

***Ab Initio* Prediction of the ${}^4\text{He}(d,\gamma){}^6\text{Li}$ Big Bang Radiative Capture**C. Hebborn^{1,2,*}, G. Hupin³, K. Kravvaris², S. Quaglioni², P. Navrátil⁴, and P. Gysbers^{4,5}¹*Facility for Rare Isotope Beams, East Lansing, Michigan 48824, USA*²*Lawrence Livermore National Laboratory, P.O. Box 808, L-414, Livermore, California 94551, USA*³*Université Paris-Saclay, CNRS/IN2P3, IJCLab, 91405 Orsay, France*⁴*TRIUMF, 4004 Wesbrook Mall, Vancouver British Columbia 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 (${}^4\text{He}$) and deuterium (d) fuse together to produce lithium-6 (${}^6\text{Li}$) and a γ ray, ${}^4\text{He}(d,\gamma){}^6\text{Li}$, is a critical puzzle piece in resolving the discrepancy between big bang predictions and astronomical observations for the primordial abundance of ${}^6\text{Li}$. The accurate determination of this radiative capture rate requires the quantitative and predictive description of the fusion probability across the big bang energy window ($30\text{ keV} \lesssim E \lesssim 400\text{ keV}$), where measurements are hindered by low counting rates. We present first-principle (or, *ab initio*) predictions of the ${}^4\text{He}(d,\gamma){}^6\text{Li}$ 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 ${}^4\text{He}$ - d scattering dynamics and bound ${}^6\text{Li}$ 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.

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The isotopes of hydrogen, helium, and lithium present a 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 ${}^7\text{Li}$ is overpredicted by a factor of 2–4, and the one of ${}^6\text{Li}$ is underpredicted by up to 3 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 ${}^6,7\text{Li}$ at BBN energies.

The production of ${}^6\text{Li}$ is dominated by the ${}^4\text{He}(d,\gamma){}^6\text{Li}$ 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 datasets. Direct measurements are hindered by the Coulomb repulsion between the ${}^4\text{He}$ 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 ${}^6\text{Li}$ in the Coulomb field of a heavy target overcome the low statistics but suffer from systematic uncertainties, caused by the difficulty of cleanly separating the nuclear and electromagnetic contributions in 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 ${}^4\text{He}$ and d reactants) [8–13] or in three-body ${}^4\text{He} + p + n$ models [14–16] with an inert ${}^4\text{He}$ 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 (${}^4\text{He}$, d , and ${}^6\text{Li}$) nuclei, but their analysis still relied on a phenomenological description of the ${}^4\text{He}$ - d scattering and suffered from the use of somewhat imprecise variational solutions for the ${}^4\text{He}$ and ${}^6\text{Li}$ wave functions. None of these models provides a fully microscopic and consistent description of the ${}^4\text{He}$ and d reactants, and of the six-body ${}^6\text{Li}$ bound and ${}^4\text{He}$ - d scattering states, they therefore 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 ${}^4\text{He}(d, \gamma){}^6\text{Li}$ radiative capture starting from nucleon degrees of freedom and their interactions. 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 ${}^4\text{He}(d, \gamma){}^6\text{Li}$ thermonuclear reaction rates is reduced by an average factor of 7 compared with 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]

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

where f and i denote respectively the final (${}^6\text{Li}$) bound-state and initial (${}^4\text{He}-d$) scattering wave function, P and T correspond to the projectile (d) and target (${}^4\text{He}$) 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 as

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

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

where e is the electric charge, μ_N is the nuclear magneton, $\mathbf{R}_{\text{cm}}^{(A)}$ 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 j th nucleon, and $g_{lj} = 1$ for proton and 0 for neutron.

In the case of ${}^4\text{He}(d, \gamma){}^6\text{Li}$, electric dipole transitions are strongly suppressed because the c.m. of the ${}^4\text{He}-d$ system corresponds to its center of charge [16]. Nevertheless, when the ${}^4\text{He}$ and d nuclei fuse together to form the bound ${}^6\text{Li}$, 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 ${}^4\text{He}$ 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 [Eq. (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 wave functions, 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 [Eqs. (2) and (3)].

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

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

where ν summarizes all the relevant quantum numbers. The unknown coefficients $c_\lambda^{J^\pi T}$ and $\gamma_\nu^{J^\pi T}$ are obtained by solving the Bloch-Schrödinger equation, 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 ${}^6\text{Li}$ and the binary ${}^4\text{He}-d$ 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 $\lambda = 2 \text{ fm}^{-1}$ [32]. The eigenstates of the aggregate ${}^6\text{Li}$, ${}^4\text{He}$, and d nuclei are obtained using a basis of many-body harmonic oscillator wave functions with frequency $\hbar\Omega = 20 \text{ MeV}$ and a maximum number $N_{\text{max}} = 11$ 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 [33] (which includes Refs. [34–38]).

Our predicted S factor agrees well with available existing experimental data [4,6,39,40] (top panel of Fig. 1). Overall, when only the SRG-evolved NN potential 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 $E_{3^+} = 0.71 \text{ MeV}$ [39] and by Robertson *et al.* around $E_{2^+} = 2.84 \text{ MeV}$ [40]. This is expected 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 ${}^6\text{Li}$ 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 $\sim 310 \text{ keV}$ (see Supplemental Material [33]). Compared to the NN-only case, the inclusion of the 3N forces modifies the ${}^6\text{Li}$ g.s. properties, namely its binding energy and asymptotic normalization constants (ANCs) in the $l = 0$ (C_0) and $l = 2$ (C_2) partial waves in the relative ${}^4\text{He}$ - d motion (see Table I), causing small changes in the magnitude and the slope of the S factor at low energy [41,42].

To improve our evaluation of the S factor at low energy [41,42], we correct the overbinding of the ${}^6\text{Li}$ g.s. by shifting only the energies of the 1^+ g.s. and 2^+ resonant eigenstates of the aggregate ${}^6\text{Li}$ system such that the full NCSMC to reproduce the experimental energies, as done in Refs. [23–25,47]. This fine-tuning (NN + $3N_{\text{loc}}$ -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 (C_0 and C_2) closer to the values inferred from the low-energy ${}^6\text{Li}$ - ${}^4\text{He}$ and ${}^4\text{He}$ - d phase shifts in Refs. [45,46] (last column of Table I). The uncertainty associated with our NN + $3N_{\text{loc}}$ -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 [33]). Because our predictions reproduce low-energy capture and elastic-scattering observables (see Supplemental Material [33]), the discrepancy between our prediction for C_0 and previous works extracting ANCs from phase shifts is most likely due to systematic uncertainties owing to the use of optical potentials [48–50] or to the extrapolation procedure to the experimental binding energy [51,52] that have not been quantified in Refs. [45,46]. Moreover, our ratio C_0/C_2 is in excellent agreement with the previously extracted evaluation of Ref. [45], for which systematic uncertainties have been accounted for.

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 nonresonant and resonant capture, in line with previous works [8–17]. Different from those studies, we obtain larger $E2$ strengths, that can be explained, as the $E2$ operator [Eq. (2)] is long ranged, by the larger amplitude of the ${}^6\text{Li}$ g.s. at large distance, i.e., by the larger value of

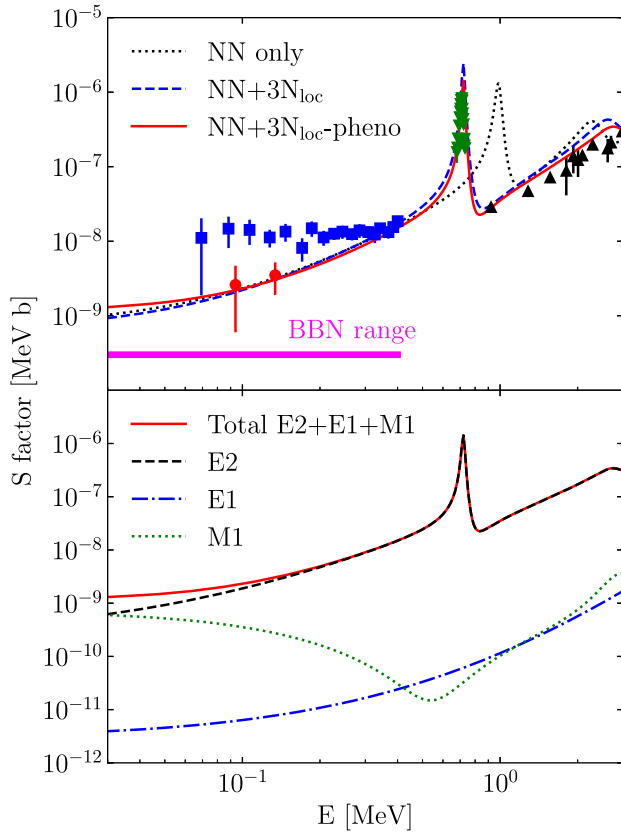


FIG. 1. Top: predicted S factor for the ${}^4\text{He}(d, \gamma){}^6\text{Li}$ compared with data taken from Refs. [4] (red circles), [6] (blue square), [39] (green down-triangles), and [40] (black up-triangles). Calculations are obtained using the SRG-evolved N3LO NN potential [43] (NN-only) with $\lambda = 2 \text{ fm}^{-1}$, the NN + $3N_{\text{loc}}$ [28,30] without (NN + $3N_{\text{loc}}$), and with the phenomenological energy adjustment (NN + $3N_{\text{loc}}$ -pheno). Bottom: $E2$, $E1$, and $M1$ components of the predicted S factor for the ${}^4\text{He}(d, \gamma){}^6\text{Li}$ obtained with the NN + $3N_{\text{loc}}$ -pheno.

TABLE I. Ground-state properties of ${}^6\text{Li}$ (binding energy $E_{g.s.}$ [MeV], ANCs C_0 , C_2 [$\text{fm}^{-1/2}$], and magnetic moment μ [μ_N]) obtained using the SRG-evolved N3LO NN potential (NN-only) with $\lambda = 2 \text{ fm}^{-1}$, the NN + $3N_{\text{loc}}$ without ($3N_{\text{loc}}$) and with the phenomenological energy adjustment ($3N_{\text{loc}}$ -pheno). The last column lists the experimental (Expt.) $E_{g.s.}$ and μ [44], and ANCs inferred from a phase shift analysis [45]. The first uncertainty is purely statistical, and the second is an estimate of the systematic error. The previous evaluation (eval.) for C_0 of Blokhintsev *et al.* [46] is also reported (third line).

	NN-only	$3N_{\text{loc}}$	$3N_{\text{loc}}$ -pheno	Expt. or eval.
$E_{g.s.}$	-1.848	-1.778	-1.474	-1.4743
C_0	2.95	2.89	2.62(4)	2.28(7) 2.29(12)
C_2	-0.0369	-0.0642	-0.0554(305)	-0.077(18)
C_2/C_0	-0.013	-0.022	-0.021(11)	-0.025(6)(10)
μ	0.85	0.84	0.84(1)	0.8220473(6)

the predicted ANC 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 ${}^6\text{Li}$ 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 [53], contrary to what is usually predicted using phenomenological prescriptions.

From the S factor at low energy, we obtain a thermonuclear reaction rate for the ${}^4\text{He}(d, \gamma){}^6\text{Li}$ (NN + $3N_{\text{loc}}$ -pheno in Fig. 2) with uncertainties reduced by an average factor of 7 compared with 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) [54]. 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 ${}^4\text{He} + d$ potential model.

In this Letter, we carried out an *ab initio* prediction of the ${}^4\text{He}(d, \gamma){}^6\text{Li}$ radiative capture at BBN energies starting from chiral effective field theory (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

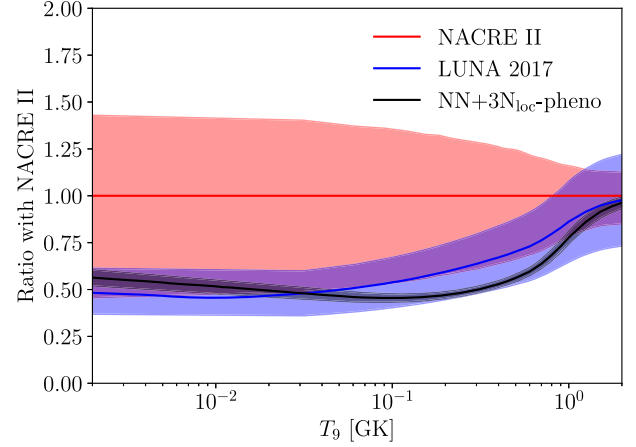


FIG. 2. Ratio of the predicted thermonuclear reaction rates (black line) for the ${}^4\text{He}(d, \gamma){}^6\text{Li}$ with the NACRE-II evaluation (red line) [18] for the ${}^4\text{He}(d, \gamma){}^6\text{Li}$ for different temperature T_9 in GK. Our results are also compared with the recent thermonuclear reaction rate derived from the measurements of the LUNA collaboration (blue line) [54]. The shaded areas correspond to the uncertainty of each calculation (see text for details).

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 Letter, 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 parametrization of the chiral NN + $3N$ Hamiltonian. We reserve that study for future work.

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