# Volume dependence of *N*-body bound states

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A B S T R A C T

We derive the finite-volume correction to the binding energy of an *N*-particle quantum bound state in a cubic periodic volume. Our results are applicable to bound states with arbitrary composition and total angular momentum, and in any number of spatial dimensions. The only assumptions are that the interactions have finite range. The finite-volume correction is a sum of contributions from all possible breakup channels. In the case where the separation is into two bound clusters, our result gives the leading volume dependence up to exponentially small corrections. If the separation is into three or more clusters, there is a power-law factor that is beyond the scope of this work, however our result again determines the leading exponential dependence. We also present two independent methods that use finite-volume data to determine asymptotic normalization coefficients. The coefficients are useful to determine low-energy capture reactions into weakly bound states relevant for nuclear astrophysics. Using the techniques introduced here, one can even extract the infinite-volume energy limit using data from a single-volume calculation. The derived relations are tested using several exactly solvable systems and numerical examples. We anticipate immediate applications to lattice calculations of hadronic, nuclear, and cold atomic systems.

## 1. Introduction

In a number of highly influential papers [1–3], Lüscher derived the volume dependence of two-particle bound states and scattering states in cubic periodic volumes. The bound-state relation connects the finite-volume correction to the asymptotic properties of the two-particle wave function, whereas the elastic scattering result relates the volume dependence of discrete energy levels to physical scattering parameters. This work has since been extended in several directions, including non-zero angular momenta [4–6], moving frames [7–11], generalized boundary conditions [12–16], particles with intrinsic spin [17], and perturbative Coulomb corrections [18].[1]

With improved numerical techniques and computational resources enabling the calculation of systems with an increasing number of constituents, understanding the volume dependence of more complex systems is of timely relevance. Currently some results are available for three-particle systems, ranging from the general theory [23–25] to explicit results for specific systems [26–29]. In this letter, we derive the volume dependence of *N*-particle bound states with finite-range interactions in *d* spatial dimensions and arbitrary total angular momentum. We also use finite-volume energies to extract asymptotic normalization coefficients, which are useful in halo effective field theory calculations of low-energy reactions of relevance for nuclear astrophysics [30–33]. The results presented here should have numerous and immediate applications for lattice QCD and lattice effective field theory calculations of nuclei. Moreover, our results also apply to lattice simulations of cold atomic systems, as discussed for example in Refs. [34–36].

When the separation is into two bound clusters, the leading correction is the same as the finite-volume correction for a two-particle system, where the clusters are treated as though they were fundamental particles. While one may have guessed this result in

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[1] In a different but related approach, two-nucleon scattering properties have been extracted by solving the system in an artificial harmonic trap [19], based on results obtained for cold atoms, where the trap is physical [20–22].

the case where the $N$-particle system is a weakly bound system of two clusters, we show that this formula continues to hold even when the $N$-particle system is more strongly bound than one or more of the constituent clusters.[2]

In the case where the separation is into three or more clusters, our derivation gives the leading exponential dependence. However, in this case there are also correction factors which scale as inverse powers of the periodic box size. We discuss these power-law factors here for a few special cases, while the general result will be addressed in a future publication.

## 2. Asymptotic behavior

We start with $N$ nonrelativistic particles in $d$ spatial dimensions with masses $m_1, \cdots m_N$. We are using units where $\hbar = c = 1$ and write the position-space wave function for a general state $|\psi\rangle$ as $\psi(\mathbf{r}_1, \cdots \mathbf{r}_N)$. The Hamiltonian we consider is of the form

$$\hat{H}_{1 \cdots N} = \sum_{i=1}^{N} \hat{K}_i + \hat{V}_{1 \cdots N}, \tag{1}$$

where $\hat{K}_i = -\nabla_i^2/(2m_i)$, and in general we have nonlocal interactions of every kind from two-particle up to $N$-particle interactions. We can write the total interaction as a sum of integral kernels,

$$V_{1 \cdots N}(\mathbf{r}_1, \cdots \mathbf{r}_N; \mathbf{r}'_1, \cdots \mathbf{r}'_N) = \sum_{i<j} W_{i,j}(\mathbf{r}_i, \mathbf{r}_j; \mathbf{r}'_i, \mathbf{r}'_j) 1_{\hat{i},\hat{j}}$$
$$+ \sum_{i<j<k} W_{i,j,k}(\mathbf{r}_i, \mathbf{r}_j, \mathbf{r}_k; \mathbf{r}'_i, \mathbf{r}'_j, \mathbf{r}'_k) 1_{\hat{i},\hat{j},\hat{k}} + \cdots, \tag{2}$$

where we use the shorthand notation

$$1_{\hat{i}_1, \cdots \hat{i}_k} = \prod_{j \neq i_1, \cdots i_k} \delta^d(\mathbf{r}_j - \mathbf{r}'_j) \tag{3}$$

for the spectator particles. We assume that the interactions respect Galilean invariance, and so the center-of-mass (c.m.) momentum is conserved, and the c.m. kinetic energy decouples from the relative motion of the $N$-particle system. We furthermore assume that every interaction has finite range, meaning that each $W_{i_1 \cdots i_k}$ vanishes whenever the separation between some pair of incoming or outgoing coordinates exceeds some finite length $R$.

We now consider an $N$-particle bound state with total c.m. momentum zero, binding energy $B_N$, and wave function $\psi_N^B(\mathbf{r}_1, \cdots \mathbf{r}_N)$. In our notation the binding energy is the absolute value of the bound-state energy. Let us consider the asymptotic properties of this wave function when one of the coordinates becomes asymptotically large, while keeping the others fixed. Without loss of generality, we take the coordinate that we pull to infinity to be $\mathbf{r}_1$.

Let $S$ refer to the set of coordinate points $\{\mathbf{r}_1, \cdots \mathbf{r}_N\}$ where $\mathbf{r}_1$ is greater than distance $R$ from all other coordinates. Therefore in $S$ there are no interactions coupling $\mathbf{r}_1$ to $\mathbf{r}_2, \cdots \mathbf{r}_N$. By the assumption of vanishing c.m. momentum, we can work with the reduced Hamiltonian

$$\sum_{i=2}^{N} \hat{K}_i - \hat{K}_{2 \cdots N}^{\mathrm{CM}} + \hat{V}_{2 \cdots N} + \hat{K}_{1|N-1}^{\mathrm{rel}}, \tag{4}$$

where $\hat{K}_{2 \cdots N}^{\mathrm{CM}} = -(\nabla_2 + \cdots \nabla_N)^2/(2m_{2 \cdots N})$ and

$$\hat{K}_{1|N-1}^{\mathrm{rel}} = -\frac{(m_{2 \cdots N}\nabla_1 - m_1 \nabla_{2 \cdots N})^2}{2\mu_{1|N-1} m_{1 \cdots N}^2}. \tag{5}$$

We have written $m_{n \cdots N} = m_n + \cdots + m_N$ for the total mass of the (sub)system for the two cases $n = 1$ and $n = 2$. We have also introduced $\mu_{1|N-1}$ as the reduced mass with $\frac{1}{\mu_{1|N-1}} = \frac{1}{m_1} + \frac{1}{m_{2 \cdots N}}$.

We note that the first three terms in Eq. (4) constitute the Hamiltonian $\hat{H}_{2 \cdots N}$ of the $\{2, \cdots N\}$ subsystem with the c.m. kinetic energy removed, while the remaining $\hat{K}_{1|N-1}^{\mathrm{rel}}$ is the kinetic energy of the relative motion between particle 1 and the center of mass of the $\{2, \cdots N\}$ subsystem. In region $S$ we use the separation of variables to expand $\psi_N^B(\mathbf{r}_1, \cdots \mathbf{r}_N)$ as a linear combination of products of eigenstates of $\hat{H}_{2 \cdots N}$ with total linear momentum zero and eigenstates of $\hat{K}_{1|N-1}^{\mathrm{rel}}$.

For the moment we assume that the ground state of $\hat{H}_{2 \cdots N}$ is a bound state with energy $-B_{N-1}$ and wave function $\psi_{N-1}^B(\mathbf{r}_2, \cdots \mathbf{r}_N)$. For simplicity we consider here the case where the relative motion wave function has zero orbital angular momentum and will relax this condition later in the discussion. Then, as $r_{1|N-1} = |\mathbf{r}_{1|N-1}|$ becomes large, we have

$$\psi_N^B(\mathbf{r}_1, \cdots \mathbf{r}_N) \propto \psi_{N-1}^B(\mathbf{r}_2, \cdots \mathbf{r}_N)$$
$$\times (\kappa_{1|N-1} r_{1|N-1})^{1-d/2} K_{d/2-1}(\kappa_{1|N-1} r_{1|N-1}), \tag{6}$$

where $K_{d/2-1}$ is a modified Bessel function of the second kind, $\mathbf{r}_{1|N-1} = \mathbf{r}_1 - (m_2\mathbf{r}_2 + \cdots + m_N\mathbf{r}_N)/m_{2 \cdots N}$, and

$$\kappa_{1|N-1} = \sqrt{2\mu_{1|N-1}(B_N - B_{N-1})}. \tag{7}$$

For the excited states of the $N-1$ system there will be terms analogous to Eq. (6), however they will be exponentially suppressed due to the larger energy difference with $B_N$.

This discussion is readily generalized to the case of two clusters with arbitrary particle content. For this case we take the center of mass of $A$ coordinates to infinity while keeping the relative separations within the $A$ and $N-A$ subsystems fixed. Without loss of generality, we can choose the $A$ coordinates to be $\mathbf{r}_1, \cdots \mathbf{r}_A$. Following steps analogous to the case $A = 1$, we again apply the separation of variables to the $N$-particle wave function and obtain

$$\psi_N^B(\mathbf{r}_1, \cdots \mathbf{r}_N)$$
$$\propto \psi_A^B(\mathbf{r}_1, \cdots \mathbf{r}_A) \psi_{N-A}^B(\mathbf{r}_{A+1}, \cdots \mathbf{r}_N)(\kappa_{A|N-A} r_{A|N-A})^{1-d/2}$$
$$\times K_{d/2-1}(\kappa_{A|N-A} r_{A|N-A}), \tag{8}$$

where

$$\mathbf{r}_{A|N-A} = \frac{m_1\mathbf{r}_1 + \cdots + m_A\mathbf{r}_A}{m_1 + \cdots + m_A} - \frac{m_{A+1}\mathbf{r}_{A+1} + \cdots + m_N\mathbf{r}_N}{m_{A+1} + \cdots + m_N}, \tag{9}$$

$$\frac{1}{\mu_{A|N-A}} = \frac{1}{m_1 + \cdots + m_A} + \frac{1}{m_{A+1} + \cdots + m_N}, \tag{10}$$

$$\kappa_{A|N-A} = \sqrt{2\mu_{A|N-A}(B_N - B_A - B_{N-A})}, \tag{11}$$

and $-B_A$ and $-B_{N-A}$ are the ground state energies of the $A$-particle and $(N-A)$-particle systems respectively. We have made the simplifying assumption that $-B_A$ and $-B_{N-A}$ are both bound-state energies. If this is not true and one or both are instead energies associated with a scattering threshold, then Eq. (8) remains correct up to additional prefactors that scale as inverse powers of $\kappa_{A|N-A} r_{A|N-A}$. These factors arise from the integration over scattering states, and will be discussed in a future publication.

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[2] In the finite volume, all energy levels are discrete states. We refer to individual levels as bound and continuum/scattering states, respectively, if their extrapolated infinite volume energy is below or above the non-interacting $N$-body threshold. In the finite volume, bound states defined this way are characterized by an exponential dependence on the volume whereas continuum/scattering states have a power-law volume dependence.

We now remove the condition that the relative motion between clusters have zero orbital angular momentum. In the general case, the relative-motion wave function has the form

$$\sqrt{\frac{2\kappa_{A|N-A}}{\pi}}\, r_{A|N-A}^{1-d/2} \sum_{\mathbf{L}} \gamma_{\mathbf{L}} Y_{\mathbf{L}}(\hat{\mathbf{r}}_{A|N-A}) K_{\ell+d/2-1}(\kappa_{A|N-A} r_{A|N-A})\,,$$

$$(12)$$

where $Y_{\mathbf{L}}$ denotes the $d$-dimensional hyperspherical harmonics for spin representation $\ell$ (see for example Ref. [37]) and $\gamma_{\mathbf{L}}$ are constant coefficients. This is exactly the same behavior as found in two-particle bound states with nonzero angular momentum. All of the various cases for $d = 2$ and $d = 3$ are discussed in Ref. [6]. For the one-dimensional case, $\ell = \mathbf{L} = 0$ corresponds with even parity and $\ell = \mathbf{L} = 1$ corresponds with odd parity. For even parity the spherical harmonic is just unity, while for odd parity it is an odd step function.

## 3. Finite volume correction

We define $B_N(L)$ as the finite-volume binding energy in a cubic periodic box of length $L$ and let $\Delta B_N(L) = B_N(L) - B_N$ be the finite-volume correction. Following steps analogous to Refs. [1,5,6,29], we find that $\Delta B_N(L)$ gets contributions from every possible breakup channel.

If the $N$-particle system can be subdivided as an $A$-particle bound state and $(N-A)$-particle bound state in a relative $\ell = 0$ state, then we get a contribution to $\Delta B_N(L)$ that is proportional to

$$(\kappa_{A|N-A}L)^{1-d/2} K_{d/2-1}(\kappa_{A|N-A}L)\,. \qquad (13)$$

In addition to this there are also terms that have a larger exponential suppression and thus can be neglected. While generally different subdivisions contribute to the overall volume dependence of a given state, the smallest value $\kappa_{A|N-A}$ determines the leading asymptotic behavior.

If the two bound states have orbital angular momentum $\ell > 0$, then the finite volume correction has the same dependence as in Eq. (13) along with subleading terms that are suppressed by powers of $\kappa_{A|N-A}L$. The functional form is exactly the same as that for the $N = 2$, $d = 2, 3$ cases derived in Refs. [5,6]. The sign of the correction oscillates with even and odd $\ell$.

For the case that the $A$-particle ground state, $(N-A)$-particle ground state, or both ground states are scattering states, we still obtain the same exponential dependence, except there is an additional power law factor of $P(\kappa_{A|N-A}L)$ due to the integration over scattering states,

$$(\kappa_{A|N-A}L)^{1-d/2} K_{d/2-1}(\kappa_{A|N-A}L) P(\kappa_{A|N-A}L)\,. \qquad (14)$$

The general functional form for this power law factor $P(\kappa_{A|N-A}L)$ is beyond the scope of this current study, but we discuss the power-law factor $P(\kappa_{A|N-A}L)$ for several notable examples below. The remaining finite-volume corrections are exponentially suppressed compared to the terms in Eq. (13) and Eq. (14).

## 4. Analytically solvable examples

We now consider several examples to check the results we have derived. We start with the exactly solvable $N$-particle system in one dimension with all equal masses $m$ and an attractive delta-function potential $-c\delta(r_i - r_j)$ between every pair of particles $i, j$. The exact ground state binding energies are

$$B_N = \frac{N(N^2-1)}{6} B_2\,, \qquad (15)$$

where $B_2 = c^2 m/4$, and the exact wave functions are

$$\psi_N^B(r_1, \cdots r_N) \propto \exp\left[-\kappa \sum_{i>j} |r_i - r_j|\right]\,, \qquad (16)$$

with $\kappa = cm/2$. Let us now pull $r_1, \cdots r_A$ in unison to infinity with $r_{A+1}, \cdots r_N$ fixed. From the exact wave function we have

$$\psi_N^B(r_1, \cdots r_N)$$
$$\propto \psi_A^B(r_1, \cdots r_A)\, \psi_{N-A}^B(r_{A+1}, \cdots r_N) e^{-A(N-A)\kappa|r_{A|N-A}|}\,. \qquad (17)$$

This result agrees precisely with the asymptotic behavior given in Eq. (8).

The next example we consider is the three-particle system at the unitarity limit in three dimensions. This corresponds with two-particle interactions with zero range and infinite scattering length. Our result for the leading finite-volume correction is

$$\Delta B_3(L) \propto (\kappa_{1|2}L)^{-1/2} K_{1/2}(\kappa_{1|2}L) P(\kappa_{1|2}L)$$
$$\propto \exp\left(-\sqrt{\frac{4mB_3}{3}}L\right)\left(\sqrt{\frac{4mB_3}{3}}L\right)^{-1} P(\kappa_{1|2}L)\,, \qquad (18)$$

where $P(\kappa_{1|2}L)$ is a power-law function arising from the scattering threshold of the two-particle system. We find the same exponential dependence as the result derived in Ref. [29],

$$\Delta B_3(L) \propto \exp\left(-\sqrt{\frac{4mB_3}{3}}L\right)\left(\sqrt{\frac{4mB_3}{3}}L\right)^{-3/2} + \cdots\,, \qquad (19)$$

and there are subleading power-law corrections in addition to exponentially suppressed corrections. In this case we find that the leading power-law behavior is $P(\kappa_{1|2}L) = (\kappa_{1|2}L)^{-1/2}$.

Finally, the third example we consider is the case of a spinless $N$-particle bound state with only an $N$-particle interaction. In this case there are no cluster substructures and we need only consider the asymptotic behavior as one of the particles is pulled away from the center of mass of the remaining ones. Without loss of generality, let the particle that we pull away be $\mathbf{r}_1$. The corresponding Jacobi coordinate is $\mathbf{r}_{1|N-1}$ with reduced mass $\mu_{1|N-1}$. As we pull $\mathbf{r}_1$ away from the center of mass of the other particles, the wave function can be shown to be proportional to

$$(\kappa_{1|N-1}r_{1|N-1})^{1-d(N-1)/2} K_{d(N-1)/2-1}(\kappa_{1|N-1}r_{1|N-1})\,. \qquad (20)$$

This result matches the same exponential dependence as our predicted result

$$(\kappa_{1|N-1}r_{1|N-1})^{1-d/2} K_{d/2-1}(\kappa_{1|N-1}r_{1|N-1}) P(\kappa_{1|N-1}r_{1|N-1})\,. \qquad (21)$$

We can further conclude that in this case the power law suppression factor is

$$P(\kappa_{1|N-1}r_{1|N-1}) \propto (\kappa_{1|N-1}r_{1|N-1})^{-d(N-2)/2}\,. \qquad (22)$$

## 5. Numerical tests

We now test our results with numerical calculations. The program used to calculate the results presented in this section has been set up to handle an arbitrary number of particles and spatial dimensions, limited only by available computational resources.

**Table 1**

Numerical results for local Gaussian potentials $V(r) = V_0 \exp(-r^2/R^2)$. All quantities are given in units of the particle mass $m = 1$ (see text).

| $N$ | $B_N$ | $L_{\min} \ldots L_{\max}$ | $\kappa_{\text{fit}}$ | $\kappa_{1|N-1}$ |
|---|---|---|---|---|
| | | $d = 1$, $V_0 = -1.0$, $R = 1.0$ | | |
| 2 | 0.356 | 20...48 | 0.59536(3) | 0.59625 |
| 3 | 1.275 | 15...32 | 1.1062(14) | 1.1070 |
| 4 | 2.859 | 12...24 | 1.539(3) | 1.541 |
| 5 | 5.163 | 12...20 | 1.916(21) | 1.920 |
| | | $d = 2$, $V_0 = -1.5$, $R = 1.5$ | | |
| 2 | 0.338 | 15...36 | 0.58195(6) | 0.58140 |
| 3 | 1.424 | 12...24 | 1.20409(3) | 1.20339 |
| 4 | 3.449 | 7...14 | 1.743(8) | 1.743 |
| | | $d = 3$, $V_0 = -5.0$, $R = 1.0$ | | |
| 2 | 0.449 | 15...24 | 0.6694(2) | 0.6700 |
| 3 | 2.916 | 4...14 | 1.798(3) | 1.814 |

This is achieved through a generator code (written in Haskell) that automatically creates scripts (to be run with GNU Octave or compatible software) for each desired case. This Haskell code is provided as supplementary material together with this letter (see Appendix A for details).

We consider equal-mass particles interacting via attractive local Gaussian potentials[3] in $d = 1, 2, 3$ dimensions. For the derivatives appearing in the kinetic energy, we write the finite difference up to $k$-th order accuracy, where $k = 2, 4, \cdots$.

Expanding the Bessel function in Eq. (13), we find that the leading finite-volume correction has the asymptotic form

$$\Delta B_N(L) \propto \exp\left(-\kappa_{A|N-A} L\right) / L^{(d-1)/2}. \qquad (23)$$

This form can be easily identified by plotting the logarithm of $\Delta B_N(L)$ times $L^{(d-1)/2}$ as a function of $L$, and linear fits can be used to extract the slopes to be compared to the expected $\kappa_{A|N-A}$.

Results for different potentials and spatial dimensions $d = 1, 2, 3$ and are shown in Figs. 1, 2, and 3. In these calculations, all physical quantities are expressed in terms of powers of the particle mass $m$, which has been set to unity. That is, energies and momenta are divided by the mass, and length scales are multiplied by the mass, and overall we set $\hbar = c = m = 1$. The lattice spacings $a_{\text{latt}}$ for the calculations were chosen to minimize discretization artifacts as much as possible while probing volumes large enough to test the asymptotic behavior of the finite-volume corrections. From the observed straight lines in the plots it is clear that Eq. (23) holds as a very good approximation. The true infinite-volume energies $B_N$ used to calculate the shifts $\Delta B_N(L)$ were obtained by minimizing the error in fitting linear functions to the data points.

As summarized in Table 1, the slopes extracted from these linear fits (performed within the ranges $L_{\min} \ldots L_{\max}$) agree very well with the prediction that the asymptotic volume dependence is dominated by the $1|N-1$ contribution. These results provide further assurance that the relations derived in this letter are correct. Similar agreement is found for other setups (involving higher-body potentials and/or relevant contributions other than $1|(N-1)$) as well; these will be presented in a forthcoming publication.
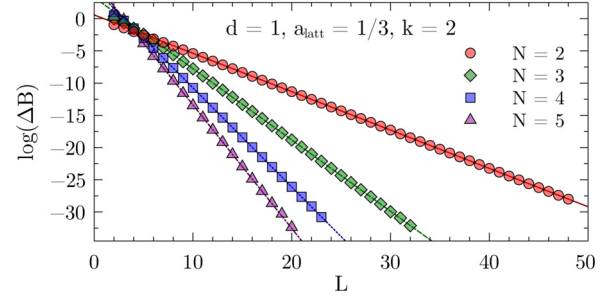


**Fig. 1.** (Color online) Finite-volume energy shift for $N = 2, 3, 4, 5$ particles interacting via a Gaussian potential ($R = 1$, $V_0 = -1$) in one dimension. All quantities are given in units of the particle mass $m = 1$ (see text).
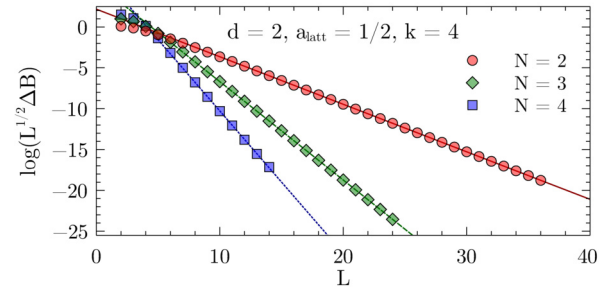


**Fig. 2.** (Color online) Finite-volume energy shift for $N = 2, 3, 4$ particles interacting via a Gaussian potential ($R = 1.5$, $V_0 = -1.5$) in two dimensions. All quantities are given in units of the particle mass $m = 1$ (see text).
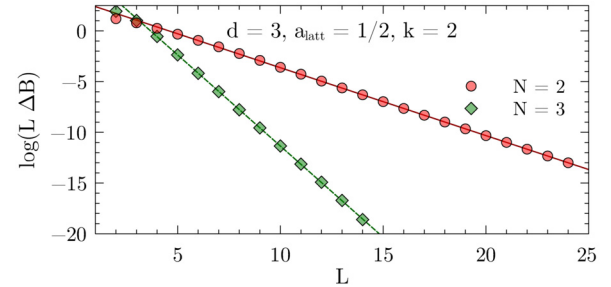


**Fig. 3.** (Color online) Finite-volume energy shift for $N = 2, 3$ particles interacting via a Gaussian potential ($R = 1$, $V_0 = -5$) in three dimensions. All quantities are given in units of the particle mass $m = 1$ (see text).

## 6. Asymptotic normalization coefficients

Let us now consider the case where both the $A$-particle and $(N-A)$-particle clusters are bound states or fundamental particles. In this case we extract an asymptotic normalization coefficient (ANC) associated with the $A + (N-A)$ threshold. ANCs play an important role for low-energy capture processes that govern nucleosynthesis in stellar environments [30–33] and are notoriously difficult to extract in terrestrial experiments due to dominance of the Coulomb repulsion at low energies. We will describe the problem of Coulomb ANCs in a future publication and focus here on the case of extracting ANCs for finite-range interactions from finite-volume data.

In the limit that separation distance $r_{A|N-A}$ between the two clusters is large, the normalized $N$-body wave function is a product of normalized $A$-body and $(N-A)$-body wave functions times the relative wave function as written in Eq. (12). The ANC is then the coefficient $\gamma_{\mathbf{L}}$ in Eq. (12), which we will write as $\gamma$ throughout the remainder of our discussion. We note for $d = 2$ our definition here

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[3] While these potentials do not have a strictly finite range, their fall-off at large distances is much faster than any expected volume dependence, such that our relations hold up to negligibly small corrections. The use of Gaussian potentials instead of, e.g., strictly finite-range step potentials has the advantage of avoiding large discretization artifacts.

differs from that used in Ref. [6]. We can extract the relative wave function by calculating the ratio

$$
\left( \frac{\langle \Psi_N^B | O_A(\mathbf{r}_{A|N-A}) O_{N-A}(\mathbf{0}) | \Psi_N^B \rangle}{\langle \Psi_A^B | O_A(\mathbf{0}) | \Psi_A^B \rangle \langle \Psi_{N-A}^B | O_{N-A}(\mathbf{0}) | \Psi_{N-A}^B \rangle} \right)^{1/2}
\tag{24}
$$

for some localized $A$-body and $(N-A)$-body operators $O_A(\mathbf{r})$, $O_{N-A}(\mathbf{r})$. We then compare this relative wave function at finite volume with the asymptotic form written in Eq. (12) plus additional copies due to the periodic boundary conditions, extracting the magnitude of the ANC. We write this as $|\gamma|_{\mathrm{WF}}$, where WF is shorthand for wave function.

We can also determine the ANC in a completely different way using the finite-volume correction $\Delta B_N(L)$. By combining our $N$-body results here with the derivations in Refs. [1,5,6], we find that $\Delta B_N(L)$ equals

$$
\frac{(-1)^{\ell+1} \sqrt{\frac{2}{\pi}} f(d) |\gamma|^2}{\mu_{A|N-A}} \kappa_{A|N-A}^{2-d/2} L^{1-d/2} K_{d/2-1}(\kappa_{A|N-A} L),
\tag{25}
$$

plus smaller corrections that are exponentially suppressed. The function $f(d)$ takes values $f(1) = 2$, $f(2) = \sqrt{8/\pi}$, and $f(3) = 3$. If there are several different ways to partition the $N$-particle system into clusters with same $\kappa_{A|N-A}$ value, then there will be contributions to the finite-volume correction from each channel. In particular, in the case of $N$ identical particles (as considered in the numerical examples presented here), there is a combinatorial factor that counts the number of ways to partition the identical particles into $A|N-A$ clusters. For $d = 3$, $\Delta B_N(L)$ is averaged over all $2\ell + 1$ elements of the angular momentum $\ell$ multiplet, while for $d = 2$ the average is taken over symmetric and antisymmetric combinations of $\mathbf{L} = \pm \ell$ for even $\ell$ [6].

Equation (25) follows directly from defining the ANC in terms of the asymptotic radial wave function, which for cluster separation $r_{A|N-A}$ large compared to the range of the interaction is universally given by

$$
\psi_{\mathrm{asympt}}(r_{A|N-A})
$$
$$
= \gamma \sqrt{\frac{2\kappa_{A|N-A}}{\pi}} (r_{A|N-A})^{1-d/2} K_{d/2-1}(\kappa_{A|N-A} r_{A|N-A}) Y(d),
\tag{26}
$$

where $Y(d)$ accounts for the angular normalization in $d$ spatial dimensions, cf. Eq. (12) specialized for the case of a bound state without angular dependence. For $d = 3$, where $Y(3) = 1/\sqrt{4\pi}$, the convention in Eq. (26) reproduces the canonical form $\gamma \exp(-\kappa_{A|N-A} r_{A|N-A})/r_{A|N-A}$ for a two-cluster S-wave state. For $d = 1$ one has $Y(1) = 1$ and the asymptotic form is simply $\gamma \exp(-\kappa_{A|N-A} r_{A|N-A})$. For $d = 2$, on the other hand, it is more natural to define the ANC directly in terms of the modified Bessel function, which does not reduce to a simple exponential in this case. The $f(d)$ quoted above have been chosen to account for this as well as the averaging over states in a cubic-group multiplet. We write the magnitude of the ANC extracted from fits using Eq. (25) as $|\gamma|_{\mathrm{FV}}$, where FV is shorthand for finite volume.

Using the same lattice examples with Gaussian potentials as discussed previously, we present results for $|\gamma|_{\mathrm{FV}}$ and $|\gamma|_{\mathrm{WF}}$ in Table 2. We use Eq. (24) with the operator $O_1$ equal to the single particle density and $O_{N-1}$ equal to the $(N-1)$-body density on a single lattice site, with all quantities extracted at the same finite volume. As seen in Table 2, the two methods for extracting the ANCs are in excellent agreement.

We furthermore note that by using the finite-volume wave function to determine $|\gamma|_{\mathrm{WF}}$ and $\kappa_{A|N-A}$, we can estimate $\Delta B_N(L)$.

**Table 2**

Extracted ANCs for local Gaussian potentials $V(r) = V_0 \exp(-r^2/R^2)$. All quantities are given in units of the particle mass $m = 1$.

| $N$ | $B_N$ | $L_{\max}$ | $|\gamma|_{\mathrm{FV}}$ | $|\gamma|_{\mathrm{WF}}$ |
|---|---|---|---|---|
| | $d = 1$, $V_0 = -1.0$, $R = 1.0$ | | | |
| 2 | 0.356 | 48 | 0.8652(4) | 0.8627(4) |
| 3 | 1.275 | 32 | 1.650(27) | 1.638(16) |
| 4 | 2.859 | 24 | 2.54(6) | 2.56(8) |
| 5 | 5.163 | 20 | 3.65(62) | 3.63(18) |
| | $d = 2$, $V_0 = -1.5$, $R = 1.5$ | | | |
| 2 | 0.338 | 36 | 1.923(2) | 1.921(9) |
| 3 | 1.424 | 24 | 5.204(4) | 5.24(2) |
| 4 | 3.449 | 14 | 11.2(4) | 10.99(4) |
| | $d = 3$, $V_0 = -5.0$, $R = 1.0$ | | | |
| 2 | 0.449 | 24 | 1.891(3) | 1.89(1) |
| 3 | 2.916 | 14 | 7.459(97) | 7.83(11) |

**Table 3**

Finite-volume corrections for local Gaussian potentials $V(r) = V_0 \exp(-r^2/R^2)$ predicted from the tail of the wave function at a single fixed volume $L$, as described in the text. All quantities are given in units of the particle mass $m = 1$.

| $N$ | $B_N$ | $L$ | $\Delta B_N(L)_{\mathrm{estimate}}$ | $\Delta B_N(L)_{\mathrm{actual}}$ |
|---|---|---|---|---|
| | $d = 1$, $V_0 = -1.0$, $R = 1.0$ | | | |
| 2 | 0.356 | 8 | $-1.32(2) \times 10^{-2}$ | $-1.42 \times 10^{-2}$ |
| 3 | 1.275 | 8 | $-3.9(4) \times 10^{-3}$ | $-3.75 \times 10^{-3}$ |
| 4 | 2.859 | 8 | $-4.3(7) \times 10^{-4}$ | $-4.69 \times 10^{-4}$ |
| 5 | 5.163 | 8 | $-0.6(2) \times 10^{-4}$ | $-0.64 \times 10^{-4}$ |
| | $d = 2$, $V_0 = -1.5$, $R = 1.5$ | | | |
| 2 | 0.338 | 8 | $-2.5(6) \times 10^{-2}$ | $-2.84 \times 10^{-2}$ |
| 3 | 1.424 | 8 | $-5.8(6) \times 10^{-3}$ | $-4.99 \times 10^{-3}$ |
| 4 | 3.449 | 8 | $-4.1(6) \times 10^{-4}$ | $-4.01 \times 10^{-4}$ |
| | $d = 3$, $V_0 = -5.0$, $R = 1.0$ | | | |
| 2 | 0.356 | 8 | $-1.3(3) \times 10^{-2}$ | $-1.34 \times 10^{-2}$ |
| 3 | 2.916 | 8 | $-6.2(6) \times 10^{-5}$ | $-4.80 \times 10^{-5}$ |

By combining this with the finite-volume binding energy $B_N(L)$, we can determine the infinite-volume binding energy from a single-volume calculation. We expect this technique to be of practical use for computationally expensive calculations of quantum bound states, perhaps making it unnecessary to perform infinite-volume extrapolations. As an illustration, we show in Table 3 results obtained by applying the method to the same potentials and states considered previously. Specifically, we calculate $\Delta B_N(L)_{\mathrm{estimate}}$ by using $|\gamma|_{\mathrm{WF}}$ and $\kappa_{A|N-A}$ obtained from the wave function at a fixed volume $L = 8$. The uncertainties quoted are based on varying the wave function tail range from which $|\gamma|_{\mathrm{WF}}$ and $\kappa_{A|N-A}$ are extracted using a fit to the known asymptotic form, and also by comparing the $\kappa_{A|N-A}$ thus determined to the result obtained directly from the energy at volume $L$.[4] Given that this error estimate does not include discretization artifacts or account for the subleading volume dependence of the states, we find overall good agreement for the single-volume extrapolation with the exact finite-volume corrections.

## 7. Summary and outlook

We have derived finite-volume corrections to the binding energy of a general $N$-particle bound state in a cubic periodic vol-

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[4] For a fixed tail range, the ANC is determined from the minimum and maximum values of the ratio of the numerical wave function compared to the asymptotic form, while $\kappa_{A|N-A}$ is treated as a fit parameter. The same technique was used to extract the $|\gamma|_{\mathrm{WF}}$ shown in Table 2, with the difference that this analysis used the $\kappa_{A|N-A}$ from the multiple-volume fit.

ume, focusing on the leading behavior in this first study of such systems. We have also derived two new methods for computing the asymptotic normalization coefficient. Our results apply to bound states with any spin and in any number of spatial dimensions, provided only they satisfy the condition of vanishing c.m. motion that is assumed in our derivation. In the future, it would be interesting to also consider the more general case of $N$-particle systems in moving frames, which is relevant for the scattering of composite particles [9,11] and as tool to reduce the overall volume dependence of calculations (see *e.g.* Ref. [10]).

The results presented here should have wide applications to many calculations of hadronic structure, nuclear structure, and bound cold atomic systems. In particular our results should be useful for lattice simulations of nuclei and hypernuclei starting from quarks and gluons in lattice quantum chromodynamics [38–46] or protons, neutrons, and hyperons in lattice effective field theory [47–49]. For such calculations performed with unphysical pion masses, one might not know *a priori* which $A + N - A$ system will give the leading finite-volume dependence. In that case we recommend a global analysis of all the available data to determine a self-consistent description.

### Acknowledgements

### Appendix A. Generator code

#### A.1. Basic principle

We provide the Haskell code `Generator.hs` as supplementary material. This program solves the general problem of diagonalizing the Hamiltonian for $N$ nonrelativistic particles (with all equal masses) interacting via local potentials in a lattice-discretized periodic finite volume. To that end, it automatically generates scripts for each desired case. These scripts are meant to be run with GNU Octave or compatible software.

The generated scripts construct the position-space Hamiltonian as a (potentially very large) sparse matrix, which is then diagonalized to find the lowest-lying energy eigenstates. The center-of-mass motion is removed by working with relative coordinates, all measured with respect to the last ($N$-th) particle. Periodic boundary conditions are implemented with index maps for each of these coordinates, and shifted versions thereof are used to generate the kinetic terms, which are differential operators in this representation, as finite differences to $k$-th order accuracy (the code supports arbitrary even $k \geq 2$). For further explanations regarding the code we refer to the comments included in the source file.

#### A.2. Usage

Using the generator code is very easy provided that a Haskell toolchain is installed on the target system; it does not require any packages beyond the Haskell standard library. `Generator.hs` can either be compiled into an executable file or, simpler yet, be invoked directly as a script. For example, the command

```
$ runhaskell Generator.hs -d 1 -n 3 -L 16
```

will generate a script for three particles in one dimension, interacting via a two-body potential that defaults to a Gaussian well with $V_0 = -1$ and $R = 1$. This, as well as many other parameters, can be changed with command-line options. The available options that can be customized are easily identified in the source code.

With the above command, the generated script code is written directly to the terminal output. From there, it can either be redirected to a file for further editing, or be conveniently passed directly to a compatible script interpreter. If GNU Octave is installed, a command like

```
$ runhaskell Generator.hs -d 1 -n 3 -L 16 | octave
```

will simply present the result of the numerical diagonalization to the terminal output.

### Appendix B. Supplementary material

Supplementary material related to this article can be found online at https://doi.org/10.1016/j.physletb.2018.01.060.

### References

[1] M. Lüscher, Commun. Math. Phys. 104 (1986) 177.
[2] M. Lüscher, Commun. Math. Phys. 105 (1986) 153.
[3] M. Lüscher, Nucl. Phys. B 354 (1991) 531.
[4] T. Luu, M.J. Savage, Phys. Rev. D 83 (2011) 114508, arXiv:1101.3347 [hep-lat].
[5] S. König, D. Lee, H.-W. Hammer, Phys. Rev. Lett. 107 (2011) 112001, arXiv:1103.4468 [hep-lat].
[6] S. König, D. Lee, H.-W. Hammer, Ann. Phys. 327 (2012) 1450, arXiv:1109.4577 [hep-lat].
[7] C.H. Kim, C.T. Sachrajda, S.R. Sharpe, Nucl. Phys. B 727 (2005) 218, arXiv:hep-lat/0507006.
[8] K. Rummukainen, S.A. Gottlieb, Nucl. Phys. B 450 (1995) 397, arXiv:hep-lat/9503028.
[9] S. Bour, S. König, D. Lee, H.-W. Hammer, U.-G. Meißner, Phys. Rev. D 84 (2011) 091503, arXiv:1107.1272 [nucl-th].
[10] Z. Davoudi, M.J. Savage, Phys. Rev. D 84 (2011) 114502, arXiv:1108.5371 [hep-lat].
[11] A. Rokash, E. Epelbaum, H. Krebs, D. Lee, U.-G. Meißner, J. Phys. G 41 (2014) 015105, arXiv:1308.3386 [nucl-th].
[12] C.T. Sachrajda, G. Villadoro, Phys. Lett. B 609 (2005) 73, arXiv:hep-lat/0411033.
[13] R.A. Briceno, Z. Davoudi, T.C. Luu, M.J. Savage, Phys. Rev. D 89 (2014) 074509, arXiv:1311.7686 [hep-lat].
[14] C. Körber, T. Luu, Phys. Rev. C 93 (2016) 054002, arXiv:1511.06598 [nucl-th].
[15] A. Cherman, S. Sen, M.L. Wagman, L.G. Yaffe, arXiv:1612.00403 [hep-lat].
[16] B. Schuetrumpf, W. Nazarewicz, P.-G. Reinhard, Phys. Rev. C 93 (2016) 054304, arXiv:1603.03743 [nucl-th].
[17] R.A. Briceno, Phys. Rev. D 89 (2014) 074507, arXiv:1401.3312 [hep-lat].
[18] S.R. Beane, M.J. Savage, Phys. Rev. D 90 (2014) 074511, arXiv:1407.4846 [hep-lat].
[19] T. Luu, M.J. Savage, A. Schwenk, J.P. Vary, Phys. Rev. C 82 (2010) 034003, arXiv:1006.0427 [nucl-th].
[20] T. Busch, B.-G. Englert, K. Rzazewski, M. Wilkens, Found. Phys. 28 (1998) 549.
[21] S.K. Yip, Phys. Rev. A 78 (2008) 013612.
[22] A. Suzuki, Y. Liang, R.K. Bhaduri, Phys. Rev. A 80 (2009) 033601.
[23] K. Polejaeva, A. Rusetsky, Eur. Phys. J. A 48 (2012) 67, arXiv:1203.1241 [hep-lat].
[24] R.A. Briceno, Z. Davoudi, Phys. Rev. D 87 (2013) 094507, arXiv:1212.3398 [hep-lat].
[25] R.A. Briceno, M.T. Hansen, S.R. Sharpe, arXiv:1609.09805 [hep-lat].
[26] S. Kreuzer, H.-W. Hammer, Phys. Lett. B 694 (2011) 424, arXiv:1008.4499 [hep-lat].
[27] S. Kreuzer, H.W. Grießhammer, Eur. Phys. J. A 48 (2012) 93, arXiv:1205.0277 [nucl-th].
[28] S. Kreuzer, H.-W. Hammer, Few-Body Syst. 54 (2013) 157.
[29] U.-G. Meißner, G. Ríos, A. Rusetsky, Phys. Rev. Lett. 114 (2015) 091602, arXiv:1412.4969 [hep-lat];
U.-G. Meißner, G. Ríos, A. Rusetsky, Phys. Rev. Lett. 117 (2016) 069902 (Erratum).
[30] H.M. Xu, C.A. Gagliardi, R.E. Tribble, A.M. Mukhamedzhanov, N.K. Timofeyuk, Phys. Rev. Lett. 73 (1994) 2027.
[31] P. Capel, R.C. Johnson, F.M. Nunes, Phys. Rev. C 88 (2013) 044602, arXiv:1309.2526 [nucl-th].

[32] X. Zhang, K.M. Nollett, D.R. Phillips, Phys. Rev. C 89 (2014) 051602, arXiv:1401.4482 [nucl-th].

[33] H.-W. Hammer, C. Ji, D.R. Phillips, arXiv:1702.08605 [nucl-th].

[34] M.G. Endres, D.B. Kaplan, J.W. Lee, A.N. Nicholson, Phys. Rev. A 87 (2013) 023615, arXiv:1203.3169 [hep-lat].

[35] S. Bour, H.-W. Hammer, D. Lee, U.-G. Meissner, Phys. Rev. C 86 (2012) 034003, arXiv:1206.1765 [nucl-th].

[36] S. Bour, D. Lee, H.-W. Hammer, U.-G. Meißner, Phys. Rev. Lett. 115 (2015) 185301, arXiv:1412.8175 [cond-mat.quant-gas].

[37] H.-W. Hammer, D. Lee, Ann. Phys. 325 (2010) 2212, arXiv:1002.4603 [nucl-th].

[38] A. Nicholson, E. Berkowitz, E. Rinaldi, P. Vranas, T. Kurth, B. Joo, M. Strother, A. Walker-Loud, PoS LATTICE 2015 (2016) 083, arXiv:1511.02262 [hep-lat].

[39] E. Berkowitz, T. Kurth, A. Nicholson, B. Joo, E. Rinaldi, M. Strother, P.M. Vranas, A. Walker-Loud, Phys. Lett. B 765 (2017) 285, arXiv:1508.00886 [hep-lat].

[40] T. Yamazaki, K.i. Ishikawa, Y. Kuramashi, A. Ukawa, Phys. Rev. D 92 (2015) 014501, arXiv:1502.04182 [hep-lat].

[41] T. Yamazaki, PACS Collaboration, PoS LATTICE 2015 (2016) 081, arXiv:1511.09179 [hep-lat].

[42] T. Inoue, et al., HAL QCD Collaboration, Phys. Rev. C 91 (2015) 011001, arXiv:1408.4892 [hep-lat].

[43] F. Etminan, et al., HAL QCD Collaboration, Nucl. Phys. A 928 (2014) 89, arXiv:1403.7284 [hep-lat].

[44] S.R. Beane, et al., Phys. Rev. Lett. 113 (2014) 252001, arXiv:1409.3556 [hep-lat].

[45] E. Chang, et al., NPLQCD Collaboration, Phys. Rev. D 92 (2015) 114502, arXiv:1506.05518 [hep-lat].

[46] M.J. Savage, et al., arXiv:1610.04545 [hep-lat].

[47] E. Epelbaum, H. Krebs, T.A. Lähde, D. Lee, U.-G. Meißner, G. Rupak, Phys. Rev. Lett. 112 (2014) 102501, arXiv:1312.7703 [nucl-th].

[48] S. Elhatisari, D. Lee, G. Rupak, E. Epelbaum, H. Krebs, T.A. Lähde, T. Luu, U.-G. Meißner, Nature 528 (2015) 111, arXiv:1506.03513 [nucl-th].

[49] S. Elhatisari, et al., Phys. Rev. Lett. 117 (2016) 132501, arXiv:1602.04539 [nucl-th].