Corrections to nucleon capture cross sections computed in truncated Hilbert spaces

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Nucleon capture cross sections enter various astrophysical processes. The measurement of proton capture on nuclei at astrophysically relevant low energies is a challenge, and theoretical computations in this long-wavelength regime are sensitive to the long-distance asymptotics of the wave functions. A theoretical foundation for estimating and correcting errors introduced in capture cross sections due to Hilbert space truncation has so far been lacking. We derive extrapolation formulas that relate the infrared regularized capture amplitudes to the infinite basis limit and demonstrate their efficacy for proton-proton fusion. Our results are thus relevant to current calculations of few-body capture reactions such as proton-proton fusion or proton capture on the deuteron, and they also open the way for the use of *ab initio* many-body wave functions represented in finite Hilbert spaces in precision calculations of nucleon capture on heavier nuclei.

Introduction. Processes in which a nucleon is captured by a nucleus occur in many areas of pure and applied physics. They play an important role in big bang nucleosynthesis and in the nuclear astrophysics of stars, novae, x-ray bursts and supernovae; see, e.g., Ref. [1] for a recent review. Capture reaction rates are essential inputs for computations of stellar models [2]. Proton capture cross sections are very difficult to measure at astrophysically relevant energies below the Coulomb barrier, forcing us to rely on theoretical results. Here, *ab initio* computations [3–6] and studies based on effective field theory [7–11] aim at achieving model-independent results with reliable uncertainty estimates.

We note that precise theoretical calculations are a challenge too, because the regime of low energies and long de Broglie wave lengths requires one to employ very large Hilbert spaces. It is therefore important to control the uncertainties in theoretical calculations of cross sections that are due to limitations of finite model spaces. This is the purpose of this work. Let us consider proton-proton fusion, i.e., $p + p \rightarrow d + \nu_e + e^+$, as the simplest example of a proton capture reaction. This reaction has been studied extensively and a calculation that reduces the uncertainty well below 1% would be an important development [2,6,11]. As we will see below, the corrections due to finite Hilbert spaces become relevant if such a precision is aimed at in *ab initio* computations.

Truncation of the Hilbert space imposes ultraviolet (UV) and infrared (IR) momentum cutoffs [12–15], leading to systematic errors in observables. Thus, capture reactions into bound states computed in finite Hilbert spaces will suffer from truncation errors regardless of how well the continuum is treated. An example of previous corrections of such shortcomings is presented in Ref. [16]. Formulas for extrapolation of various bound-state observables to the infinite-basis limit were derived in Refs. [17–20]. In the same spirit, we study and quantify the IR corrections to the capture and fusion cross sections calculated from wave functions represented in truncated Hilbert spaces. We make use of the dependence of the IR length scale L on the parameters of the oscillator basis, which is known for the two-body problem [18], the no-core shell model [21], and many-body product spaces [22]. Below, we also present the IR length relevant for hyperspherical harmonics with Laguerre polynomials as radial wave functions.

Recent progress in *ab initio* computations of reactions and scattering states [23–29] (see also Ref. [30] for a recent review) has made it possible to calculate capture cross sections of medium-mass and heavy nuclei using discrete-basis representations of bound state wave functions. This makes it a timely issue to understand and correct the shortcomings pertaining to the finite Hilbert space treatment of the bound states involved.

Theoretical derivation. In what follows, we focus on the nucleon-nucleon (*NN*) processes as examples where the truncation error can be fully understood. This allows us to derive IR extrapolation formulas that have a more general applicability. The generalization to heavier nuclei will be discussed below. We assume that the nuclear interaction vanishes beyond the range R. Thus, at relative distances $r \geqslant R$ the bound state radial wave function calculated in a truncated basis has the asymptotic form [18]

$$u^{(L)}(r) \rightarrow A_\infty e^{-\gamma_\infty r}[1 - e^{-2\gamma_\infty(L-r)}]. \tag{1}$$

Here, γ_∞ and A_∞ are, respectively, the binding momentum and the asymptotic normalization coefficient in the infinite volume limit [18]. Equation (1) is asymptotically valid for all partial waves. However, its higher order corrections for *s* wave are of $O(e^{-\gamma_\infty(2L+r)})$, much smaller than the $O[1/(\gamma_\infty r)]$ corrections for higher partial waves.

Calculations of capture cross sections in a truncated basis, therefore, effectively involve the radial matrix elements

$$\mathcal{I}_\lambda(k;\eta;L) \equiv \int_0^L dr\, u^{(L)}(r)\, r^\lambda\, u_k(r), \tag{2}$$

where k is the momentum of the scattering wave function $u_k(r)$ in the initial state, η is the Sommerfeld parameter, and λ defines the multipolarity of the transition. For an electromagnetic

capture process, the multipolarity is equal to λ for electric transitions and to $\lambda + 1$ for magnetic transitions. For the weak process, the dominant contribution at low energies comes from $\mathcal{I}_0(k; \eta; L)$.

At $r \geqslant R$ and $kr \gg \eta$, the radial wave function of the initial state has the form

$$u_k(r) \rightarrow \cos\delta_l \, \sin\left[kr - \eta \log(2kr) + \sigma_l - \frac{\pi l}{2} \right]$$
$$+ \sin\delta_l \, \cos\left[kr - \eta \log(2kr) + \sigma_l - \frac{\pi l}{2} \right], \quad (3)$$

with σ_l being the Coulomb phase shift. For the case of neutron capture, $\sigma_l = 0 = \eta$. Apart from the subleading η dependence, Eq. (3) has additional $O[1/(kr)]$ corrections for $l > 0$ even in the absence of Coulomb interaction.

We now proceed to derive the IR truncation error, $\Delta\mathcal{I}_\lambda(k; \eta; L)$, in the matrix element $\mathcal{I}_\lambda(k; \eta; L)$ calculated in Hilbert spaces with $L \gg R$. However, to use the asymptotically valid approximations for the wave functions given in Eqs. (1) and (3), we additionally require $kL \gg \eta$ for proton capture and fusion reactions, and $kL \gg l$ for capture in partial waves with orbital angular momentum l.

We begin by splitting the radial integral, Eq. (2), into two regions,

$$\mathcal{I}_\lambda(k; \eta; L) = \left(\int_0^R + \int_R^L \right) dr \, u_L(r) \, r^\lambda \, u_k(r). \quad (4)$$

The second integral, which is independent of the details of the nuclear interaction, can be evaluated analytically using Eqs. (1) and (3) to give

$$\int_R^L dr \, u^{(L)}(r) \, r^\lambda \, u_k(r) = \int_R^\infty dr \, u^{(\infty)}(r) \, r^\lambda \, u_k(r)$$
$$+ 2\,\text{Re}[f_\lambda(k; \eta; L)], \quad (5)$$

where $u^{(\infty)}(r)$ is $u^{(L)}(r)$ at $L \rightarrow \infty$, and

$$f_\lambda(k; \eta; L) = \frac{i}{2} A_\infty \, e^{i(\delta_l + \sigma_l - \pi l/2)} \, (2k)^{-i\eta} [(\gamma_\infty - ik)^{(-\lambda - 1 + i\eta)}$$
$$\times \, \Gamma(\lambda + 1 - i\eta, \gamma_\infty L - ikL)$$
$$- e^{-2\gamma_\infty L} (-\gamma_\infty - ik)^{(-\lambda - 1 + i\eta)}$$
$$\times \, \Gamma(\lambda + 1 - i\eta, -\gamma_\infty L - ikL)], \quad (6)$$

is the result of an overlap integral of the asymptotic incoming and outgoing scattering wave function with the finite volume bound state wave function.

Here $\Gamma(c, z)$ is the complex continuation of the incomplete gamma function [31]. We have dropped terms of $O(e^{-\gamma_\infty(2L-R)})$ in Eq. (5). For asymptotically large values of $\gamma_\infty L$, we can also replace $u^{(L)}(r)$ in the first integral in Eq. (4), which includes the contribution from the $r \ll L$ region, by $u^{(\infty)}(r)$. Equation (4) can then be written as

$$\Delta\mathcal{I}_\lambda(k; \eta; L) = \mathcal{I}_\lambda(k; \eta; \infty) - \mathcal{I}_\lambda(k; \eta; L)$$
$$= -2\,\text{Re}[f_\lambda(k; \eta; L)], \quad (7)$$

where

$$\mathcal{I}_\lambda(k; \eta; \infty) = \int_0^\infty dr \, u^{(\infty)}(r) \, r^\lambda \, u_k(r) \quad (8)$$

is the radial matrix element $\mathcal{I}_\lambda(k; \eta; L)$ at $L \rightarrow \infty$.

In addition to the exponentially suppressed term we explicitly dropped above, we have also neglected the contributions to $\Delta\mathcal{I}_\lambda(k; \eta; L)$ from the higher-order η dependence and higher partial wave corrections to Eqs. (1) and (3). These terms scale as $\Delta\mathcal{I}_{\lambda-1}(k; \eta; L)$ and are therefore only suppressed by a factor of $1/L$. Using the leading-order approximation in the asymptotic expansion of the Γ function,

$$\Gamma(c, z) = z^{c-1} e^{-z} \left(1 + \frac{c-1}{z} + \cdots \right), \quad (9)$$

valid for $|z| \gg 1$ and $|\arg z| < 3\pi/2$, in Eq. (6), the IR truncation error in the capture matrix element reduces to a much simpler form,

$$\Delta\mathcal{I}_\lambda(k; \eta; L) = \frac{2A_\infty \gamma_\infty}{\gamma_\infty^2 + k^2} L^\lambda e^{-\gamma_\infty L}$$
$$\times \sin\left(\delta_l + \sigma_l - \frac{\pi l}{2} + kL - \eta \log 2kL \right), \quad (10)$$

for asymptotically large values of $\gamma_\infty L$. We note that the approximation for $\Gamma(c, z)$ used here in order to arrive at Eq. (10) is exact for $\lambda = 0$ neutron capture. However, at larger values of λ and η, this approximation gets worse and it may be necessary to obtain the IR truncation error using Eqs. (6) and (7) instead.

Since the relative error in the cross section is twice that in the matrix element, we find from Eq. (10) that the IR truncation error in the cross section scales as $e^{-\gamma_\infty L}$. We note that this $e^{-\gamma_\infty L}$ convergence with increasing $\gamma_\infty L$ is much slower than the $e^{-2\gamma_\infty L}$ behavior found for bound-state observables such as energies and radii [17].

The extrapolation formula, Eq. (7), and its asymptotic form, Eq. (10), are the main results of this work. These equations hold for heavier nuclei and for all reasonable models of the nuclear Hamiltonian because the single-particle wave functions have the asymptotic forms given in Eqs. (1) and (3) in the range $R \leqslant r < L$. They are valid for neutron capture as well as for proton capture unless the energy is low enough to warrant the use of Coulomb wave functions $F_l(kr)$ and $G_l(kr)$ for all $r \lesssim L$ instead of the sine and the cosine functions in Eq. (3). Furthermore, the same radial matrix elements contribute to break-up cross sections as well.

Numerical results. For numerical calculations, we use the chiral effective field theory (EFT) interaction from Ref. [32]. We obtain the pp and np scattering states by solving the momentum-space Schrödinger equation. We then calculate the radial matrix elements, $\mathcal{I}_\lambda(k; \eta; L)$, numerically for a range of L values by expanding the deuteron wave function in HO bases of varying dimensionality.

In the IR regime, the finite harmonic oscillator basis we use is indistinguishable from a spherical box with radius [18]

$$L = \sqrt{2(N + 3/2 + 2)} \, b. \quad (11)$$

Here N is the maximum number of oscillator quanta and $b = \sqrt{1/(\mu\Omega)}$, the oscillator length for a system with reduced mass μ and oscillator frequency Ω, respectively. The hyperspherical harmonics basis is popular in few-body problems [33,34] and has also been used in the computation of capture
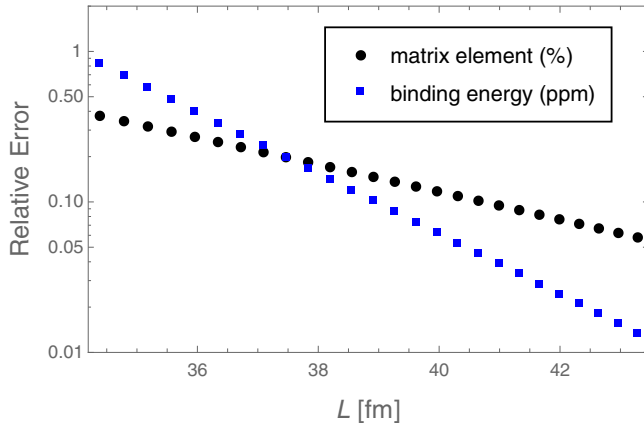
FIG. 1. IR truncation error in the axial-vector matrix element of pp fusion at 50-keV center-of-mass energy (black circles) and in the deuteron binding energy (blue squares). The relative errors for the axial-vector matrix elements and those for the binding energy are expressed in percentage and parts per million (ppm) respectively.

reactions [3,6]. For this reason, we also discuss the IR length L_{HH} relevant for this method. Using the hyperradius ρ and a momentum scale β, the hyperradial basis functions

$$\sqrt{\frac{m!\beta^{3A-3}}{\Gamma(a+m+1)}}(\beta\rho)^{\frac{a-3A+4}{2}}e^{-\frac{1}{2}\beta\rho}L_m^a(\beta\rho)$$

are orthonormal under the hyperradial integration measure $d\rho\rho^{3A-4}$, which is adequate for a translationally invariant A-body system [35,36]. Here L_m^a denotes the associated Laguerre polynomial and a is a parameter. Noting the similarity between the hyperradial wave functions and the radial wave functions of the three-dimensional harmonic oscillator, i.e., identifying $a = l + 1/2$ and $N = 2n + l$ in Eq. (11), where n is the largest degree of the Laguerre polynomial used, we infer that the IR length for the hyperspherical radial basis is

$$L_{\mathrm{HH}} = (4n + 2a + 6)\beta^{-1}. \qquad (12)$$

For the NN processes, it is computationally feasible to calculate $\mathcal{I}_\lambda(k;\eta;L)$ in a large enough basis and obtain an accurate numerical approximation to $\mathcal{I}_\lambda(k;\eta;\infty)$. We begin by comparing the numerical truncation error, $\Delta\mathcal{I}_\lambda(k;\eta;L)$, thus obtained with those predicted by Eq. (10).

In Fig. 1, we plot the relative error due to a IR cutoff in the matrix element of the Gamow-Teller operator between the deuteron s-wave and the pp $^1S_0$ wave functions at 50-keV center-of-mass energy, $\Delta\mathcal{I}_0(k;\eta;L)/\mathcal{I}_0(k;\eta;\infty)$. For comparison, we also show the relative IR truncation error in the deuteron binding energy. The error in the matrix element at $L = 35$ fm is about 0.3%, which translates to an error in the cross section of about 0.6%. The size of this error is relevant for computing pp fusion cross sections to percentage precision, which recent calculations [6] aim at. In contrast, the deuteron binding energy shows a much faster IR convergence—the relative error at $L = 35$ fm is about 0.5×10^{-6}—reinforcing our claim that a basis that gives highly accurate results for bound state observables may still yield large systematic errors in capture cross section calculations. Furthermore, we have
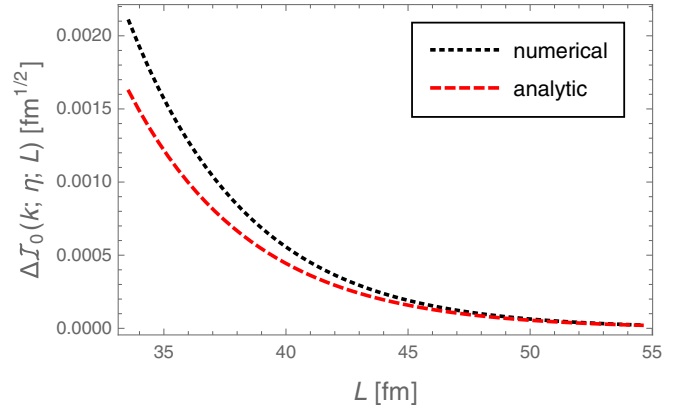
checked and verified that the L dependences of these errors are consistent with theoretical predictions: approximate $e^{-\gamma_\infty L}$ behavior for the capture matrix element as derived above, and $e^{-2\gamma_\infty L}$ for deuteron binding energy [18].

In Fig. 2, we plot the truncation error for the pp fusion matrix element shown earlier in Fig. 1 along with the analytic result given by Eq. (10). Since $\eta = 0.5$ is not particularly small, we get good agreement between the analytic formula and numerical data at larger values of L, where the corrections to Eq. (10) due to higher-order η dependence are less important.

For comparison, we plot $\Delta\mathcal{I}_\lambda(k;\eta;L)$ for the same process at 1-MeV center-of-mass energy for the same range of L values in Fig. 3. Since $\eta = 0.11 \ll 1$ at this energy, we find a much better agreement even at smaller L.

Finally, in Fig. 4, we plot the IR truncation error in the matrix element of the electric dipole ($E1$) operator between the deuteron s wave and the np $^3P_1$ wave functions, which contributes to the radiative np capture,

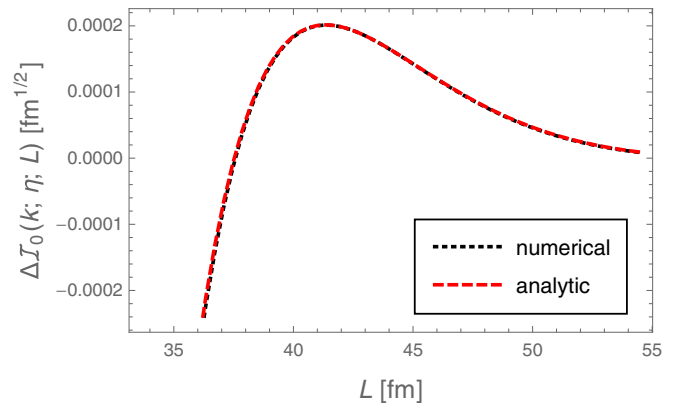$$n + p \rightarrow d + \gamma, \qquad (13)$$

FIG. 2. Numerical and analytic results for the correction $\Delta\mathcal{I}_0(k;\eta;L)$ to the radial overlap between the $^1S_0$ pp scattering wave function at 50-keV center-of-mass energy and the deuteron s-wave state.

FIG. 3. Numerical and analytic results for the correction $\Delta\mathcal{I}_0(k;\eta;L)$ to the radial overlap between the $^1S_0$ pp scattering wave function at 1-MeV center-of-mass energy and the deuteron s-wave state.
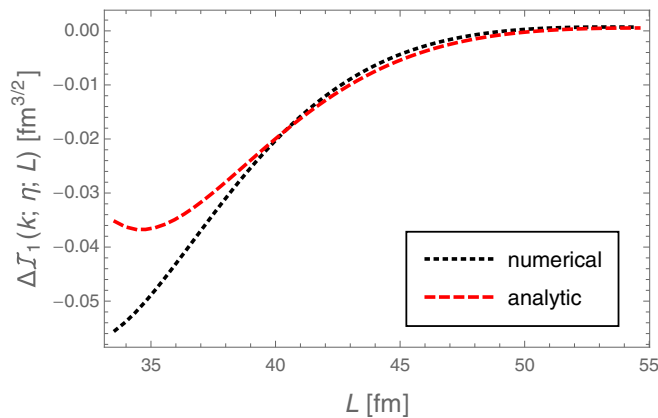
FIG. 4. Numerical and analytic results for the correction $\Delta\mathcal{I}_1(k;\eta;L)$ to the radial matrix element of the $E1$ operator between the np $^3P_1$ scattering wave function at 1-MeV center-of-mass energy and the deuteron s-wave state.

and its reverse process, deuteron photodisintegration. Here the analytic formula for $\Delta\mathcal{I}_\lambda(k;\eta;L)$ has neglected terms from the $O[1/(kr)]$ corrections to Eq. (3). Since these terms are suppressed by a factor of $1/L$, we get a better agreement between the analytic and the numerical results at larger L values.

The analytic results shown above in Figs. 2–4 were not fit to the data. The quantities A_∞, γ_∞, and δ_l were known *a priori* from the wave functions, and the IR truncation error was thus completely predicted by Eq. (10). For systems with $A > 2$, however, extracting values for the single-particle separation energies, asymptotic normalization coefficients, and phase shifts might not be as straightforward. Moreover, the use of our analytic results in practical applications is to obtain $\mathcal{I}_\lambda(k;\eta;\infty)$ by extrapolation when the size of the basis is constrained due to unavailability of computational resources. One computes $\mathcal{I}_\lambda(k;\eta;L)$ at several large values of L, and fits Eq. (10) [or, if required, Eq. (7)] to these data with $\mathcal{I}_\lambda(k;\eta;\infty)$, A_∞, γ_∞, and δ_l treated as fit parameters. We present the results of such extrapolations for the pp fusion process in Table I. The extrapolations are robust not only at 1 MeV but also at 50-keV center-of-mass energy, where the neglected contributions to our extrapolation formula are larger. We found that the differences in $\mathcal{I}_\lambda(k;\eta;\infty)$ values for different sets of input data are very small compared to those of the other fit parameters, A_∞, γ_∞, and δ_l (data not shown). These are

not determined very well by the fit because of the relatively large number of fit parameters in Eq. (10). However, we want to remark that in any standard calculation these could be fit to several other observables such as finite volume binding energies or radii thereby increasing the constraints on these parameters significantly.

Since Eq. (10) is valid at asymptotically large values of L, we obtain better fits when the input data contain larger L values. However, even for smaller L, the extrapolation error is much smaller than the IR truncation error one would make by avoiding extrapolation and simply using $\mathcal{I}_0(k;\eta;L_{max})$ instead.

Summary. We studied the dependence of the nucleon capture cross section on the radius L of the hard wall with Dirichlet boundary condition, which arises as an effective infrared cutoff when the bound state wave function is represented in a truncated basis. We presented an expression of this radius for computations based on hyperspherical harmonics. We showed that the infrared convergence of the cross section thus calculated is much slower than that of bound state properties whose errors generally scale as $e^{-2\gamma_\infty L}$ [17,18,20]. We also showed that this feature can lead to errors in the pp fusion cross section that are comparable in size to uncertainties induced by the nucleon-nucleon interaction and the electroweak current operator in state-of-the-art calculations [6,11]. We derived a simple analytic formula for controlled extrapolation of the cross section to the infinite basis limit. By exploiting our ability to calculate the two-body wave function for a very wide range of basis size while concurrently maintaining ultraviolet convergence, we tested our predictions for two different two-nucleon capture processes. Our extrapolation formula also holds for $A > 2$ nuclei since their single-particle bound- and scattering-state wave functions also have the form given respectively by Eqs. (1) and (3). However, for the proton capture process, the large value of η in heavier nuclei restricts the domain of validity of our extrapolation formula to very high energies. In such case, one needs to replace Eq. (3) by the full Coulomb wave function to compute the IR correction numerically. An analytic derivation of such results, which could facilitate calculations at the energy regime relevant to the rp-process, is left for future work.

TABLE I. Values of $\mathcal{I}_0(k;\eta;\infty)$ (in fm$^{1/2}$) for pp fusion at 50 keV ($\eta = 0.50$) and 1 MeV ($\eta = 0.11$) center-of-mass energies, obtained by fitting Eq. (10) to the $(L,\mathcal{I}_0(k;\eta;L))$ data for L ranging from L_{min} to L_{max} (in fm). The fit results agree very well with the numerically approximated values of $\mathcal{I}_0(k;\eta;\infty)$, which are 0.4711 and 2.592 fm$^{1/2}$ for $\eta = 0.50$ and $\eta = 0.11$, respectively, for all fit intervals.

		$\eta = 0.50$			$\eta = 0.11$		
L_{min}	L_{max}	$\mathcal{I}_0(k;\eta;L_{min})$	$\mathcal{I}_0(k;\eta;L_{max})$	$\mathcal{I}_0(k;\eta;\infty)$	$\mathcal{I}_0(k;\eta;L_{min})$	$\mathcal{I}_0(k;\eta;L_{max})$	$\mathcal{I}_0(k;\eta;\infty)$
15.30	20.29	0.4063	0.4440	0.4704	2.585	2.621	2.590
20.29	24.28	0.4440	0.4583	0.4712	2.621	2.611	2.592
15.30	24.28	0.4063	0.4583	0.4706	2.585	2.611	2.591
15.30	39.51	0.4063	0.4708	0.4711	2.585	2.592	2.592

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