Ab Initio Calculation of the Alpha-Particle Monopole Transition Form Factor

Ulf-G. Meißner,[1,2,3] Shihang Shen,[4,*] Serdar Elhatisari,[5,1] and Dean Lee[6]
[1]*Helmholtz-Institut für Strahlen- und Kernphysik and Bethe Center for Theoretical Physics, Universität Bonn, D-53115 Bonn, Germany*
[2]*Institut für Kernphysik, Institute for Advanced Simulation and Jülich Center for Hadron Physics, Forschungszentrum Jülich, D-52425 Jülich, Germany*
[3]*Tbilisi State University, 0186 Tbilisi, Georgia*
[4]*Institute for Advanced Simulation and Institut für Kernphysik, Forschungszentrum Jülich, D-52425 Jülich, Germany*
[5]*Faculty of Natural Sciences and Engineering, Gaziantep Islam Science and Technology University, Gaziantep 27010, Turkey*
[6]*Facility for Rare Isotope Beams and Department of Physics and Astronomy, Michigan State University, East Lansing, Michigan 48824, USA*

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We present a parameter-free *ab initio* calculation of the α-particle monopole transition form factor in the framework of nuclear lattice effective field theory. We use a minimal nuclear interaction that was previously used to reproduce the ground state properties of light nuclei, medium-mass nuclei, and neutron matter simultaneously with no more than a few percent error in the energies and charge radii. The results for the monopole transition form factor are in good agreement with recent precision data from Mainz.

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Introduction.—The ^{4}He nucleus, the α particle, is considered to be a benchmark nucleus for our understanding of the nuclear forces and the few-body methods to solve the nuclear A-body problem [1]. The attractive nucleon-nucleon interaction makes this highly symmetric four-nucleon system enormously stable. Furthermore, its first excited state has the same quantum numbers as the ground state, $J^P = 0^+$ with $J(P)$ the spin (parity), but is located about 20 MeV above the ground state. This large energy of the first quantum excitation makes the system difficult to perturb. This isoscalar monopole resonance of the ^{4}He nucleus presents a challenge to our understanding of nuclear few-body systems and the underlying nuclear forces [2]. Within pionless effective field theory, the ground state and the first excited state of the alpha particle could already be reproduced in Ref. [3], although with some uncertainty in the position of the first excited state to the proton-triton threshold. The recent precision measurement of the corresponding transition form factor of the first excited state to the ground state at the Mainz Microtrom MAMI [4] compared with *ab initio* calculations based on the Lorentz-integral transformation method [5] using phenomenological potentials as well as potentials based on chiral effective field theory, e.g. [6–10], revealed sizable discrepancies as shown in Fig. 3 of Ref. [4].

These new results have spurred a number of theoretical investigations, stressing especially the role of the continuum when including the resonant state which is located close to the two-body breakup threshold [11,12]. In particular, Ref. [12] showed that employing an explicit coupled-channel representation of the no-core Gamow shell model with the $^3\mathrm{H} + p$, $^3\mathrm{He} + n$, and $^2\mathrm{H} + {}^2\mathrm{H}$ reaction channels allows to reproduce the Mainz data. In that paper, the effects of three-nucleon forces were neglected. We remark that the Mainz data are also reproduced by the pioneering work of Ref. [13], which also pointed out the importance of the loosely bound $3N + N$ system, where N denotes a nucleon. However, as noted in Ref. [4], that calculation does not reproduce the low-energy data, more precisely, the two first parameters in the low-momentum expansion of the transition form factor. It was also pointed out that the shape of the transition density obtained from the data in Ref. [4] is significantly different from that obtained theoretically in the literature [14].

Here, we will use the framework of nuclear lattice effective field theory (NLEFT) to present an *ab initio* solution to the problem [15,16]. In particular, we want to address the issue whether one possibly misses parts of the nuclear force which, given a simple spin-0 and isospin-0 nucleus like ^{4}He, would be rather striking. We make use of a so-called minimal nuclear interaction, that has been successfully used to describe the gross properties of light and medium-mass nuclei and the equation of state of neutron matter to a few percent accuracy [17]. It was used in nuclear thermodynamics calculations [18] and *ab initio* studies of clusters in hot dilute matter using the method of light-cluster distillation [19]. A similar action was also successfully applied to investigate the emergent geometry and intrinsic cluster structure of the low-lying states of ^{12}C [20]. In particular, the transition form factor from the Hoyle state to the ground state measured at Darmstadt [21] could be excellently reproduced without any parameter

adjustment. In this context, we mention the work of Ref. [3], which stated that pairs of a deep ground state and a shallow excited state with the same quantum numbers as in ^{4}He also occur in larger nuclei like ^{12}C and ^{16}O. Consequently, it is worth mentioning that within NLEFT, the first *ab initio* calculation of the Hoyle state in ^{12}C was performed [22], which, together with the ground state, is arguably the most known of such pairs. Taking these achievements into account, we believe that the NLEFT framework is well suited to address the issue of the α-particle transition form factor.

Formalism.—In Ref. [17] a minimal nuclear interaction was constructed that reproduces the ground state properties of light nuclei, medium-mass nuclei, and neutron matter simultaneously with no more than a few percent error in the energies and charge radii. It is given by the SU(4)-invariant leading-order effective field theory without pions, formulated on a periodic cubic box of L^3. The Hamiltonian reads

$$H_{\mathrm{SU(4)}} = H_{\mathrm{free}} + \frac{1}{2!}C_2\sum_{\boldsymbol{n}}\tilde{\rho}(\boldsymbol{n})^2 + \frac{1}{3!}C_3\sum_{\boldsymbol{n}}\tilde{\rho}(\boldsymbol{n})^3, \qquad (1)$$

where $\boldsymbol{n} = (n_x, n_y, n_z)$ are the lattice coordinates, H_{free} is the free nucleon Hamiltonian with nucleon mass $m = 938.9$ MeV. The lattice spacing is $a = 1.32$ fm, which corresponds to a momentum cutoff $\Lambda = \pi/a \simeq 471$ MeV, which is also the optimal resolution scale to unravel the hidden spin-isospin symmetry of QCD in the limit of a large number of colors [23]. The density operator $\tilde{\rho}(\boldsymbol{n})$ is defined in the same manner as introduced in Ref. [24],

$$\tilde{\rho}(\boldsymbol{n}) = \sum_i \tilde{a}_i^\dagger(\boldsymbol{n})\tilde{a}_i(\boldsymbol{n}) + s_L\sum_{|\boldsymbol{n}'-\boldsymbol{n}|=1}\sum_i \tilde{a}_i^\dagger(\boldsymbol{n}')\tilde{a}_i(\boldsymbol{n}'), \qquad (2)$$

where i is the joint spin-isospin index, s_L is the local smearing parameter, and the nonlocally smeared annihilation and creation operators with parameter s_{NL} are defined as

$$\tilde{a}_i(\boldsymbol{n}) = a_i(\boldsymbol{n}) + s_{NL}\sum_{|\boldsymbol{n}'-\boldsymbol{n}|=1} a_i(\boldsymbol{n}'). \qquad (3)$$

The summation over the spin and isospin implies that the interaction is SU(4) invariant. The parameter s_L controls the strength of the local part of the interaction, while s_{NL} controls the strength of the nonlocal part of the interaction. The parameters C_2 and C_3 give the overall strength of the two-body and three-body interactions, respectively. For a given value of s_{NL}, C_2, C_3, and s_L are determined by fitting to $A \leq 3$ data. Then, the optimal strength and range of the local and nonlocal parts of the interactions are defined by parametrizing the nuclear binding energies with nuclei with $A \geq 16$ with the Bethe-Weizsäcker mass formula. Note that the local part the interactions is an important factor in nuclear binding, especially for the α-α interaction [25]. These parameters have been determined in Ref. [17] as $C_2 = -3.41 \times 10^{-7}$ MeV^{-2}, $C_3 = -1.4 \times 10^{-14}$ MeV^{-5}, $s_{NL} = 0.5$, and $s_L = 0.061$, and they will be used throughout this work. The effects from the Coulomb interaction are included in perturbation theory. For details, see Ref. [17].

The transition form factor $F(q)$ of the monopole transition is related to the transition density $\rho_{\mathrm{tr}}(r)$ by

$$F(q) = \frac{4\pi}{Z}\int_0^\infty \rho_{\mathrm{tr}}(r) j_0(qr) r^2 dr = \frac{1}{Z}\sum_{\lambda=1}^{\infty}\frac{(-1)^\lambda}{(2\lambda+1)!}q^{2\lambda}\langle r^{2\lambda}\rangle_{\mathrm{tr}}, \qquad (4)$$

with Z the charge of the nucleus under consideration. Here, $Z = 2$, and $\rho_{\mathrm{tr}}(r) = \langle 0_1^+|\hat{\rho}(\vec{r})|0_2^+\rangle$ is the matrix element of the charge density operator $\hat{\rho}(\vec{r})$ between the ground state 0_1^+ and the first excited 0_2^+ state. This definition differs from the one used in Ref. [4] by a factor of $Z/\sqrt{4\pi}$. It is also interesting to consider the low-q expansion of the transition form factor. We use the definition of Ref. [4],

$$\frac{Z|F(q^2)|}{q^2} = \frac{1}{6}\langle r^2\rangle_{\mathrm{tr}}\left[1 - \frac{q^2}{20}\mathcal{R}_{\mathrm{tr}}^2 + \mathcal{O}(q^4)\right], \qquad (5)$$

with $\mathcal{R}_{\mathrm{tr}}^2 = \langle r^4\rangle_{\mathrm{tr}}/\langle r^2\rangle_{\mathrm{tr}}$. The corresponding parameters were extracted in Ref. [4] as $\langle r^2\rangle_{\mathrm{tr}} = 1.53 \pm 0.05$ fm^2 and $\mathcal{R}_{\mathrm{tr}} = 4.56 \pm 0.15$ fm.

Results and discussion.—The first excited state of ^{4}He is a resonance that sits just above the $^3\mathrm{H} + p$ threshold. In order to study this continuum state, we perform calculations using three different cubic periodic boxes with lengths $L = 10$, 11, 12 in lattice units, corresponding to $L = 13.2$ fm, 14.5 fm, 15.7 fm. We then compare results for the different box sizes in order to quantify the residual uncertainties in the resonance energy and wave function due to the finite volume and decay width. The lattice calculations performed in this work follow the same methods as presented in Ref. [20] for the low-lying states of ^{12}C. We use the Euclidean time projection operator $\exp(-Ht)$ to prepare the low-lying states of ^{4}He, starting from some set of initial states with the desired quantum numbers. The operator $\exp(-Ht)$ is implemented using auxiliary-field Monte Carlo simulations with time step size $a_t = (1000\ \mathrm{MeV})^{-1} = 0.197$ fm^{-1}. The total number of time steps is denoted L_t, and so $t = L_t a_t$. While we do not compute the decay width of the 0_2^+ state in this work, new computational algorithms for computing widths of resonances from finite-volume lattice Monte Carlo simulations are currently under development.

We perform coupled channel calculations using three different initial states composed of shell-model wave functions. The first channel contains four particles in the $1s_{1/2}$ state with oscillator frequency $\hbar\omega = 20$ MeV. The second channel has all three particles for ^{3}H in the $1s_{1/2}$

TABLE I. Energy of the ^{4}He ground state (0_1^+) and the first excited state (0_2^+) for different box sizes L. Here, $\Delta E = E(0_2^+) - E(^3\mathrm{H})$ for the same box length L. The error bars include stochastic errors and uncertainties in the Euclidean time extrapolation.

L [fm]	$E(0_1^+)$ [MeV]	$E(0_2^+)$ [MeV]	ΔE [MeV]
13.2	−28.32(3)	−8.37(14)	0.28(14)
14.5	−28.30(3)	−8.02(14)	0.42(14)
15.7	−28.30(3)	−7.96(9)	0.40(9)

state and an excited proton in the $2s_{1/2}$ state. The third channel has one neutron in the $2s_{1/2}$ state and the remaining nucleons in the $1s_{1/2}$ state. In these channels, we use $\hbar\omega =$ 6 MeV for the initial state of the excited particle and $\hbar\omega =$ 14 MeV for the initial state of the $3N$ system. The three-channel calculation accelerates the exponential convergence of the two lowest lying 0^+ states in the limit of infinite Euclidean time, $L_t \to \infty$. In fact, the values of $\hbar\omega$ in the second and third channel were tuned to optimize this convergence, however, the final results do not depend on these particular choices, see Ref. [26] for details. The corresponding ground and first excited state energies are collected in Table I. These compare well with the experimental values of $E(0_1^+) = -28.30$ MeV and $E(0_2^+) = -8.09$ MeV. The ground state energies of the $3N$ systems using an exact calculation at $L = 12$ are $E(^3\mathrm{H}) = -8.36$ MeV and $E(^3\mathrm{He}) = -7.65$ MeV, which compare well with the experimental values of −8.48 and −7.72 MeV, respectively. We note some difference to the energies given in Ref. [17], which can be traced back to the use of larger volumes here. However, for the cases of $L = 8$, 9, 10, our results align with those presented in Ref. [17], albeit with slightly enlarged uncertainties. We have performed calculations with the Coulomb interaction treated nonperturbatively, the resulting energy differences are below 1 per mille, see Ref. [26]. For $L = 12$, we find $\Delta E = E(0_2^+) - E(^3\mathrm{H}) = 0.40(9)$ MeV, consistent with the main finding of Ref. [12]. We note that a recent paper finds that $E(0_2^+)$ and $E(^3\mathrm{H})$ are much closer together [27], in contrast with experimental observations. The results for $L = 10$ and $L = 11$ give very similar results for ΔE. We also find only small differences in the transition form factor results for $L = 10$, 11, 12. In the following we represent results for $L = 12$, corresponding to a box volume of $V = (15.7\ \mathrm{fm})^3$. Note further that when switching off the 3NF, the value of ΔE and the transition form factor increase, entirely consistent with the findings of Ref. [12], see Ref. [26] for details.

Since we are using a short-ranged SU(4) interaction, we can resort to the Efimov analysis of Refs. [28,29] to give an additional argument in favor of explaining why the 0_2^+ state can be accurately predicted by NLEFT using a minimal nuclear interaction. We employ the universal Efimov tetramer relation between the second state in ^{4}He and the triton energy, $E(0_2^+) = 1.01 \times E(^3\mathrm{H})$. In the absence of the Coulomb interaction, the 0_2^+ state should be $0.01 \times 8.48 =$ 0.084 MeV below the triton threshold. The Coulomb energy has no effect on the triton. Adding the Coulomb energy for 0_2^+ from our lattice calculations with $L = 12$, we get $0.46(2) - 0.08 = 0.38(2)$ MeV, which is very close to the observed value of 0.40 MeV.

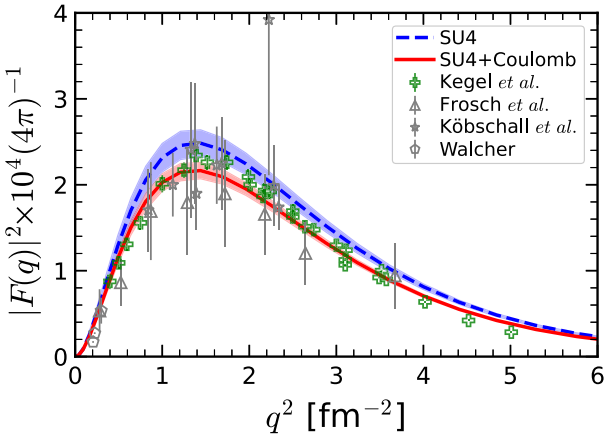

FIG. 1. Calculated monopole form factor of the $0_2^+ \to 0_1^+$ transition in ^{4}He compared to the recent data from Mainz [4] (green squares) and the older data from Refs. [31–33] (gray symbols). Blue dashed line: SU(4) symmetric strong interaction with all parameters determined in Ref. [17]. Red solid line: adding the Coulomb interaction perturbatively. The uncertainty bands in the lattice results include stochastic errors and uncertainties in the Euclidean time extrapolation.

Next, we turn to the analysis of the transition form factor, denoted as $F(q)$. In the framework of NLEFT, observables such as nucleon density distributions, charge radii, and form factors can be computed using the pinhole algorithm [24], which performs a Monte Carlo sampling of the A-body density of the nucleus in position space. Furthermore, the pinhole algorithm can be combined with the first order perturbation theory to compute the corrections to these observables [17]. In this work, we compute the transition form factor $F(q)$ using the pinhole algorithm while the Coulomb interaction is treated using perturbation theory. Further details and additional calculations extending this work will be presented in Ref. [30]. First, we consider the SU(4)-symmetric interactions without Coulomb. The resulting form factor is depicted by the blue dashed line in Fig. 1. It somewhat overshoots the data, although the error band associated with stochastic errors and the large L_t extrapolation almost encompasses the data. Including the Coulomb interaction leads to an overall reduction of the transition form factor as shown by the red solid line in Fig. 1. Overall, we achieve a good reproduction of the data and the uncertainty band is also somewhat reduced. This is due to the fact that inclusion of

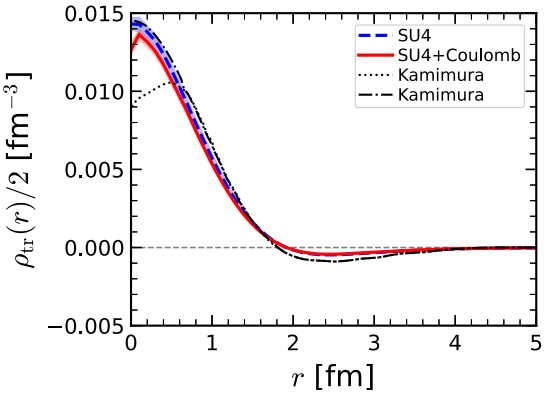

FIG. 2. The transition charge density for the SU(4) interaction (blue dashed line) and the SU(4) plus Coulomb interaction (red solid line) in comparison to the results of Kamimura in Ref. [14]. The black dotted (dash dotted) line corresponds to no node (a node in the transition form factor near $q^2 = 14$ fm^{-2}). The uncertainty bands in the lattice results include stochastic errors and uncertainties in the Euclidean time extrapolation.

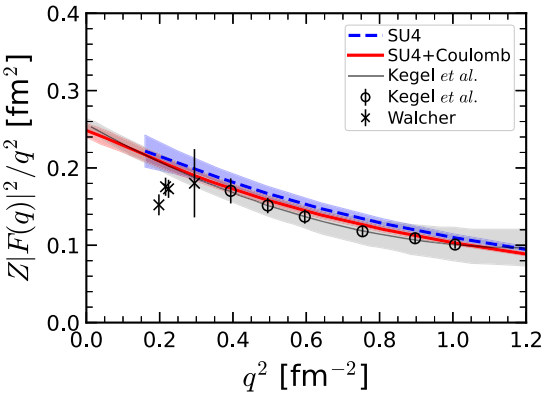

FIG. 3. The low-momentum expansion of the transition form factor for the SU(4) interaction (blue dashed line) and the SU(4) plus Coulomb interaction (red solid line) in comparison to the results of Refs. [4,32]. The uncertainty bands for the NLEFT results are due to the L_t extrapolation. The gray band is from Ref. [4].

the Coulomb interaction leads to smaller fluctuations in the Monte Carlo data when extrapolating to large L_t. Consequently, we find that the nuclear interaction defined in Ref. [17], which has already been shown to reproduce the essential elements of nuclear binding, also leads to a good description of the α-particle transition $0_2^+ \to 0_1^+$ form factor without adjusting any parameters. Note that we have also analyzed the many-body uncertainty underlying our minimal interaction, as detailed in [26]. For $A \leq 4$, this error is much smaller than the statistical errors from the MC simulation and the L_t extrapolation.

The transition density $\rho_{\rm tr}(r)$ underlying the form factor is displayed in Fig. 2, for the SU(4) interaction and the inclusion of the Coulomb interaction. The corresponding curves are very similar to the results of Ref. [14], though we find a less pronounced central depletion when the Coulomb force is included. Note, however, that the definition used there is based on averaging over all four nucleons, while our definition is the charge (proton) density. We account for the charge radius of the proton, $r_p = 0.84$ fm [34], while in Ref. [14] a more phenomenological proton size factor is used.

Now, we consider the low-momentum expansion as given in Eq. (5). The resulting curves for the SU(4) and SU(4) plus Coulomb interactions are shown in Fig. 3. Our results are in good agreement with the results of Ref. [4], which is shown by the gray band. We note again that the error band of the NLEFT calculation is reduced when the Coulomb interaction is included. The corresponding moments of the low-q expansion are $\langle r^2 \rangle_{\rm tr} = 1.48(1)$ fm^2 and $\mathcal{R}_{\rm tr} = 3.61(3)$ fm for the SU(4) interaction fitted in the range $q^2 = 0.09$–0.49 fm^{-2}, and $\langle r^2 \rangle_{\rm tr} = 1.49(1)$ fm^2 and $\mathcal{R}_{\rm tr} = 4.00(4)$ fm for the SU(4) plus Coulomb interaction, fitted in the range $q^2 = 0.04$–0.25 fm^{-2}, as the signals are less noisy at low q^2 when the Coulomb interaction is included.

Summary and discussion.—In this Letter, we have used a minimal nuclear interaction that allows us to describe the gross features of nuclei and nuclear matter with no more than a few percent error to postdict the α particle transition form factor from the first excited to the ground state. This interaction accounts for SU(4) symmetric two- and three-body terms as well as the Coulomb interaction with only four parameters that previously had been determined in Ref. [17]. First, we reproduce the energies of the ground state and the first excited state of ^{4}He. This is a known prerequisite to properly describe the form factor due to the closeness of the first excited state to the ^{3}H + p threshold [12,13]. Having met that prerequisite, we find that the description of the transition form factor and its low-energy expansion is quite satisfactory. The nuclear forces relevant to this system are under good control, and we do not find the puzzle mentioned in Ref. [4]. We were able to accurately reproduce the position of the energy 0_2^+ relative to ^{3}H with a simple interaction and no parameter tuning. This strongly suggests a link between the tuning of the α-α interaction already performed in Ref. [17] and the required tuning of the p-^{3}H interaction to get the correct energy of 0_2^+ relative to ^{3}H. In the future, calculations of the monopole transition form factor can be made more systematic and accurate by using high-fidelity chiral interactions and the machinery of wave function matching [35].

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*Corresponding author: s.shen@fz-juelich.de

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