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C. Hebborn, G. Hupin, K. Kravvaris, S. Quaglioni, P. Navrátil, and P. Gysbers

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Ab initio prediction of the ^{4}He$(d,\gamma)\,^6$Li big bang radiative capture

C. Hebborn,[1,2,*] G. Hupin,[3] K. Kravvaris,[2] S. Quaglioni,[2] P. Navrátil,[4] and P. Gysbers[4,5]

[1] *Facility for Rare Isotope Beams, East Lansing, MI 48824, USA*
[2] *Lawrence Livermore National Laboratory, P.O. Box 808, L-414, Livermore, CA 94551, USA*
[3] *Universit Paris-Saclay, CNRS/IN2P3, IJCLab, 91405 Orsay, France*
[4] *TRIUMF, 4004 Wesbrook Mall, Vancouver BC, V6T 2A3, Canada*
[5] *Department of Physics and Astronomy, University of British Columbia, Vancouver, British Columbia, V6T 1Z1, Canada*

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The rate at which helium (^{4}He) and deuterium (d) fuse together to produce lithium-6 (^{6}Li) and a γ ray, ^{4}He$(d,\gamma)^6$Li, is a critical puzzle piece in resolving the discrepancy between big bang predictions and astronomical observations for the primordial abundance of ^{6}Li. The accurate determination of this radiative capture rate requires the quantitative and predictive description of the fusion probability across the big bang energy window (30 keV $\lesssim E \lesssim$ 400 keV), where measurements are hindered by low counting rates. We present first-principles (or, *ab initio*) predictions of the ^{4}He$(d,\gamma)^6$Li astrophysical S-factor using validated nucleon-nucleon and three-nucleon interactions derived within the framework of chiral effective field theory. By employing the *ab initio* no-core shell model with continuum to describe ^{4}He-d scattering dynamics and bound ^{6}Li product on an equal footing, we accurately and consistently determine the contributions of the main electromagnetic transitions driving the radiative capture process. Our results reveal an enhancement of the capture probability below 100 keV owing to previously neglected magnetic dipole (M1) transitions and reduce by an average factor of 7 the uncertainty of the thermonuclear capture rate between 0.002 and 2 GK.

The isotopes of hydrogen, helium and lithium present few minutes after the big bang seeded all nucleosynthetic processes responsible for the creation of chemical elements in the Universe. Although the big bang nucleosynthesis (BBN) predictions for the abundances of hydrogen and helium are in agreement with astrophysical observations, they fall short in the cases of lithium isotopes: the abundance of ^{7}Li is overpredicted by a factor of 2-4, and the one of ^{6}Li is underpredicted by up to three orders of magnitude [1]. The origin of these discrepancies could be traced to beyond standard model physics or to systematic uncertainties in inferring the primordial abundances from the composition of metal-poor stars [2, 3]. A third possibility is that part of the discrepancy could be explained by inaccuracies in the nuclear reaction rates that are the main inputs to the BBN reaction network. To arrive at a complete solution of these cosmological lithium problems, it is therefore essential to accurately pin down the astrophysical reaction rates responsible for the formation of ^{6,7}Li at BBN energies.

The production of ^{6}Li is dominated by the ^{4}He$(d,\gamma)\,^6$Li radiative capture at BBN energies, from 30 keV to 400 keV, which is poorly known. On the experimental side, there are large discrepancies between existing data sets. Direct measurements are hindered by the Coulomb repulsion between the ^{4}He and d nuclei, that strongly suppresses the counting statistics. Consequently, there exist only two direct measurements in the BBN energy range, at 94 and 134 keV [4]. Indirect estimates relating the capture rate with the disintegration of ^{6}Li in the Coulomb field of a heavy target overcome the low statistics but suffer from systematic uncertainties, caused by difficulty to cleanly separate the nuclear and electromagnetic contributions to the breakup cross section [5–7]. Accurate theoretical predictions are therefore needed to guide the extrapolation of the existing direct measurements to the whole BBN range of energies. On the theory side, most calculations were carried out in either two-body potential models (that neglect the internal structure of the ^{4}He and d reactants) [8–13] or in three-body ^{4}He+p+n models [14–16] with an inert ^{4}He core. In both cases, typically the contributions owing to the electromagnetic dipole transitions are approximated. In the early 2000s, Nollett *et al.* [17] improved these theoretical predictions by including an *ab initio* treatment of all relevant (^{4}He, d and ^{6}Li) nuclei, but their analysis still relied on a phenomenological description of the ^{4}He-d scattering and suffered from the use of somewhat imprecise variational solutions for the ^{4}He and ^{6}Li wave functions. Because none of these models provides a fully microscopic and consistent description of the ^{4}He and d reactants, and of the six-body ^{6}Li bound and ^{4}He-d scattering states, they use phenomenological prescriptions to evaluate the electric dipole (E1) transitions and the magnetic dipole (M1) matrix elements are often not computed. Using these approximations, quadrupole electric (E2) transitions are predicted to drive the capture above 100 keV, below which E1 transitions become dominant. This work constitutes the first calculations that do not rely on these phenomenological prescriptions and we evaluate the electromagnetic operators exactly.

In this Letter, we present a fully *ab initio* and consistent prediction of the ^{4}He$(d,\gamma)\,^6$Li radiative capture starting from nucleon degrees-of-freedom and their inter-

actions. Scattering and bound states are treated within the same theoretical framework. Contrary to previous studies, E1 transitions are found to be negligible. An enhancement of the capture below 100 keV is instead driven by previously neglected M1 transitions. The uncertainty of the predicted ^{4}He$(d,\gamma)\,^6$Li thermonuclear reaction rates is reduced by an average factor 7 compared to previous evaluations [18].

For capture reactions below the Coulomb barrier, the typical observable is the astrophysical S-factor, which is proportional to the cross section σ but is not exponentially suppressed at low energies. At these energies, the capture cross section can be safely approximated by [19]

$$\sigma(E) = \frac{64\pi^4}{4\pi\epsilon_0\hbar v}\sum_{\kappa\lambda}\frac{k_\gamma^{2\lambda+1}}{[(2\lambda+1)!!]^2}\frac{\lambda+1}{\lambda} \times \sum_{J_i l_i s_i}\frac{\hat{J}_f^2}{\hat{s}_P^2\hat{s}_T^2\hat{l}_i^2}\left|\left\langle \Psi^{J_f^{\pi_f}T_f}\middle|\middle|\mathcal{M}^{\kappa\lambda}\middle|\middle|\Psi^{J_i^{\pi_i}T_i}_{l_i s_i}\right\rangle\right|^2, \quad (1)$$

where f and i denote respectively the final (^{6}Li) bound-state and initial (^{4}He-d) scattering wavefunction, P and T correspond to the projectile (d) and target (^{4}He) nuclei, v is the initial relative P-T velocity, λ is the multipolarity of the electric ($\kappa=$E) and magnetic ($\kappa=$M) transition operator and the notation $\hat{J}_f$ stands for $\sqrt{2J_f+1}$. The quantum numbers J, l, s, π, and T are respectively the total and orbital angular momenta, spin, parity, and isospin. The matrix element in Eq. (1) is evaluated for E1, E2 and M1 operators, which read

$$\mathcal{M}^{E\lambda} = e\sum_{j=1}^{A}\frac{1+\tau_{jz}}{2}(\boldsymbol{r}_j - \boldsymbol{R}_{\rm cm}^{(A)})^\lambda \quad (2)$$

$$\mathcal{M}^{M1} = \frac{\mu_N}{\hbar c}\sqrt{\frac{3}{4\pi}}\sum_{j=1}^{A}(g_{lj}L_j + g_{sj}S_j) \quad (3)$$

where e is the electric charge, μ_N is the nuclear magneton, $\boldsymbol{R}_{\rm cm}^{(A)}$ is the center-of-mass (c.m.) coordinate of the A-nucleon system, g_{sj}, τ_{jz}, S_j and L_j are respectively the gyromagnetic factor, the isospin, spin and orbital angular momentum (defined with respect to the c.m.) operator of the jth nucleon and $g_{lj}=1$ for proton and 0 for neutron.

In the case of ^{4}He$(d,\gamma)\,^6$Li, electric dipole transitions are strongly suppressed because the c.m. of the ^{4}He-d system corresponds to its center-of-charge [16]. Nevertheless, when the ^{4}He and d nuclei fuse together to form the bound ^{6}Li, this is no longer true and these E1 transitions can become important. Models which do not treat the internal structure of these nuclei explicitly [8, 10–13] evaluate E1 transitions by adopting the experimental masses of the ^{4}He and d nuclei, effectively shifting the c.m. away from the center-of-charge and thus generating a small dipole strength. Recently, the validity of this phenomenological prescription has been questioned since it cannot reproduce the physical energy slope of the S-factor [16]. Moreover, M1 transitions are usually assumed to be negligible, based on the fact that the operator (3) can be seen as the sum of a spin S_j and total angular momentum J_j contributions, with the second term canceling exactly due to the orthogonality of the initial and final wavefunctions, which are both eigenstates of the underlying microscopic Hamiltonian [16, 17, 20]. Because both E1 and M1 transitions are predicted to be small, the E2 component typically dominates the capture. In the present work, we do not rely on these assumptions and compute the transition operators microscopically starting from the operators (2)–(3).

The no-core shell model with continuum method (NCSMC, see Ref. [21] for a recent review) is a tool of choice to predict ^{4}He$(d,\gamma)\,^6$Li as it describes accurately both the static properties of light nuclei and their dynamics [22–27]. The NCSMC 6-body wavefunction for the ^{4}He+d system is given in terms of ^{6}Li no-core shell model (NCSM) wavefunctions $|A\lambda J^\pi T\rangle$ and continuous ^{4}He-d cluster states $\mathcal{A}_\nu\left|\Phi_{\nu r}^{J^\pi T}\right\rangle$, built from the ^{4}He and d NCSM states

$$\left|\Psi^{J^\pi T}\right\rangle = \sum_\lambda c_\lambda^{J^\pi T}|A\lambda J^\pi T\rangle + \sum_\nu\int_0^{+\infty} dr\, r^2\,\frac{\gamma_\nu^{J^\pi T}(r)}{r}\hat{\mathcal{A}}_\nu\left|\Phi_{\nu r}^{J^\pi T}\right\rangle. \quad (4)$$

The unknown coefficients $c_\lambda^{J^\pi T}$ and $\gamma_\nu^{J^\pi T}$ are obtained by solving the Bloch-Schrödinger equations, as detailed in Ref. [21]. The E1 matrix elements within the NCSMC formalism are also derived in Ref. [21] and expressions for E2 and M1 operators can be obtained in an analogous way, with the exception that they rely on closure relationships with respect to the NCSM ^{6}Li and the binary ^{4}He-d cluster bases, respectively.

Our prediction starts from state-of-the-art nucleon-nucleon (NN) and three-nucleon (3N) interactions [28–30] derived from low-energy quantum chromodynamics via chiral effective field theory [31], that provide an accurate description of both bound and scattering physics. These interactions are softened using the similarity renormalization group (SRG) transformation in three-body space with a momentum resolution scale of $\lambda = 2$ fm^{-1} [32]. The eigenstates of the aggregate ^{6}Li, ^{4}He, and d nuclei are obtained using a basis of many-body harmonic oscillator wavefunctions with frequency $\hbar\Omega = 20$ MeV and a maximum number $N_{\rm max} = 11$ of particle excitation quanta above the lowest energy configuration of the system. Discussions on the choice of the microscopic Hamiltonian, the influence of the SRG transformation on the electromagnetic operators and the convergence of our predictions can be found in the Supplemental material (which includes Refs. [33–37]).

Our predicted S-factor agrees well with available existing experimental data [4, 6, 38, 39] (top panel of Fig. 1). Overall, when only the SRG-evolved NN po-

	NN-only	$3N_{loc}$	$3N_{loc}$-pheno	Exp. or Eval.
$E_{g.s.}$	-1.848	-1.778	-1.474	-1.4743
$\mathcal{C}_0$	2.95	2.89	2.62(4)	2.28(7) 2.29(12)
$\mathcal{C}_2$	-0.0369	-0.0642	-0.0554(305)	-0.077(18)
$\mathcal{C}_2/\mathcal{C}_0$	-0.013	-0.022	-0.021(11)	-0.025(6)(10)
μ	0.85	0.84	0.84(1)	0.8220473(6)

TABLE I. Ground-state properties of ^{6}Li (binding energy $E_{g.s.}$ [MeV], ANCs $\mathcal{C}_0$, $\mathcal{C}_2$ [fm$^{-1/2}$] and magnetic moment μ [μ_N]) obtained using the SRG-evolved N3LO NN potential (NN-only) with $\lambda = 2$ fm^{-1}, the NN+$3N_{loc}$ without ($3N_{loc}$) and with the phenomenological energy adjustment ($3N_{loc}$-pheno). The last column lists the experimental $E_{g.s.}$ and μ [43], and ANCs inferred from a phase shift analysis [44]. The first uncertainty is purely statistical and the second is an estimate of the systematic error. The previous evaluation for $\mathcal{C}_0$ of Blokhsintsev *et al.* [45] is also reported (third line).

tential is considered (NN-only), our calculation reproduces well the magnitude of the data, particularly at low energies where it agrees with the direct measurements of the LUNA collaboration [4]. Our results are however incompatible with the ones inferred from breakup data [6], which, as discussed before, have been shown to suffer from model-dependence [7]. However, this NN-only prediction misses the positions of the 3^+ and 2^+ resonance peaks respectively measured by Mohr *et al.* around $E_{3^+} = 0.71$ MeV [38] and by Robertson *et al.* around $E_{2^+} = 2.84$ MeV [39]. This is unexpected because both the chiral and SRG-induced 3N forces strongly affect the splitting between the 3^+ and 2^+ states [22]. When both NN and 3N forces (both chiral and SRG-induced) are considered, the ^{6}Li 3^+ and 2^+ resonances are in excellent agreement with the direct measurements of Mohr *et al.* and Robertson *et al.*, but the ground state (g.s.) is overbound by ~ 310 keV (see Supplemental Material). Compared to the NN-only case, the inclusion of the 3N forces modifies the ^{6}Li g.s. properties, namely its binding energy and asymptotic normalization constants (ANCs) in the $\ell = 0$ ($\mathcal{C}_0$) and $\ell = 2$ ($\mathcal{C}_2$) partial-waves in the relative ^{4}He-d motion (see Table I), causing small changes in the magnitude and the slope of the S-factor at low energy [40, 41].

To improve our evaluation of the S-factor at low energy [40, 41], we correct the overbinding of the ^{6}Li g.s. by shifting only the energies of the 1^+ g.s. and 2^+ resonant eigenstates of the aggregate ^{6}Li system for the full NCSMC to reproduce the experimental energies, as done in Refs. [23–25, 46]. This fine-tuning (NN+$3N_{loc}$-pheno) impacts mainly the low-energy part of the S-factor and the energy region close to the 2^+ resonance. This phenomenological correction also brings the predicted ANCs ($\mathcal{C}_0$ and $\mathcal{C}_2$) closer to the values inferred from the low-energy ^{6}Li-^{4}He and ^{4}He-d phase shifts in Refs. [44, 45] (last column of Table I). The uncertainty associated with our NN+$3N_{loc}$-pheno results are estimated from the errors arising from the truncation of the model space in the number of excitation quanta N_{max} and the choice of the chiral 3N force (see Supplemental material). Because our predictions reproduce low-energy capture and elastic-scattering observables (see Supplemental material), the discrepancy between our prediction for $\mathcal{C}_0$ and previous works extracting ANCs from phase shifts is most likely due to systematic uncertainties owing to the use of optical potentials [47–49] or to the extrapolation procedure to the experimental binding energy [50, 51] that have not been quantified in Refs. [44, 45]. Moreover, our ratio $\mathcal{C}_0/\mathcal{C}_2$ is in excellent agreement with the previously extracted evaluation of Ref. [44], for which systematic uncertainties have been accounted for.

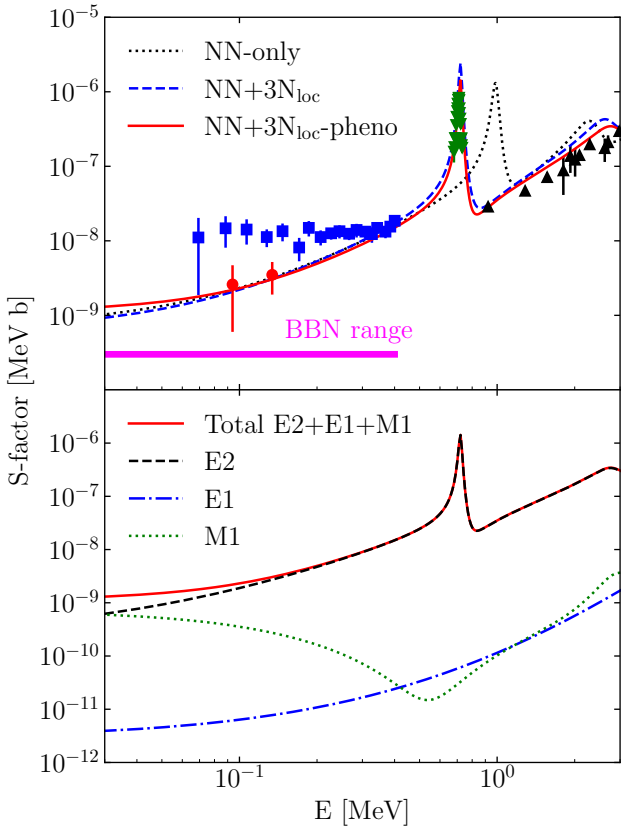

FIG. 1. Top: Predicted S-factor for the ^{4}He$(d,\gamma)^6$Li compared with data taken from Refs. [4] (red circles), [6] (blue square), [38] (green down-triangles) and [39] (black up-triangles). Calculations are obtained using the SRG-evolved N3LO NN potential [42] (NN-only) with $\lambda = 2$ fm^{-1}, the NN+$3N_{loc}$ [28, 30] without (NN+$3N_{loc}$) and with the phenomenological energy adjustment (NN+$3N_{loc}$-pheno). Bottom: E2, E1 and M1 components to the predicted S-factor for the ^{4}He$(d,\gamma)^6$Li obtained with the NN+$3N_{loc}$-pheno.

The relative importance of the electromagnetic E2, E1 and M1 transitions varies with energy (bottom panel of Fig. 1). We find that the E2 transitions dominate the non-resonant and resonant capture, in line with previous works [8–17]. Different from those studies, we obtain

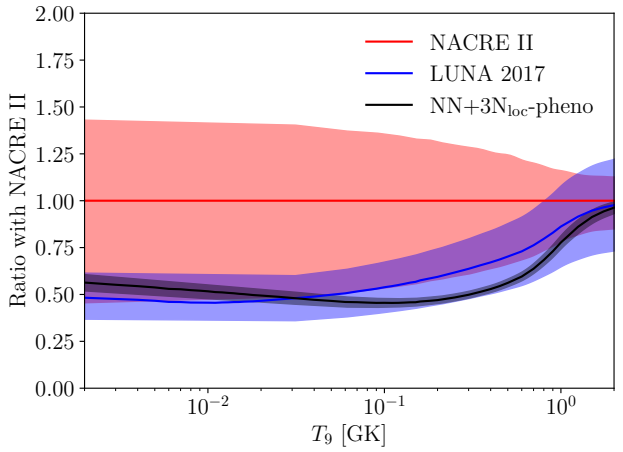

FIG. 2. Ratio of the predicted thermonuclear reaction rates (black line) for the ^{4}He$(d,\gamma)\,^6$Li with the NACRE-II evaluation (red line) [18] for the ^{4}He$(d,\gamma)\,^6$Li for different temperature T_9 in GK. Our results are also compared with the recent thermonuclear reaction rate derived from the measurements of the LUNA collaboration (blue line) [53]. The shaded areas correspond to the uncertainty of each calculation (see text for details).

larger E2 strengths, that can be explained, as the E2 operator (2) is long-ranged, by the larger amplitude of the ^{6}Li g.s. at large distance, i.e., by the larger value of the predicted ANC $\mathcal{C}_0$ (second line of Table I). Moreover, we find a sizeable M1 component that has not been predicted in previous works [8–17]. This M1 contribution arises from the internal dipole magnetic moments of the ^{6}Li and d nuclei, making a full microscopic description essential for an accurate calculation. The good agreement between our predicted magnetic moment and the experimental one corroborates our evaluation (last line in Table I). Finally, our calculations show that the E1 transitions have a negligible influence on the S-factor [52], contrary to what it is usually predicted using phenomenological prescriptions.

From the S-factor at low energy, we obtain a thermonuclear reaction rate for the ^{4}He$(d,\gamma)\,^6$Li (NN+3N$_{\rm loc}$-pheno in Fig. 2) with uncertainties reduced by an average factor of 7 compared to the Nuclear Astrophysics Compilation of REaction rates (NACRE II) [18]. Because the low-energy S-factor is dominated by the binding energy and the ANCs of the g.s., the description of which is improved as an effect of the phenomenological correction of the g.s. energy, the uncertainties remain small for all $T_9 \lesssim 2$ GK. Our result is systematically smaller than the NACRE II rate, but agrees well with the rates reported by the LUNA collaboration (LUNA 2017) [53]. Contrary to our first-principle prediction, both the NACRE II and LUNA evaluations rely on an extrapolation of experimental data informed by a two-body ^{4}He+d potential model.

In this Letter, we carried out an *ab initio* prediction for the ^{4}He$(d,\gamma)\,^6$Li radiative capture at BBN energies starting from chiral EFT NN and 3N forces, treating both bound and scattering states within the same formalism and consistently evaluating the underlying electromagnetic transitions. In line with previous studies, we find that the E2 transitions dominate the capture at all relevant BBN energies. However, different from the earlier understanding, our results indicate that the M1 transitions become increasingly important at low energies, while the E1 component remains negligible over the whole energy range. The validity of our evaluation is demonstrated by the excellent agreement with available S-factor data (both those at low-energy measured by the LUNA collaboration and those in the vicinity of the 3^+ resonance) and with the experimental magnetic dipole moment. Our microscopic prediction leads to a systematically lower reaction rate, with an average reduction of 9%, and a factor of 7 smaller uncertainty than the recent NACRE II evaluation [18]. In this work, we have accounted for systematic uncertainties related to the convergence of our calculations and the choice of the 3N force. However, we have not accounted for the statistical uncertainties owing to the parameterization of the chiral NN+3N Hamiltonian. We reserve that study for future work.

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* hebborn@frib.msu.edu

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[52] Note1, because only isovector E1 transitions from $T_i = 0$ scattering state to the $T_f = 1$ component of the ^{6}Li g.s. contribute at low energy [16], the E1 strength is closely related to the isospin mixing of the ^{6}Li 1^+ g.s.. In our NCSMC calculation, this mixing is mainly caused by the $T_f = 1$ component of the aggregate ^{6}Li g.s., which stays small, i.e., $T_f \leq 0.0003$, and therefore leads to negligible E1 transitions.

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