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Local Two- and Three-Nucleon Chiral Interactions

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Abstract Understanding the structure and reactions of nuclei from first principles has been a long-standing goal of nuclear physics. In this respect, few- and many-body systems provide a unique laboratory for studying nuclear interactions. In the past couple of decades, the modeling of nuclear interactions has progressed significantly owing, in particular, to the development of chiral effective field theory (χ EFT), a low-energy effective representation of quantum chromodynamics. Within χ EFT, many studies have dealt with the construction of both two- and three-nucleon interactions. The aim of the present article is to provide a concise account of chiral interaction models that are local in configuration space, and to report on a selection of recent results for nuclear systems obtained with these interactions.

1 Introduction

The modeling of nuclei as systems of nucleons (protons and neutrons) interacting with each other via effective forces and with external electroweak probes via effective currents has a long and venerable history. We refer to it as the basic model of nuclear physics. When combined with accurate methods to solve the many-body Schrödinger equation, the basic model presents us with the opportunity and challenge to understand and explain nuclear structure and reactions in terms of the underlying dynamics of interacting nucleons. A calculation carried out in such a framework is commonly referred to as an *ab-initio* one. Examples of *ab initio* calculations are those based on the no-core shell model (NCSM) $[1,2]$ $[1,2]$, the coupled cluster (CC) $[3,4]$ $[3,4]$ $[3,4]$ or hyperspherical harmonics (HH) [\[5](#page-5-4)] expansions, similarity renormalization group (SRG) approaches [\[6,](#page-5-5)[7](#page-6-0)], self-consistent Green's function techniques [\[8](#page-6-1),[9\]](#page-6-2), quantum Monte Carlo (QMC) methods [\[10](#page-6-3),[11\]](#page-6-4), and nuclear lattice effective field theory (NLEFT) [\[12\]](#page-6-5). While significant progress has been made in recent years, enabled by advances in the input nuclear interactions and currents based on chiral effective field theory (χ EFT), improved and novel many-body frameworks, and increasingly powerful computer facilities, these *ab initio* calculations remain challenging and their domain of applicability is, at present, limited to provide a quantitative description of light and medium-mass nuclei $[1,4,7-11,13]$ $[1,4,7-11,13]$ $[1,4,7-11,13]$ $[1,4,7-11,13]$ $[1,4,7-11,13]$ $[1,4,7-11,13]$ and their reactions $[14-17]$ $[14-17]$. The main challenge is to describe diverse physical phenomena within a single coherent picture. The reasons are twofold. First, at the moment, there exist no interactions and electroweak currents which are able to correctly predict, simultaneously, different nuclear few- and many-body observables over a wide range of mass number, including infinite matter, within quantified theoretical uncertainties. This can be probably traced back to fundamental questions regarding

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inconsistencies in the derivation and implementation of nuclear interactions and current operators, and the complexity of the optimization procedures needed for estimating the parameters entering the nuclear models. Second, the difficulty in the solution of the nuclear many-body problem is exacerbated by limitations inherent to the different many-body frameworks utilized for atomic nuclei and nuclear matter. These drawbacks include the scaling behavior as a function of mass number, the convergence of observables as a function of basis states, the validity of many-body truncations, and constraints regarding which nuclear interactions can be used. A special but related challenge is the development, within the basic model, of approaches accounting for the coupling to the continuum—these are mandatory to describe, for instance, weakly bound nuclear systems [\[18](#page-6-9)[,19](#page-6-10)].

Of course, nucleons are composite particles, and it could be argued that an understanding of nuclei that is truly fundamental can only be realized on the basis of approaches explicitly (as opposed to effectively) accounting for the dynamics of quarks and gluons, the degrees of freedom of Quantum Chromodynamics (QCD). Such approaches, which are computationally very demanding, attempt to solve the nuclear many-body problem on a discretized (Euclidean) space-time lattice. Albeit there have been many advances [\[20](#page-6-11)[–23\]](#page-6-12), lattice QCD calculations are still limited to small nucleon numbers and/or large pion masses, and hence, at the present time, can only be used to address a limited set of representative key-issues. As a consequence, most theoretical studies of nuclear systems must turn to the basic model to address the full complexity of the nuclear many-body problem.

2 Nuclear Interactions

The basic model assumes that a Hamiltonian consisting of non-relativistic kinetic energy, and two-nucleon (2*N*) and three-nucleon (3*N*) interaction, provides a good approximation to the energy of interacting nucleons.

Two-nucleon interactions are characterized by a long-range component, due to one-pion exchange (OPE) [\[24\]](#page-6-13), for inter-nucleon separation $r \gtrsim 2$ fm, and intermediate- and short-range components for 1 fm \lesssim $r \le 2$ fm and $r \le 1$ fm, respectively. Up until the mid-1990's, these interactions [\[25](#page-6-14)[–27\]](#page-6-15) were based essentially on meson-exchange phenomenology, with parameters characterizing the short- and intermediaterange components that were constrained by fits to the 2*N* elastic scattering data up to lab energies of 350 MeV (that is, slightly above the threshold for pion production). The χ^2 /datum achieved in these fits was close to 1 relative to the database available at the time [\[28](#page-6-16)]. Two well-known, and still widely used, examples in this class of phenomenological 2*N* interactions are the Argonne v_{18} (AV18) [\[26](#page-6-17)] and CD-Bonn [\[27](#page-6-15)].

Already in the early 1980's, accurate Faddeev calculations had shown that 2*N* interactions (those available at the time) did not provide enough binding for the three-body nuclei, ${}^{3}H$ and ${}^{3}He$ [\[29\]](#page-6-18). In the late 1990's and early 2000's this conclusion was shown to hold also for the energy spectra (ground and low-lying excited states) of light p-shell nuclei in calculations based on the phenomenological interactions mentioned earlier, and using quantum Monte Carlo (QMC) [\[30](#page-6-19)] and no-core shell-model (NCSM) [\[31\]](#page-6-20) methods. This led to the realization that the basic model without the inclusion of (at least) 3*N* interaction is definitely incomplete.

Because of the composite nature of the nucleon and, in particular, the dominant role of the Δ-resonance in pion-nucleon scattering, multi-nucleon interactions arise quite naturally in the meson-exchange phenomenology. In particular, the Illinois 3*N* interactions [\[32\]](#page-6-21) consist of a dominant two-pion exchange (TPE) component with a single intermediate Δ—the Fujita-Miyazawa interaction [\[33](#page-6-22)]—and smaller multi-pion exchange components resulting from the excitation of multiple intermediate Δ 's. The most recent version, Illinois-7 (IL7) [\[34\]](#page-6-23), also contains phenomenological isospin-dependent central terms. The few (4) parameters characterizing the IL7 model have been determined by fitting the low-lying spectra of nuclei in the mass range *A* = 3–10. The resulting AV18 + IL7 Hamiltonian, generally utilized with QMC methods, then leads to predictions of about 100 ground- and excited-state energies up to $A = 12$, including the ¹²C ground- and Hoyle-state energies, in good agreement with the corresponding empirical values [\[10](#page-6-3)]. However, when used to compute the equation of state of neutron star matter, the AV18 + IL7 Hamiltonian does not provide sufficient repulsion to ensure the stability of the observed stars against gravitational collapse [\[35](#page-6-24)]. Thus, it would appear that, in the context of phenomenological nuclear interactions, we do not have models that can predict simultaneously the properties of light p-shell nuclei and dense nuclear and neutron matter. It is also important to emphasize that these interactions are affected by several additional limitations, most notably the missing link with the (approximate) chiral symmetry exhibited by QCD, and the absence of rigorous schemes to consistently derive nuclear electroweak currents.

The advent of chiral effective field theory (χ EFT) [\[36](#page-6-25)[–38\]](#page-6-26) in the early 1990's has spurred a new phase in the evolution of the basic model, and has renewed interest in its further development. χ EFT is a low-energy

effective theory of QCD based on pions and nucleons (and, in some instances, Δ 's) as effective degrees of freedom. For momenta *p* ∼ *m*_π, such a framework is expected to be accurate, since shorter-range structures, e.g., the quark substructure, or heavier meson exchanges, e.g., ρ -meson exchanges, are not resolved, and can be absorbed in short-range contact interactions between nucleons. This *separation of scales* between typical momenta $p \sim m_\pi$ and much harder momenta of the order of the ρ -meson or nucleon mass can be used to systematically derive a general scheme, which accommodates all possible interactions among the relevant degrees of freedom (pions, nucleons, and, in some formulations, Δ 's), and which is consistent with the symmetries of QCD.

The starting point in χ EFT is the most general Lagrangian in terms of the chosen degrees of freedom, which contains all interaction mechanisms allowed by the symmetries of QCD. This Lagrangian contains an infinite number of terms and needs to be truncated using a given power-counting scheme. Most chiral interactions used in nuclear structure calculations use Weinberg's power counting, which itself is based on naive dimensional analysis of interaction contributions. Within Weinberg's power counting, the interactions are expanded in powers of the typical momentum *p* over the breakdown scale Λ_b , that is, the expansion parameter is $Q = p/\Lambda_b$, where the breakdown scale denotes momenta at which the short distance structure becomes important and cannot be neglected and absorbed into contact interactions any longer (see Refs. [\[39](#page-6-27)[–43](#page-6-28)] for recent review articles). It is worthwhile mentioning that alternative power-counting schemes have been also suggested, see Refs. [\[44](#page-6-29)[–49](#page-7-0)].

This expansion defines an order by order scheme, defined by the power ν of the expansion parameter *Q* in each interaction contribution: leading order (LO) for $\nu = 0$, next-to-leading order (NLO) for $\nu = 2$, next-to-next-to-leading order (N²LO) for $v = 3$ and so on. Similarly as for nuclear interactions, such a scheme can also be developed for electroweak currents [\[50](#page-7-1)]. Therefore, χ EFT provides a rigorous scheme to systematically construct nuclear many-body forces and consistent electroweak currents, and tools to estimate their uncertainties [\[51](#page-7-2)[–56\]](#page-7-3).

Nuclear interactions in χEFT are separated into pion-exchange terms, associated with the long- and intermediate-range components, and contact terms that encode short-range physics. The strength of these contact terms is specified by unknown low-energy constants (LECs), which are constrained by fitting experimental data. Nuclear interactions (and electroweak currents) suffer from ultraviolet (UV) divergencies, which need to be removed by a proper regularization and renormalization procedure. As a matter of fact, there are two sources of UV divergencies that require regularization: one from loop corrections and the other when solving the Schrödinger equation (or when calculating matrix elements of nuclear currents). Loop divergences can be treated via dimensional regularization (DR) or spectral-function regularization (SFR), where the latter is implemented by including a finite cutoff in the spectral functions. If this cutoff is taken to be infinity, then SFR coincides with DR. To remove divergencies occurring in the solution of the Schrödinger equation, nuclear interactions are multiplied by regulator functions that remove momenta larger than a preset cutoff scale. The regularization of interactions (and currents) is followed by a renormalization procedure, that is, dependencies on the regularization scheme and cutoff are reabsorbed, order by order, by the LECs characterizing these interactions (and currents).

Nucleon–nucleon scattering has been extensively studied in χ EFT in the past two decades following the pioneering work by Weinberg [\[36](#page-6-25)[–38\]](#page-6-26) and Ordonez *et al.* [\[57](#page-7-4)]. In particular, 2*N* interactions at N3LO in the chiral expansion are available since the early 2000's [\[58](#page-7-5)[,59\]](#page-7-6) and have served as a basis for numerous *ab initio* calculations of nuclear structure and reactions. More recently, models up to the fifth order in the chiral expansion, i.e., N4LO, have been developed [\[60](#page-7-7)[–63\]](#page-7-8), which lead to accurate descriptions of 2*N* databases up to laboratory energies of 300 MeV with χ^2 per datum close to 1. These databases have been provided by the Nijmegen group [\[25,](#page-6-14)[28](#page-6-16)], the VPI/GWU group [\[64\]](#page-7-9), and more recently the Granada group [\[65](#page-7-10)[–67](#page-7-11)]. In the standard optimization procedure, the 2*N* interactions are first constrained through fits to neutron–proton (np) and proton–proton (pp) phase shifts, and then refined by minimizing the total χ^2 obtained from a direct comparison with the 2*N* scattering data. However, new optimization schemes are being explored in Refs. [\[68](#page-7-12)[,69](#page-7-13)]. For instance, the optimization strategy of Ref. [\[69\]](#page-7-13) is based on a simultaneous fit of low-energy 2*N* data, the deuteron binding energy, and the binding energies and charge radii of hydrogen, helium, carbon, and oxygen isotopes using consistent 2*N and* 3*N* interactions at N2LO.

Three-nucleon interactions and their impact on nuclear structure and reactions have become a nuclearphysics topic of intense current interest, see Refs. [\[70](#page-7-14)[–72\]](#page-7-15) for review articles. Three-nucleon interactions have been derived up to N4LO in χ EFT [\[73](#page-7-16)[–77\]](#page-7-17). However, few- and many-nucleon calculations are, with very few exceptions, still limited to chiral 3*N* interactions at N2LO. At this order, they are characterized by two unknown LECs, one in a OPE-contact term and the other in a purely contact 3*N* term; these LECs are commonly denoted as c_D and c_E , respectively. They have been constrained either by fitting exclusively strong-interaction observables [\[78](#page-7-18)[–81\]](#page-7-19) or by relying on a combination of strong- and weak-interaction observables [\[82](#page-8-0)[–86](#page-8-1)]. This last approach is made possible by the relation between c_D and the LEC entering the 2*N* contact axial current [\[82](#page-8-0)[,83](#page-8-2),[87\]](#page-8-3). This relation emerges naturally in χ EFT, and allows one to use nuclear properties governed by either strong or weak interactions to constrain simultaneously the 3*N* interaction and 2*N* axial current.

Since *x* EFT is a low-momentum expansion, many of the chiral interactions available in the literature are naturally formulated in momentum space and have the feature of being strongly non-local in coordinate space. This makes them ill-suited for certain numerical algorithms, for example, Quantum Monte Carlo (QMC) methods. This strong non-locality comes about on account of two factors: (i) the specific choice made for the cutoff function needed to remove large momenta, and (ii) contact terms involving high-order derivatives of the nucleon field.

3 Local Chiral Interactions

In recent years, local chiral interactions suitable for QMC calculations have been developed by two different groups using Δ -less [\[79](#page-7-20)[,80](#page-7-21),[88](#page-8-4)[–91](#page-8-5)] and Δ -full [\[81](#page-7-19)[,84](#page-8-6)[,92](#page-8-7)[–94](#page-8-8)] χ EFT formulations. At LO, both Δ -less and Δ-full interactions have the same operator structure. At this order, only the leading contact terms (involving no derivatives of the nucleon field) and one-pion exchange (OPE) term contribute (the latter is often taken to include also the charge-independence breaking induced by the difference between the neutral and charged pion masses).

At higher orders, additional momentum-dependent contact as well as two-pion exchange (TPE) terms appear. The TPE coordinate-space expressions at NLO and N2LO for both the Δ-less and Δ-full approaches are given in Refs. [\[88](#page-8-4)[,89](#page-8-9)[,95](#page-8-10)] and Ref. [\[93\]](#page-8-11), respectively. For the NLO contact interactions, the most general form consists of 14 terms [\[40](#page-6-30)]. However, only 7 out of these 14 terms are linearly independent; they turn out to be fully local. Moreover, at this order, a leading contact charge-dependent (CD) term is also accounted for, needed to reproduce the *pp* and *nn* singlet scattering length.

At the next order, N3LO, contact interactions cannot be written down in a purely local fashion, since Fierz identities prove ineffective in removing all non-localities. A possible way forward is the definition of *minimally non-local* N3LO interactions, which have been constructed in the Δ-full approach as reported in Ref. [\[93\]](#page-8-11). The local versions of these Δ-full *minimally non-local* 2*N* interactions have been defined by dropping terms proportional to **p**² that remain after Fierz rearrangement [\[92](#page-8-7)] (here, **p** is the relative momentum operator). The inclusion of these terms was shown to yield no significant improvement in the fit to the 2*N* database [\[92\]](#page-8-7). As a matter of fact, three combinations of such terms vanish off the energy shell [\[62](#page-7-22)] and their effect can be absorbed into a redefinition of the 3*N* interaction [\[96\]](#page-8-12). In these models, four charge-dependent (CD) operators at N3LO are also retained [\[92](#page-8-7)].

In order to use these interaction models in many-body calculations, it is necessary to specify a regularization scheme. For the \triangle -less interactions, the following long- and short-range regulators are used [\[88](#page-8-4)[,89\]](#page-8-9),

$$
f_{\text{long}}(r) = \left[1 - e^{-(r/R_0)^{n_1}}\right]^{n_2}, \quad f_{\text{short}}(r) = \frac{n}{4\pi R_0^3 \Gamma(3/n)} e^{-(r/R_0)^n}, \tag{1}
$$

with $n_1 = 4$, $n_2 = 1$, and $n = 4$.

The long-range regulator multiplies each radial function in the OPE and TPE contributions, while the shortrange regulator replaces all δ-functions in the contact terms. The regulator functions depend on the cutoff scale R_0 that is taken in the range of $R_0 = (1.0-1.2)$ fm. There are 11 LECs associated with contact terms in the Δ -less (NLO) models. They are fixed by performing χ^2 fits to 2*N* phase shifts from the Nijmegen partial-wave analysis (PWA) up to 150 MeV laboratory energy [\[88](#page-8-4),[89\]](#page-8-9).

In the Δ-full interactions, the long- and short-range regulators are, instead, given by the following functions

$$
f_{\text{long}}^{\Delta}(r) = 1 - \frac{1}{(r/R_{\text{L}})^6 e^{(r-R_{\text{L}})/a_{\text{L}}} + 1}, \quad f_{\text{short}}^{\Delta}(r) = \frac{1}{\pi^{3/2} R_{\text{S}}^3} e^{-(r/R_{\text{S}})^2},\tag{2}
$$

where three values for the radius R_L are considered: $R_L = (0.8, 1.0, 1.2)$ fm with the diffuseness a_L fixed at $a_L = R_L/2$ in each case. In combination with R_L , the R_S values considered are (0.6, 0.7, 0.8) fm, corresponding to typical momentum-space cutoffs $\Lambda_{\rm S} = 2/R_{\rm S}$ ranging from about 660 MeV down to 500 MeV. The interactions with cutoffs (R_L, R_S) equal to $(1.2, 0.8)$ fm, $(1.0, 0.7)$ fm, and $(0.8, 0.6)$ fm are denoted, respectively, as model a, b, and c. There are 26 LECs that enter these (N^2LO) interactions. The optimization procedure to fix these 26 LECs utilizes *pp* and *np* scattering data (including normalizations), as assembled in the Granada database [\[65\]](#page-7-10), the 2*N* scattering lengths, and the deuteron binding energy. For each of the three different sets of cutoff radii (R_S, R_L) , two classes of local interactions have been developed, which only differ in the range of laboratory energy over which the fits were carried out, either 0–125 MeV in class I or 0–200 MeV in class II. The χ^2 /datum achieved by the fits in class I (II) was $\lesssim 1.1 (\lesssim 1.4)$ for a total of about 2700 (3700) data points. In the literature, these 2*N* interactions are generically referred to as the Norfolk interactions (NV2s). Those in class I are designated as NV2-Ia, NV2-Ib, and NV2-Ic, and those in class II as NV2-IIa, NV2-IIb, and NV2-IIc.

Both the Δ -less and Δ -full formulations account for 3*N* interactions. In the Δ -less version, the leading 3*N* contributions appear at N2LO in the power counting. They consist of (i) a long-range TPE term (V_C) , depending on the subleading pion-nucleon LECs *c*1, *c*3, and *c*4, that already appear in the 2*N* sector; (ii) a OPE-contact term (V_D) dependent on the LEC c_D , and (iii) a purely contact 3*N* term (V_E) dependent on the LEC c_E . The LECs c_D and c_E are adjusted so as to fit properties of $A \geq 3$ systems. In the Δ -less approach, these observables have been chosen to be the 4He binding energy and *n*-α scattering *P* wave phase shifts. In Fig. 1 of Ref. [\[79\]](#page-7-20), the parameter curves for the 3*N* LECs corresponding to different 3*N* cutoffs *R*3N, chosen similarly to R_0 , are shown.

In the Δ -full formulation, the 3*N* interaction consists of the three N2LO terms above (V_C , V_D and V_E) plus a NLO TPE term involving the excitation of a Δ in the intermediate state, the well-known Fujita–Miyazawa interaction [\[33](#page-6-22)] (V_{Δ}). In the Δ -less approach, it is expected to be subsumed in V_C . In the Δ -full chiral EFT, two different sets for the values of c_D and c_E were obtained, leading to two different parametrizations of the 3*N* interaction [\[81,](#page-7-19)[84](#page-8-6)]. In the first, these LECs were determined by simultaneously reproducing the experimental trinucleon ground-state energies and the neutron–deuteron (*nd*) doublet scattering length, as shown in Ref. [\[81\]](#page-7-19). In the second set, these c_D and c_E were constrained by fitting, in addition to the trinucleon energies, the empirical value of the Gamow-Teller matrix element in tritium β decay [\[84\]](#page-8-6). Because of the much reduced correlation between binding energies and the GT matrix element, the second procedure leads to a more robust determination of c_D and c_E than attained in the first one. Note that these observables have been calculated with hyperspherical-harmonics (HH) expansion methods [\[5\]](#page-5-4) as described in Refs. [\[81](#page-7-19)[,84\]](#page-8-6).

4 Applications

In this section, we briefly discuss some illustrative applications of local chiral interactions to the few- and many-body systems.

Figure [1](#page-5-6) shows the binding energies of nuclei up to ¹⁶O as calculated with the Green's function Monte Carlo (GFMC) method for one of the Δ -full models (NV2 + 3-Ia) [\[81\]](#page-7-19), and with the Auxiliary Diffusion Monte Carlo (AFDMC) method for one of the \triangle -less models (GT + Eτ-1.0) [\[90](#page-8-13),[98\]](#page-8-14). The calculated energies are compared to the experimental values. GFMC results only carry Monte Carlo statistical uncertainties, while for AFDMC results, theoretical uncertainties coming from the truncation of the chiral expansion are also included. These uncertainties are estimated accordingly to the prescription of Epelbaum *et al.* [\[61\]](#page-7-23). In addition to energies, local chiral interactions describe charge radii extremely well as shown in Fig. 4 of Ref. [\[11\]](#page-6-4) (see this reference for a more extensive discussion).

The Δ-full models have been recently used in benchmark calculations of the energy per particle of pure neutron matter (PNM) as a function of density using three independent many-body methods [\[99](#page-8-15)]: Brueckner-Bethe-Goldstone (BBG), Fermi hypernetted chain/single-operator chain (FHNC/SOC), and AFDMC. These calculations are especially useful in providing a quantitative assessment of systematic errors associated with the different many-body approaches and how they depend on the chosen interaction. A selection of results is reported in Fig. [2,](#page-5-7) where the energy per particle of pure neutron matter as obtained from AFDMC calculations with the phenomenological AV18 and the NV2 models is reported. The inclusion of 3*N* interactions is essential for a realistic description of neutron matter. Preliminary AFDMC calculations of the equation of state of PNM carried out with the NV2 + 3-Ia/b and NV2 + 3-IIa/b models are not compatible with the existence of two solar masses neutron stars, in conflict with recent observations [\[100](#page-8-16)[,101](#page-8-17)]. On the other hand, the smaller values of c_E characterizing the 3*N* interactions entering the NV2 + 3-Ia*/b* and NV2 + 3-IIa*/b* models mitigate, if not resolve, this problem. There are indications that these models also predict the energies of low-lying states in light nuclei reasonably well, than 4% away from the experimental values. Studies along this line are currently in progress.

Fig. 1 From Ref. [\[11](#page-6-4)]. Ground-state energies in $A \le 16$ nuclei. For each nucleus, experimental results [\[97](#page-8-18)] are shown in green at the center. GFMC (AFDMC) results for the NV2 $+$ 3-Ia [\[81\]](#page-7-19) (GT+E τ -1.0 [\[90\]](#page-8-13)) interactions are shown in red (blue) to the left (right) of the experimental values. For the NV2 + 3-Ia (GT + E τ -1.0) interactions, the colored bands include statistical (statistical plus systematic) uncertainties

Fig. 2 From Ref. [\[99](#page-8-15)]. AFDMC energy per particle of PNM as a function of density for the AV18 (black triangles), NV2-Ia (red triangles), NV2-Ib (solid blue points), NV2-IIa (green diamonds), and NV2-IIb (grey squares) interactions

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