemingly inconsistent results of these strategies. In this letter, we report the first results for the evolution with Eq. (1) of realistic nuclear NN and 3N forces in such a basis. A similar approach has been used recently for the evolution of bosonic interaction models in one dimension [16]. As we will discuss below, however, the coupling of partial waves makes the RG evolution more challenging in three dimensions.

We adopt the notation and conventions of Ref. [13] and write the interaction in the form $V_s = V_{12} + V_{13} + V_{23} + V_{123}$ and the kinetic energy as $T_{\rm rel} = T_{12}+T_3 = T_{13}+T_2 = T_{23}+T_1$. Here $V_{ij}$ denotes NN interactions between particle $i$ and $j$ and $V_{123}$ the irreducible three-body potential. The kinetic energy terms $T_{jk}$ and $T_i$ correspond to the contributions of the Jacobi momenta $p_i$ and $q_i$, respectively. We recast Eq. (1) as separate RG flow equations for the two- and three-body interactions [13]:

$$\frac{dV_{ij}}{ds} = \left[\left[T_{ij}, V_{ij}\right], T_{ij} + V_{ij}\right], \tag{2}$$

$$\begin{aligned}\frac{dV_{123}}{ds} &= \left[\left[T_{12}, V_{12}\right], V_{13} + V_{23} + V_{123}\right] \\ &\quad + \left[\left[T_{13}, V_{13}\right], V_{12} + V_{23} + V_{123}\right] \\ &\quad + \left[\left[T_{23}, V_{23}\right], V_{12} + V_{13} + V_{123}\right] \\ &\quad + \left[\left[T_{\rm rel}, V_{123}\right], H_s\right].\end{aligned} \tag{3}$$

Compared to Eq. (1), this system of differential equations has the important advantage that terms resulting from spectator particles in two-body interaction processes have been eliminated explicitly. In a momentum basis, the spectator particles lead to delta functions that make the representation of Eq. (1) problematic [17].

The flow equation (2) is solved in a two-body basis and then embedded in Eq. (3) by using

$$V_{12} = P_{132} V_{23} P_{132}^{-1}, \quad V_{13} = P_{123} V_{23} P_{123}^{-1}. \tag{4}$$

Here $P_{123} = P_{12}P_{23}$ ($P_{132} = P_{13}P_{23}$) permutes three particles cyclically (anti-cyclically) with $P_{ij}$ denoting two-particle transpositions. We represent Eq. (2) in a standard partial-wave basis of the form $|p;(LS)JT\rangle$, where $L$, $S$, $J$ and $T$ denote the orbital angular momentum, spin, total angular momentum and isospin of the interacting pair of particles with relative momentum $p$. For the three-body basis we choose [17, 18]

$$|pq\alpha\rangle_i \equiv |p_i q_i; \left[(LS)J(ls_i)j\right] \mathcal{J}\mathcal{J}_z (Tt_i)\mathcal{T}\mathcal{T}_z\rangle\,, \tag{5}$$

where $p_i$ and $q_i$ denote the three-body Jacobi momenta of particle $i$. The quantum numbers $l$, $s_i = 1/2$, $j$ and $t_i = 1/2$ label the orbital angular momentum, spin, total angular momentum and isospin of particle $i$ relative to the center-of-mass of the pair with momentum $p$. $\mathcal{J}$ and $\mathcal{T}$ denote the total three-body angular momentum and isospin, which are equal to $1/2$ in the three-nucleon bound states. For details we refer the reader to Refs. [17, 18]. The basis states (5) are not completely antisymmetric. It is most natural to evolve the antisymmetrized interaction

$$\langle pq\alpha|\overline{V}_{123}|p'q'\alpha'\rangle \equiv {}_i\langle pq\alpha|\mathcal{A}_{123} V_{123}^{(i)} \mathcal{A}_{123}|p'q'\alpha'\rangle_i\,, \tag{6}$$

with $\mathcal{A}_{123} = (1 + P_{123} + P_{132})$ and $V_{123}^{(i)}$ being the $i$-th Faddeev component of the three-body interaction [17].

We solve Eqs. (2) and (3) for a set of five different initial NN and 3N interaction potentials derived from chiral EFT at next-to-next-to-leading order (N$^2$LO) [19]. The 3N forces low energy constants $c_D$ and $c_E$ have been fitted for five different cutoff combinations $\Lambda$ and $\tilde{\Lambda}$ to the $^3$H binding energy and the $nd$ doublet scattering length $^2a_{np}$ [19, 20]. For this first exploratory work we represent the initial Hamiltonian at $s = 0$ in a basis with $N_\alpha^0 = 26$ three-body partial-wave channels ($J \leq 3$). The corresponding ground state energies are shown in Fig. 1. They are found to be within 12 keV of the converged values based on the antisymmetrized interaction (6). We neglect the effects of charge symmetry breaking, i.e., we use the neutron-proton interaction in all isospin channels of the NN force. Due to this we obtain ground state energies that are about 150–260 keV more bound than

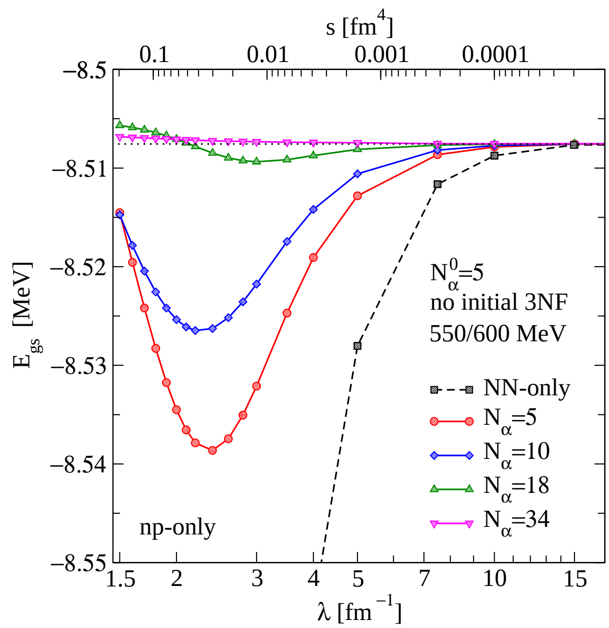


FIG. 2. (Color online) Ground state energy of $^3$H as a function of the flow parameter $\lambda = s^{-1/4}$ for different SRG model space sizes $N_\alpha$ and a fixed model space for the initial Hamiltonian $N_\alpha^0 = 5$ (for a detailed definition of the 3N channels see Ref. [17]). The dotted line shows the energy at $\lambda = \infty$. Only $np$ NN interactions have been used.

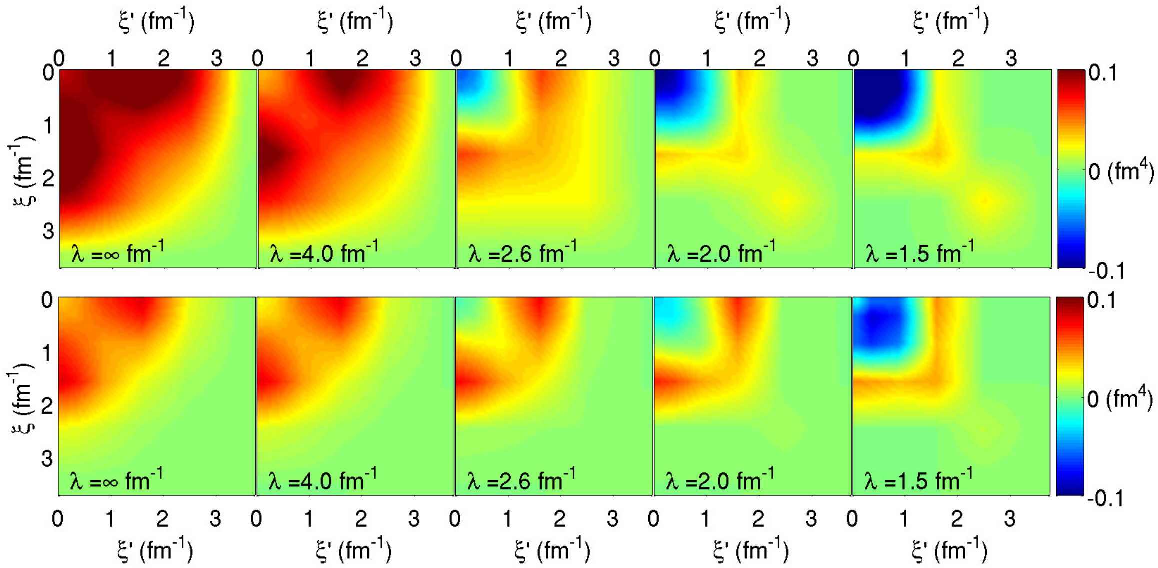


FIG. 3. (Color online) Contour plots of the evolved 3N potential $\langle \xi\, \alpha = 1 | \overline{V}_{123} | \xi'\, \alpha' = 1 \rangle$ at the hyperangle $\theta = \pi/12$ (see Ref. [17] for definition of partial waves). The upper panel shows the potential with $\Lambda/\tilde{\Lambda} = 550/600$ MeV and the lower panel $\Lambda/\tilde{\Lambda} = 450/500$ MeV.

the experimental value $E_{\rm gs} = -8.481821(5)$ [21] for all studied potentials. For future applications it will be possible to incorporate the charge dependence of the nuclear interactions, as well the Coulomb potential, in the flow equations.

The SRG evolution is performed in a larger model space with $N_\alpha = 42 > N_\alpha^0$ channels ($J \leq 5$). This basis size is also used for the solutions of the Faddeev equations at the different resolution scales. As can be seen in Fig. 1, the ground state energy is not perfectly invariant under the RG transformations. This is because a finite basis of the form (5) is not complete under cyclic and anticyclic permutations of particles, as the permuation operator ${}_i\langle pq\alpha | P_{ijk} | p'q'\alpha' \rangle_i$ couples in general all partial waves $\alpha$ and $\alpha'$ [17, 18]. As a consequence, non-vanishing matrix elements in all three-body partial waves are induced when two-body operators are embedded in a three-body momentum basis (5) via Eq. (4). This problem is absent in one dimension [16] or in a discrete oscillator basis [14], where the permutation operator is block-diagonal in a given model space of size $N_{\rm max}$. The violation of unitarity is correlated with the value of the cutoff values $\Lambda/\tilde{\Lambda}$. For intermediate values $\Lambda/\tilde{\Lambda} = 550/600$ MeV we find a maximal variation of 5 keV of the ground state energy, compared to about 400 keV if induced 3N forces are completely neglected. For small values $\Lambda = 450$ MeV the variation is even smaller ($\leq 2$ keV), whereas for $\Lambda = 600$ MeV it is about 16 keV. This is natural since high momentum modes couple stronger with higher partial waves under permutation of particles. A signifcant part of the variations for large $\Lambda$ results from an insufficient antisymmetrization of the initial 3N forces based on a partial-wave representation of $\mathcal{A}_{123}$ (see Eq. (6)). For future applications it will be possible to optimize the evolution by using exactly antisymmetrized initial 3N forces (see Refs. [22, 23]).

The RG evolution can be improved systematically by increasing the model space size $N_\alpha$. This is demonstrated in Fig. 2. For illustrative purposes we restrict the initial Hamiltonian at $s = 0$ to a small model space with $N_\alpha^0 = 5$ channels, which includes the ${}^1$S$_0$ and ${}^3$S$_1$-${}^3$D$_1$ pair partial waves (see Ref. [17]). The figure shows the triton ground state energy for different SRG model space sizes $N_\alpha$ as a function of the resolution. For the largest basis size shown, the resolution dependence is smaller than 1 keV, in contrast to about 30 keV for the smallest basis.

Low-resolution NN interactions have been found to be quantitatively very similar [2, 13]. This universality can be attributed to common long-range pion physics and phase-shift equivalence of all potentials, which is reflected in the matrix elements at low resolution. It is an interesting question if the same is true for 3N forces since there are important differences: First, 3N forces are fixed by fitting only two low-energy constants $c_D$ and $c_E$, in contrast to numerous couplings in NN interactions. Second, 3N forces give only subleading contributions to observables. Since universality is only approximate in NN interactions, it is not obvious to what extent 3N forces are constrained by long-range physics at low resolution.

In Fig. 3 we show representative examples of 3N forces matrix elements at different resolution scales. To do so we introduce the hyperradius $\xi = p^2 + 3/4q^2$ and the hyperangle $\tan\theta = 2p/(\sqrt{3}q)$ and choose an arbitrary value $\theta = \pi/12$. The upper panel shows the matrix elements of the channel $\alpha = \alpha' = 1$ for $\Lambda/\tilde{\Lambda} = 550/600$ MeV and the lower panel for $\Lambda/\tilde{\Lambda} = 450/500$ MeV. At large resolution

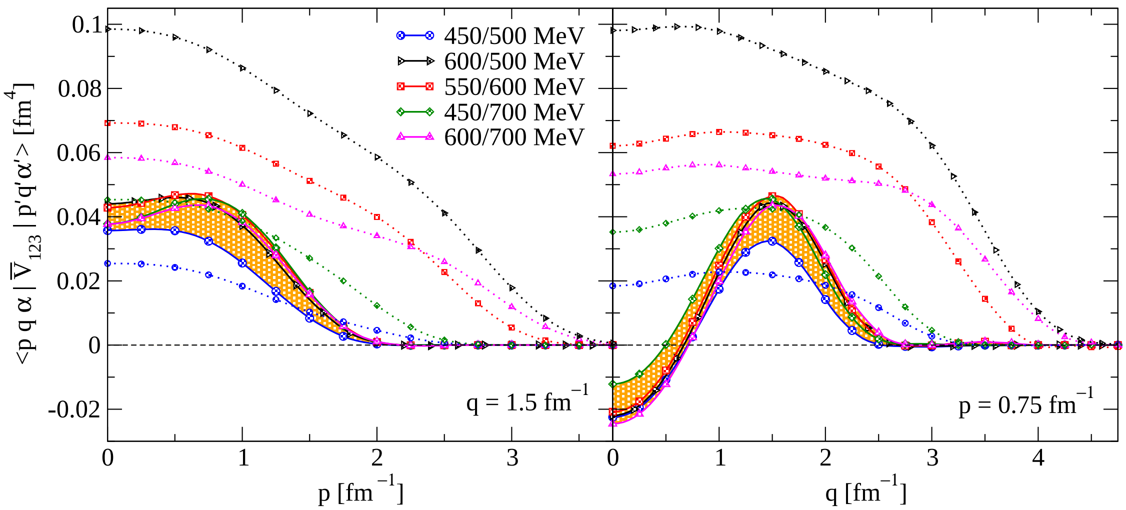


FIG. 4. (Color online) Matrix elements of the initial 3N forces (dotted lines) compared to evolved 3N forces (solid lines) at $\lambda = 1.5\,\mathrm{fm}^{-1}$ for different interactions labeled by the values of the cutoffs $\Lambda/\tilde{\Lambda}$. We choose $p' = 1.0\,\mathrm{fm}^{-1}$, $q' = 1.25\,\mathrm{fm}^{-1}$ and $\alpha = \alpha' = 2$ (see Ref. [17]). In the left panel we fixed $q = 1.5\,\mathrm{fm}^{-1}$ and in the right panel $p = 0.75\,\mathrm{fm}^{-1}$. The shaded band marks the maximal variation between different evolved 3N force matrix elements.

scales $\lambda = \infty$ ($s = 0$) the off-diagonal couplings are much stronger for larger cutoffs $\Lambda$ and the potential is in general more repulsive. As we evolve to lower resolution, the repulsive off-diagonal couplings get successively suppressed and finally at $\lambda = 1.5\,\mathrm{fm}^{-1}$ we find matrix elements of significant size only below $\xi, \xi' \lesssim 2\,\mathrm{fm}^{-1}$ and around the diagonal $\xi \simeq \xi'$. These features are general and hold for matrix elements at all hyperangles and partial waves. In addition, the overall effects of the SRG evolution are stronger for initial potentials with large cutoffs $\Lambda/\tilde{\Lambda}$. In summary, the evolved 3N matrix elements show the same tendencies found in evolved matrix elements of NN interactions [13].

In Fig. 4 we show in more detail initial and low-resolution ($\lambda = 1.5\,\mathrm{fm}^{-1}$) matrix elements for $\alpha = \alpha' = 2$ (see Ref. [17]) at some typical fixed momenta $p', q' \sim 1\,\mathrm{fm}^{-1}$ for all five different chiral interactions. We find a remarkably reduced model dependence for evolved interactions in this kinematical region. We find that this approximate collapse of matrix elements is most pronounced in the 3N channels in which the three-body contact interaction $c_E$ contributes ($\alpha, \alpha' = \{1, 2\}$). This suggests that the coupling constant $c_E$ is flowing to an approximately universal value at low resolution. In addition, new momentum-dependent universal structures are induced at low resolution, as can be seen in the right panel. If one or more momenta becomes very small the model dependence of the matrix elements tends to become larger. However, the phase space of these matrix elements is suppressed and are less relevant for physical observables. We emphasize that all these observations are based on initial potentials that have been derived at $\mathrm{N^2LO}$ in chiral EFT. At this order, phase shifts at higher energies are not as well described as at $\mathrm{N^3LO}$, which reduces the degree of universality of NN interactions at low resolution. It will be very interesting to investigate if universality of 3N forces becomes more pronounced by including contributions at $\mathrm{N^3LO}$ [24, 25].

The low-resolution interactions derived here are ideal for microscopic calculations of nuclear systems. Evolution in a momentum basis has several advantages compared to a discrete oscillator basis. First, the oscillator basis has intrinsic infrared and ultraviolet cutoffs that depend on the basis size and oscillator parameter $\hbar\Omega$ [3], which lead to convergence issues for 3N forces. The problems can be avoided by first evolving in momentum space and then using a straightforward transformation to an oscillator basis with *any* $\hbar\Omega$. This enables new tests of SRG interactions in finite nuclei within the no-core-shell model [26] and coupled cluster [27] that allow systematic studies of the role of induced 4N forces. Second, the momentum-space interactions can be used directly in calculations of infinite systems within many-body perturbation theory. This will test whether consistently evolved NN plus 3N forces, initially fit only to few-body properties, predict empirical nuclear saturation properties within theoretical errors, as found previously for evolved NN forces combined with fitted 3N forces [9].

Finally, since SRG transformations are usually characterized by the coupling of momentum eigenstates, the momentum basis is a natural basis in which to construct the SRG generator $\eta_s$. In particular, momentum-diagonal generators such as $T_{\mathrm{rel}}$ (as chosen here) can be implemented very efficiently in a momentum basis and it is straightforward to generalize to the Hamiltonian-diagonal form advocated by Wegner [12]. Other generators can significantly improve the efficiency of the RG evolution [28] or achieve alternative RG decoupling patterns, such as a flow towards a block-diagonal Hamiltonian [29]. The possibility of using the generator to suppress the growth of many-body forces is also under active investigation.


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[1] E. Epelbaum, H.-W. Hammer and U.-G. Meissner, Rev. Mod. Phys. **81**, 1773 (2009).
[2] S. K. Bogner, R. J. Furnstahl and A. Schwenk, Prog. Part. Nucl. Phys. **65**, 94 (2010).
[3] E. D. Jurgenson, P. Navratil and R. J. Furnstahl, Phys. Rev. C **83**, 034301, (2011).
[4] R. Roth *et al.*, Phys. Rev. Lett. **107**, 072501 (2011).
[5] T. Otsuka *el al.*, Phys. Rev. Lett. **105**, 032501 (2010).
[6] J. D. Holt *et al.*, arXiv:1009.5984.
[7] S. Bacca *et al.* Phys. Rev. Lett. **102**, 162501 (2009).
[8] K. Hebeler and A. Schwenk, Phys. Rev. C **82**, 014314 (2010).
[9] K. Hebeler *et al.*, Phys. Rev. C **83**, 031301(R) (2011).
[10] K. Hebeler *et al.* Phys. Rev. Lett. **105**, 161102 (2010).
[11] S. D. Glazek and K. G. Wilson, Phys. Rev. D **48**, 5863 (1993).
[12] F. Wegner, Ann. Phys. (Leipzig) **3**, 77 (1994).
[13] S. K. Bogner, R. J. Furnstahl and R. J. Perry, Phys. Rev. C **75**, 061001(R) (2007).
[14] E. D. Jurgenson, P. Navratil and R. J. Furnstahl, Phys. Rev. Lett. **103**, 082501 (2009).
[15] R. Roth *et al.*, arXiv:1112.0287.
[16] O. Akerlund *et al*, Eur. Phys. J. A **47**, 122 (2011).
[17] W. Glöckle, *The Quantum Mechanical Few-Body Problem* (Springer-Verlag, Berlin, 1983).
[18] A. Stadler, W. Glöckle and P. U. Sauer, Phys. Rev. C **44**, 2319 (1991).
[19] E. Epelbaum, Prog. Part. Nucl. Phys. **57**, 654 (2006).
[20] E. Epelbaum, private communication.
[21] G. Audi and A. H. Wapstra, Nucl. Phys. A **595**, 409 (1995).
[22] J. Golak *et al.*, Eur. Phys. J. A **43**, 241 (2010).
[23] R. Skibinski *et al.*, Eur. Phys. J **47**, 48 (2011).
[24] V. Bernard *et al.*, Phys. Rev. C **77**, 064004 (2008).
[25] V. Bernard *et al.*, Phys. Rev. C **84**, 054001 (2011).
[26] P. Navratil *et al.* J. Phys. G **36**, 083101 (2009).
[27] G. Hagen *et al.* Phys. Rev. C **76**, 034302 (2007).
[28] W. Li, E. R. Anderson and R. J. Furnstahl, Phys. Rev. C **84**, 054002 (2011).
[29] E. Anderson *et al.*, Phys. Rev. C **77**, 037001 (2008).