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Charged-particle bound states in periodic boxes

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We consider the binding energy of a two-body system with a repulsive Coulomb interaction in a finite periodic volume. We define the finite-volume Coulomb potential as the usual Coulomb potential, except that the distance is defined the shortest separation between the two bodies in the periodic volume. We investigate this problem in one and three-dimensional periodic boxes and derive the asymptotic behavior of the volume dependence for bound states with zero angular momentum in terms of Whittaker functions. We benchmark our results against numerical calculations and show how the method can be used to extract asymptotic normalization coefficients for charged-particle bound states. The results we derive here have immediate applications for calculations of atomic nuclei in finite periodic volumes for the case where the leading finite-volume correction is associated with two charged clusters.

Finite-volume (FV) simulations in cubic boxes with periodic boundary conditions have emerged as a well established theoretical technique to study quantum systems. Pioneered by Lüscher in a series of highly influential papers [1–3] that showed how real-world properties of a quantum system are encoded in how its discrete energy levels change as volume size is varied, the method has become a standard approach for example in Lattice Quantum Chromodynamics (LQCD) to extract scattering information for hadronic systems. Over the past decade, driven by progress in computing that enables simulations of increasingly complex systems, extending the technique in various directions has become an area of very active research [4–20]. Moreover, few-body approaches formulated in FV can be used to match and extrapolate LQCD results to an effective field theory (EFT) description [21–24].

When simulated in FV, bound-state energy levels have an exponential dependence on the size L of the periodic box that encodes asymptotic properties of the state's wavefunction in infinite volume [1, 25, 26]. For a general bound state of $N \geq 2$ particles with lowest breakup into two clusters with A and $N - A$ particles, respectively, the volume dependence of the (binding) energy, $\Delta E_N(L) \equiv E_N(\infty) - E_N(L)$ with $E_N(L) = -B_N(L)$ denoting the energy at volume L , has been shown to be [27, 28]

$$\Delta E_N(L) = (-1)^{\ell+1} \sqrt{\frac{2}{\pi}} f(d) \mu_{A|N-A}^{-1} |A_\infty|^2 \times \kappa_{A|N-A}^{2-d/2} L^{1-d/2} K_{d/2-1}(\kappa_{A|N-A} L), \quad (1)$$

with d the number spatial dimensions, $f(d)$ a normalization factor, and $K_{d/2-1}$ a modified Bessel function. $\kappa_{A|N-A} = \sqrt{2\mu_{A|N-A}(B_N - B_A - B_{N-A})}$ with the reduced mass $\mu_{A|N-A}$ of the two-cluster system and the cluster binding energies B_A and B_{N-A} is the relevant momentum scale. Moreover, A_∞ is the asymptotic normalization coefficient (ANC) of the cluster wavefunction, a quantity that plays an important role for the descrip-

tion of low-energy capture processes. Eq. (1) implies that both $\kappa_{A|N-A}$ and A_∞ can be extracted by fitting the volume dependence of numerical simulations. This is in principle an efficient way to compute ANCs from *ab initio* calculations at finite volume. Unfortunately, most cases of astrophysical interest involve two clusters each with nonzero electric charge, and the analogous expression for Eq. (1) for charged clusters had not been derived.

In this letter we address this problem and determine the leading volume dependence for bound states composed of two charged particles. While there have been studies of finite-volume electromagnetic corrections using perturbation theory [29–34], we derive the analytic form with fully nonperturbative Coulomb repulsion. The non-perturbative nature of the Coulomb interaction becomes important in medium-mass and heavy nuclei with a significant number of protons. The work presented here has immediate applications to finite-volume simulations of bound nuclei using *ab initio* Lattice EFT [35–39], and the definition of the finite-volume Coulomb interaction we use here is the same as in Lattice EFT. We derive the analog for Eq. (1) when the relevant continuum threshold corresponds to two charged particles. While we focus on the case of two charged point particles, our results can be regarded as the leading term for the multipole expansions of the permanent and/or induced cluster charge densities.

Derivation We consider a two-body system of particles interacting via a finite-range central potential V plus a repulsive Coulomb potential V_C . For simplicity we assume that V is local, $\langle \mathbf{r} | V | \mathbf{r}' \rangle = V(r) \delta^{(3)}(\mathbf{r} - \mathbf{r}')$, but all results remain valid for a general non-local short-range potential. The interaction range R is the smallest distance for which it holds that $V(r) = 0$ if $r = |\mathbf{r}| > R$. The Coulomb potential is given by

$$V_C(r) = \frac{\gamma}{2\mu r}, \quad \gamma = 2\mu\alpha Z_1 Z_2 > 0, \quad (2)$$

where μ denotes the reduced mass of the two-body system, $\alpha \approx 1/137$ is the electromagnetic fine-structure con-

stant, and $Z_{1,2}$ are the charges of the two particles. The Hamiltonian of the system is given by $H = H_0 + V + V_C$ with the kinetic-energy operator H_0 . If we consider the system enclosed in a periodic cubic box with edge length L , the Hamiltonian becomes

$$H_L = H_0 + V_{\{L\}} + V_{C,\{L\}}. \quad (3)$$

The finite-range potential is easily made periodic by defining $V_{\{L\}}(\mathbf{x}) = \sum_{\mathbf{n}} V(\mathbf{x} - \mathbf{n}L)$. Such a definition remains valid up to negligible corrections for short-range potentials that do not have a strict finite range but fall off faster than any power law. For the Coulomb potential, however, the long-range tail $\sim r^{-1}$ complicates matters. To obtain a well-defined periodic extension of V_C , we let $V_{C,\mathbf{n}L}$ be a shifted version of V_C , centered at $\mathbf{n}L$ and clipped such that it is non-zero only within the box of edge length L around its center. With d the dimension of our space and $B = [-L/2, L/2]$, we define $V_{C,\mathbf{n}L} = \theta_{B^d}(\mathbf{r} - \mathbf{n}L)V_C(\mathbf{r} - \mathbf{n}L)$ with $\theta_{B^d}(\mathbf{r}) = 1$ for $\mathbf{r} \in B^d$ and vanishing otherwise. Equipped with these clipped and shifted potentials we can now define

$$V_{C,\{L\}}(\mathbf{r}) = \sum_{\mathbf{n}} V_{C,\mathbf{n}L}(\mathbf{r}). \quad (4)$$

Effectively, this definition implies that we simply let the Coulomb tail grow with the box. We note that Lattice QCD+QED calculations use a different approach and define a periodic FV Coulomb potential $U_L(\mathbf{r})$ by subtracting the ‘‘zero mode’’ in momentum space [30]. In the Supplemental Material [40] we show that this $U_L(\mathbf{r})$ can be expanded to have exactly $V_{C,\{L\}}(\mathbf{r})$ as first term, with a dominant correction contributing an $\mathcal{O}(1/L)$ constant shift to the binding energy.

We assume now that the total potential $V + V_C$ is such that the system supports an S -wave bound state $|\psi_\infty\rangle$ with energy $-E_\infty < 0 = -\kappa_\infty^2/(2\mu)$ in infinite-volume, *i.e.*, $H|\psi_\infty\rangle = (H_0 + V_C + V)|\psi_\infty\rangle = -E_\infty|\psi_\infty\rangle$, and our goal is to derive an expression for the finite-volume energy shift $\Delta E(L) = E_\infty - E(L)$, where $E(L)$ denotes the energy of the state at volume L , *i.e.*, $H_L|\psi_L\rangle = E(L)|\psi_L\rangle$. In a simplified setup that considers the Coulomb potential (2) in one spatial dimension, it is possible to directly use the boundary condition imposed on the finite-volume wavefunction at the edge of the box to obtain the energy shift as

$$\Delta E(L) = \frac{\kappa_\infty A_\infty^2}{\mu} e^{i\pi\bar{\eta}} \frac{W'_{-\bar{\eta}, \frac{1}{2}}(\kappa L)}{W'_{\bar{\eta}, \frac{1}{2}}(-\kappa L)} + \mathcal{O}[e^{-2\kappa L}], \quad (5)$$

where A_∞ is the ANC of the infinite-volume wavefunction, $W_{\bar{\eta}, \frac{1}{2}}(z)$ with $\bar{\eta} = \gamma/(2\kappa_\infty)$ is a Whittaker function, and the prime denotes the derivative with respect to the argument. We point out that phase factor in Eq. (5) is crucial to ensure that overall $\Delta E(L)$ is real. A full derivation of this result is provided in the Supplemental Material [40].

For the three-dimensional system, the infinite-volume bound-state wavefunction for $r = |\mathbf{x}| \geq R$ is given by $\psi_\infty(\mathbf{x}) = A_\infty W_{-\bar{\eta}, 1/2}(2\kappa r)/(\sqrt{4\pi r})$. A simple treatment of the 3D system based on the periodic boundary condition is not possible because the long-range tail r^{-1} combined with the breaking of spherical symmetry by the box-shaped finite volume renders the setup too complicated. We therefore use an alternative formalism, starting with an intermediate Hamiltonian $\tilde{H}_L = H_0 + V_{C,\{L\}} + V$ that includes the truncated periodic Coulomb potential, but leaves the short-range potential V as in infinite volume. We can write $\tilde{H}_L = H + \epsilon\Delta V_C$ for $\epsilon \rightarrow 1$, with

$$\begin{aligned} \Delta V_C &= V_{C,\{L\}} - V_C = \sum_{\mathbf{n} \in \mathbb{Z}^3} \Delta V_{C,(\mathbf{0},\mathbf{n})L}, \quad (6) \\ \Delta V_{C,(\mathbf{n},\mathbf{n}')L}(\mathbf{x}) &= \theta_{B^3}(\mathbf{x} - \mathbf{n}'L) \\ &\quad \times [V_{C,\mathbf{n}'L}(\mathbf{x}) - V_C(\mathbf{x} - \mathbf{n}L)]. \quad (7) \end{aligned}$$

For the exact ground state $|\tilde{\psi}_L\rangle$ of \tilde{H}_L we have $\tilde{H}_L|\tilde{\psi}_L\rangle = -\tilde{E}(L)|\tilde{\psi}_L\rangle$, and we can now treat ΔV_C as a perturbation on top of this state. To that end we write

$$\begin{aligned} (H + \epsilon\Delta V_C)(|\tilde{\psi}_L^{(0)}\rangle + \epsilon|\tilde{\psi}_L^{(1)}\rangle + \dots) \\ = (\tilde{E}^{(0)} + \epsilon\Delta\tilde{E}^{(1)} + \dots)(|\tilde{\psi}_L^{(0)}\rangle + \epsilon|\tilde{\psi}_L^{(1)}\rangle + \dots), \quad (8) \end{aligned}$$

where to lowest order we have $|\tilde{\psi}_L^{(0)}\rangle = |\psi_\infty\rangle$ and $\tilde{E}^{(0)} = -E_\infty$. The leading volume dependence will be found below in terms of just $|\tilde{\psi}_L^{(0)}\rangle$, and the main purpose of the perturbative treatment is that it allows us to derive explicit bounds for subleading corrections. To conclude the basic setup, we note that at this stage all L dependence comes from the definition of ΔV_C , and there is no L -periodic boundary condition imposed on $|\tilde{\psi}_L\rangle$. We use $|\tilde{\psi}_L\rangle$ in order to construct an ansatz for the actual ground state $|\psi_L\rangle$ of H_L . In the following we write equations explicitly in configuration space and define

$$\tilde{\psi}_{L,0}(\mathbf{x}) = \sum_{\mathbf{n} \in \mathbb{Z}^3} \tilde{\psi}_L(\mathbf{x} - \mathbf{n}L), \quad (9)$$

i.e., we approximate the exact finite-volume solution by summing shifted copies of the exact eigenstate of \tilde{H}_L introduced above. Using the ansatz $\tilde{\psi}_{L,0}(\mathbf{x})$, we can follow steps very similar to the derivation for neutral particles [1, 25]. Applying H_L to $\tilde{\psi}_{L,0}(\mathbf{x})$, we obtain

$$\begin{aligned} H_L\tilde{\psi}_{L,0}(\mathbf{x}) &= -\tilde{E}(L)\tilde{\psi}_{L,0}(\mathbf{x}) + \sum_{\mathbf{n}, \mathbf{n}' \neq \mathbf{n}} V(\mathbf{x} - \mathbf{n}'L) \\ &\quad \times \tilde{\psi}_L(\mathbf{x} - \mathbf{n}L) \equiv -\tilde{E}(L)\tilde{\psi}_{L,0}(\mathbf{x}) + \zeta(\mathbf{x}), \quad (10) \end{aligned}$$

with $\zeta(\mathbf{x}) = \sum_{\mathbf{n}} \sum_{\mathbf{n}' \neq \mathbf{n}} V(\mathbf{x} - \mathbf{n}'L)\tilde{\psi}_L(\mathbf{x} - \mathbf{n}L)$. This function only involves the short-range interaction V and scales as $\zeta(\mathbf{x}) \sim \mathcal{O}(e^{-\kappa L})$ for large $|\mathbf{x}|$. For the exact finite-volume solution $|\psi_L\rangle$, it holds that $|\psi_L\rangle =$

$\beta|\tilde{\psi}_{L,0}\rangle + |\tilde{\psi}'_L\rangle$, with $|\tilde{\psi}'_L\rangle = \mathcal{O}(e^{-\kappa L})$ and β chosen so that $\langle\tilde{\psi}'_L|\tilde{\psi}_{L,0}\rangle = 0$. We emphasize here that if instead we had used the naive ansatz $\psi_{L,0}(\mathbf{x})$ that replaces $\tilde{\psi}_L$ with ψ_∞ in Eq. (9), as it is appropriate for neutral particles, we would end up with the weaker asymptotic scaling $\mathcal{O}(e^{-\kappa L/2})$ for $|\tilde{\psi}'_L\rangle$, which would lead to unacceptably large subleading corrections. We now write the overall energy shift at volume L as $\Delta E(L) = \Delta E^*(L) + \Delta\tilde{E}(L)$, where $\Delta\tilde{E}(L) = E_\infty - \tilde{E}(L)$ and

$$\Delta E^*(L) = E(L) - \tilde{E}(L) = \frac{\langle\tilde{\psi}_{L,0}|\zeta\rangle}{\langle\tilde{\psi}_{L,0}|\tilde{\psi}_{L,0}\rangle} + \mathcal{O}(e^{-3\kappa L/2}). \quad (11)$$

The leading volume dependence stems from $\Delta E^*(L)$, for which with

$$\zeta(\mathbf{x}) = \sum_{|\mathbf{n}|=1} V(\mathbf{x})\tilde{\psi}_L(\mathbf{x} - \mathbf{n}L) + \mathcal{O}(e^{-\sqrt{2}\kappa L}), \quad (12)$$

and $\langle\tilde{\psi}_{L,0}|\tilde{\psi}_{L,0}\rangle = 1 + \mathcal{O}(e^{-\kappa L})$ we obtain

$$\Delta E^*(L) = \sum_{|\mathbf{n}|=1} \int_{B^3} d^3x \tilde{\psi}_L(\mathbf{x})V(\mathbf{x})\tilde{\psi}_L(\mathbf{x} - \mathbf{n}L) \quad (13)$$

up to terms $\mathcal{O}(e^{-\sqrt{2}\kappa L})$. This expression can be further evaluated by considering explicitly $\mathbf{n} = -\hat{z}$ and exploiting the symmetry of the wavefunction. As we explain further in the Supplemental Material [40], this ultimately leads to

$$\Delta E(L) = \underbrace{-\frac{3A_\infty^2}{\mu L} \left[W_{-\bar{\eta}, \frac{1}{2}}(\kappa L) \right]^2}_{\equiv \Delta E_0(L)} + \Delta\tilde{E}(L) + \Delta\tilde{E}'(L) + \mathcal{O}(e^{-\sqrt{2}\kappa L}). \quad (14)$$

Besides higher-order exponential corrections—which actually involve Whittaker functions but can be expressed as $\mathcal{O}(e^{-\sqrt{2}\kappa L})$ asymptotically—there are two correction terms in Eq. (14): $\Delta\tilde{E}(L)$ has been defined already in above Eq. (11), and $\Delta\tilde{E}'(L)$ is explained further in the Supplemental Material [40]. Our perturbative setup makes it possible to derive the asymptotic scaling of both these correction terms, the full details of which are also presented in the Supplemental Material [40]. It turns out that although their detailed forms are quite different, both terms actually scale the same asymptotically, namely

$$\Delta\tilde{E}(L), \Delta\tilde{E}'(L) = \mathcal{O}\left(\frac{\bar{\eta}}{(\kappa L)^2}\right) \times \Delta E_0(L), \quad (15)$$

where $\Delta E_0(L)$ is the leading volume dependence as defined in Eq. (14).

Numerical examples We evaluate the performance of Eq. (14) with explicit numerical calculations. To that end we use the “generator code” of Ref. [27], extended to

include the Coulomb interaction, to compute 1D and 3D bound states in boxes with a range of sizes. The volume dependence of these energies we then fit the appropriate expressions for $\Delta E(L)$ to extract the infinite-volume binding momenta and ANCs. We use units that set $\hbar = 1$ and express all physical quantities in terms of the particle mass m , which we also set to unity.

The generator code constructs the finite-volume Hamiltonian based on a simple lattice discretization (see Ref. [28] for details). Because $V_C(r)$ is singular at $r = 0$, we regularize it at short distances. While the simplest way to achieve this is a simple cut (setting $V_C(r) = 0$ for r less than some small range), we instead multiply $V_C(r)$ by a Gauss regulator $(1 - e^{-r^2/R_C^2})$. Such a smooth regulator is preferable for our lattice setup, which would suffer from substantial discretization artifacts with a sharp cutoff. We choose $R_C < R$ (the range of the short-range potential V) so that we can interpret the short-distance Coulomb regularization as merely a redefinition of V , which we otherwise choose as attractive local Gaussian potentials, $V(r) = V_0 e^{-r^2/R^2}$. We use $R = 1$ and $R_C^2 = 0.1$ in all calculations and we emphasize that the actual concrete form of the potential at small r is irrelevant because the expression for $\Delta E(L)$ is universal and does not depend on any particular choice for the short-range interaction.

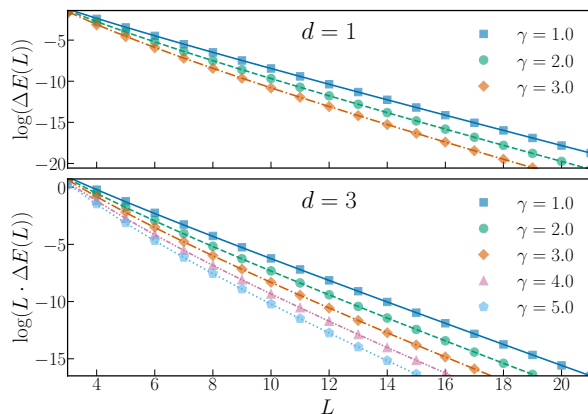


Figure 1. Finite-volume energy shifts for two-body system with attractive Gaussian interaction plus repulsive Coulomb force of varying strength γ in one (upper panel) and three (lower panel) dimensions. For each γ the attraction is adjusted to fix the ground state at $\kappa_\infty \approx 0.86$ in infinite volume. All quantities are given in units of the mass $m = 1$ (see text).

In Fig. 1 we show our numerical results for 1D and 3D systems (in the upper and lower panels, respectively). For each case we use a logarithmic scale for the vertical axis, and we have scaled $\Delta E(L)$ with a factor L for the 3D results to account for the overall factor $1/L$ in Eq. (14). For each choice of γ , we adjust the strength of the attractive Gaussian potential to keep the binding momentum κ_∞ roughly constant in infinite volume. The precise val-

ues for V_0 that we use for the different cases are given in the Supplemental Material [40]. In the limit $\gamma \rightarrow 0$ our expressions for $\Delta E(L)$ reduce to the known results for systems with only short-range interaction, and with the axis scalings chosen in Fig. 1 the data points would follow straight lines in that case. We can clearly observe how the actual behavior deviates more and more from the straight-line behavior with increasing γ , highlighting the importance of knowing the precise analytical form of the volume dependence in the presence of Coulomb repulsion. Indeed, the lines in the figures show the results of fitting Eqs. (5) and (14) to the numerical data, with excellent agreement. In Table I we show the values for κ_∞ and A_∞ that we extract from the FV fits for the various cases. The uncertainties quoted were obtained by varying the volume range for the fits as indicated in the table, and for all calculations we have approximated E_∞ from an $L = 32$ calculation. For comparison, the table includes also binding momenta and ANC's determined with direct continuum calculations (explained further in the Supplemental Material [40]). We find excellent agreement up to minor deviations, which we attribute primarily to small discretization errors in the lattice data. For 1D, we used a lattice spacing $a_{\text{latt}} = 1/30$, while the 3D calculations were performed with $a_{\text{latt}} = 1/6$. The finer lattice spacing required for good accuracy in 1D is an artifact of using the 3D Coulomb potential in a 1D setup, which causes significant sensitivity to the regularization of the Coulomb singularity at $r = 0$. In 3D, the reduced radial wavefunction vanishes at $r = 0$, which suppresses sensitivity to regularization details. In practical applications for example to analyzing Lattice EFT data, one would expect other uncertainties to dominate. Overall, our numerical calculations confirm conclusively that FV fits can be used for accurate ANC determinations even in the presence of strong Coulomb repulsion.

γ	Finite-volume fit			Continuum result	
	κ_∞	A_∞	L range	κ_∞	A_∞
$d = 1$					
1.0	0.861110(3)	2.1286(1)	12 ~ 24	0.860	2.1284
2.0	0.861125(9)	4.4740(9)	12 ~ 23	0.860	4.4782
3.0	0.86108(6)	10.386(2)	12 ~ 20	0.858	10.435
$d = 3$					
1.0	0.8610(3)	5.039(2)	17 ~ 28	0.861	5.049
2.0	0.8607(3)	11.71(4)	15 ~ 26	0.860	11.79
3.0	0.8605(7)	29.95(20)	14 ~ 24	0.859	30.31
4.0	0.8604(1)	83.14(10)	14 ~ 22	0.858	84.76
5.0	0.8604(2)	247.9(5)	14 ~ 18	0.857	255.4

Table I. Fit results for the calculations shown in Fig. 1. All quantities are given in units of the mass $m = 1$ (see text).

We furthermore consider a three-nucleon system on a lattice with $SU(4)$ -invariant contact interaction that cor-

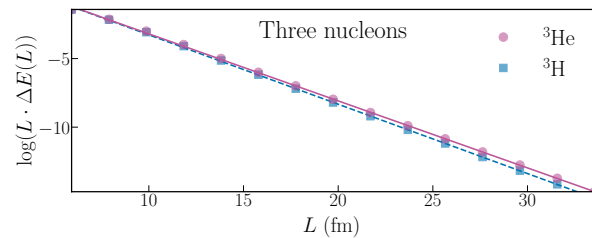


Figure 2. Finite-volume energy shifts for ${}^3\text{He}$ and ${}^3\text{H}$ calculated with an $SU(4)$ -invariant contact interaction (see text for details).

responds to a Pionless EFT description (see Ref. [41] for a review of nuclear EFTs). For this calculation, which we describe in more detail in the Supplemental Material [40], we tune a two-body single-lattice-site coupling to produce a deuteron with binding energy 1 MeV (in infinite volume), and in addition a three-body single-lattice-site coupling to reproduce the triton at its physical binding energy. For ${}^3\text{He}$ we add a repulsive Coulomb interaction between protons and tune a short-distance parameter associated with pp contact interaction to reproduce the ${}^3\text{He}$ binding energy in infinite volume. In Fig. 2 we show the energy shift for both the ${}^3\text{H}$ and ${}^3\text{He}$ energies for a range of volumes between 3 and 17 lattice units, with infinite-volume energies approximated by $L_\infty \approx 39.5$ fm (20 lattice units). We fit the numerical results with the analytic expression for the volume dependence and find that already for a system with relatively weak Coulomb repulsion like ${}^3\text{He}$ it is important for the pd breakup channel to make use of the relation derived in this work, which for general two-cluster states is the leading term in multipole expansions of the permanent and/or induced charge densities. In particular, the ANC extracted as $A_\infty = 1.44(1)$ fm $^{-1/2}$ would be off by about 5% if we were to fit the volume dependence assuming neutral clusters, already for γ as small as 0.046 fm $^{-1}$ here. This importance will increase for systems with more protons and/or weaker binding energy, such as proton halo nuclei. As an additional check, we can compare the ANC that we obtain from fitting the energy volume dependence to a direct extraction from the finite-volume wave function (as discussed in Ref. [27] and described further in the Supplemental Material [40]). From that procedure we obtain a value of 1.46(1) fm $^{-1/2}$, in good agreement with the result from the energy fit. Moreover, considering the $SU(4)$ -symmetric scenario that we consider here, our ANC is in reasonably good agreement with Ref. [42], which reports an S-wave ANC for ${}^3\text{He}$ of 1.82(1) fm $^{-1/2}$, converted to our conventions.

Summary and outlook We have derived the leading finite-volume energy correction for bound states of two charged clusters in a periodic volume. Numerical calculations for several examples in 1D and 3D systems give confidence that the analytical results are correct. Our

derivation does not rely on perturbation theory and is therefore applicable to medium-mass and heavy nuclei with large numbers of protons. The results should be immediately useful for *ab initio* calculations of bound nuclei in periodic boxes, which is standard practice in lattice EFT calculations. The form of the finite-volume energy correction provides a better extrapolation for the binding energy at infinite volume. Even more importantly, it yields a new efficient method for calculating ANCs that play an important role in low-energy astrophysical capture reactions. The extension to bound states of charged particles with nonzero angular momentum is currently under investigation.

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