Radius extrapolations for two-body bound states in finite volume

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Simulations of quantum systems in finite volume have proven to be a useful tool for calculating physical observables. Such studies to date have focused primarily on understanding the volume dependence of binding energies, from which it is possible to extract asymptotic properties of the corresponding bound state, as well as on extracting scattering information. For bound states, all properties depend on the size of the finite volume, and for precision studies it is important to understand such effects. In this work, we therefore derive the volume dependence of the mean squared radius of a two-body bound state, using a technique that can be generalized to other static properties in the future. We test our results with explicit numerical examples and demonstrate that we can robustly extract infinite-volume radii from finite-volume simulations in cubic boxes with periodic boundary conditions.

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I. INTRODUCTION

Finite-volume (FV) simulations of quantum systems in periodic cubic boxes are a powerful tool that is used to study properties of nuclear bound states and scattering. A series of highly influential papers [1–3] established in the 1980s and 90s that real-world properties of a quantum system are encoded in how its discrete energy levels change as volume size is varied. Over the past decades, this fruitful idea has spurred a lot of activity, with recent focus on the study of three-body systems [4–25], motivated primarily by applications to lattice quantum chromodynamics (lattice QCD). For two-cluster bound states, the volume dependence of the binding energy is known for an arbitrary number of constituents [26]; see also Refs. [27,28] for studies of general N-body states in finite volume. Recent work derived the volume dependence of two-body bound states comprised of charged particles, with a full nonperturbative account for the repulsive Coulomb interaction [29], and Ref. [30] extended the method to resonances. An important motivation for understanding the volume dependence of bound states is that knowledge of the functional form makes it possible to extract asymptotic normalization coefficients (ANCs) from FV calculations, for example based on lattice effective-field theory (lattice EFT) simulations of atomic nuclei [31–35].

In this paper, we extend studies of the volume dependence for bound states beyond what is known for binding energies. As simplest observable, we consider mean squared radii $\langle r^2\rangle$ of two-body bound states, defined (in more detail in the following section) as the expectation value of an operator that measures the average distance of the constituents from their common center of mass. Just like the binding energy, $\langle r^2\rangle$ will be shifted from its physical value in FV, and the magnitude of this shift can be traced back to changes in the wave function induced by being confined to a periodic box. We derive in detail the functional form of the radius finite-volume shift, which makes it possible to perform extrapolations from a set of finite-volume calculations to the real world, i.e., infinite volume.

Unlike the binding energy, which is known to depend to leading exponential order only on asymptotic properties of the the wave function (and is thus universal with respect to the details of the short-range interaction that gives rise to the bound state [1,26,29,36,37]), one should expect $\langle r^2\rangle$ to be sensitive in principle to the form of the wave function at all relative distances. This has indeed been observed for radii and other static properties of bounds states calculated in truncated harmonic-oscillator bases [38–40].

We derive in this work analytical expressions for the leading volume dependence of the mean-squared radius for two-body states bound by a short-range interaction. Based on an appropriate ansatz for the relevant volume dependence of the wave function, we obtain explicit formulas for states within the A_1^+ and T_1^- representations of the cubic symmetry group, which correspond approximately to S- and P-wave states in infinite volume. A constructive prescription is given for the general case. Our results are relevant, for example, for lattice QCD studies of the deuteron radius, and the formalism we develop paves the way for deriving analogous relations for other static observables, as well as for bound states comprised of more than two particles. Relations of this form will have applications not only in lattice QCD studies of multinucleon bound states, but also to precision studies of atomic nuclei with lattice EFT.

This paper is organized as follows: In Sec. II we develop the formalism for deriving the finite-volume radius shift $\Delta\langle r^2\rangle(L)$, starting with a discussion of how the bound-state wave function changes when it is confined to a periodic box.

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Subsequently, in Sec. III we present closed-form analytical expressions that describe the radius shift for bound states within the A_1^+ and T_1^- cubic representations, and we verify these the results with explicit numerical calculations. Finally, in Sec. IV we close with a summary and outlook.

II. FORMALISM

A. General setup in infinite volume

We consider a system of two particles with reduced mass μ and relative coordinate denoted $\mathbf{r}$ interacting via a finite-range, spherically symmetric potential, i.e., for $R > 0$ and

$$B = \{\mathbf{x} \in \mathbb{R}^3 : |\mathbf{x}| \leqslant R\}, \tag{1}$$

it holds that

$$V(\mathbf{r}, \mathbf{r}') = 0 \quad \text{if} \quad \mathbf{r}, \mathbf{r}' \notin B, \tag{2}$$

and V depends only on the magnitude of $\mathbf{r}$ and $\mathbf{r}'$. To be as general as possible, we allow V to have a nonlocal form and we emphasize that our main results to do not depend on the detailed form of $V(\mathbf{r}, \mathbf{r}')$. We furthermore note that, although for convenience we assume a strict finite range R in the following, our results remain valid with negligible corrections for short-range potentials that fall off faster than any power law at large distances.

We write the Schrödinger equation for a state $|\psi\rangle$ as

$$\hat{H}|\psi\rangle = E|\psi\rangle, \tag{3}$$

with the Hamiltonian given by

$$\hat{H}\psi(\mathbf{r}) = -\frac{1}{2\mu}\nabla^2\psi(\mathbf{r}) + \int d^3\mathbf{r}'\, V(\mathbf{r}, \mathbf{r}')\psi(\mathbf{r}'). \tag{4}$$

We define $|\psi_\infty\rangle$ to be a solution with positive binding energy E_∞ such that

$$\hat{H}|\psi_\infty\rangle = -E_\infty|\psi_\infty\rangle. \tag{5}$$

For $\mathbf{r} \notin B$ the Hamiltonian simplifies to

$$\hat{H}\psi(\mathbf{r}) \overset{\mathbf{r}\notin B}{=} -\frac{1}{2\mu}\nabla^2\psi(\mathbf{r}), \tag{6}$$

and we can write the asymptotic wave function as

$$\psi_\infty(\mathbf{r}) \overset{\mathbf{r}\notin B}{\equiv} \psi_{\infty,\mathrm{asm}}(\mathbf{r}) = -\mathrm{i}^\ell \gamma h_\ell^{(1)}(i\kappa r) Y_\ell^m(\mathbf{r}/r), \tag{7}$$

where $h_\ell^{(1)}$ is the spherical Hankel function of the first kind and

$$\kappa^2 = 2\mu E_\infty. \tag{8}$$

The asymptotic normalization coefficient (ANC) γ is fixed via the normalization condition $\langle\psi_\infty|\psi_\infty\rangle = 1$ and Eq. (7). For later use we also define a state $|\psi_{E,\mathrm{asm}}\rangle$ to be the purely asymptotic form of a bound state with binding energy E, satisfying

$$\hat{H}\psi_{E,\mathrm{asm}}(\mathbf{r}) \overset{\mathbf{r}\notin B}{=} -E\psi_{E,\mathrm{asm}}(\mathbf{r}). \tag{9}$$

We are not making any assumption here about the behavior of $\psi_{E,\mathrm{asm}}(\mathbf{r})$ for $\mathbf{r} \in B$ and just note that in all applications $\psi_{E,\mathrm{asm}}$ will be multiplied by an indicator function that is zero for $\mathbf{r} \in B$.

B. Finite-volume wave function

Now we consider the same system confined to a cubic periodic box of edge length $L \gg R$. The potential becomes periodic, taking the form

$$V_L(\mathbf{r}, \mathbf{r}') = \sum_{\mathbf{n}\in\mathbb{Z}} V(\mathbf{r} + \mathbf{n}L, \mathbf{r}' + \mathbf{n}L), \tag{10}$$

and it satisfies

$$V_L(\mathbf{r}, \mathbf{r}') = 0 \quad \text{if} \quad \mathbf{r} \in A \text{ or } \mathbf{r}' \in A, \tag{11}$$

where A, called the asymptotic domain, is defined as

$$A = \{\mathbf{x} \in \mathbb{R}^3 : (\mathbf{x} + \mathbf{n}L) \notin B\ \forall\, \mathbf{n} \in \mathbb{Z}^3\}. \tag{12}$$

The action of the finite-volume Hamiltonian on a generic state $|\psi\rangle$, written in configuration space, is then

$$\begin{aligned}\hat{H}_L\psi(\mathbf{r}) &= -\frac{1}{2\mu}\nabla^2\psi(\mathbf{r}) + \int d^3\mathbf{r}'\, V_L(\mathbf{r}, \mathbf{r}')\psi(\mathbf{r}') \\ &= \hat{H}\psi(\mathbf{r}) + \sum_{|\mathbf{n}|\neq 0}\int d^3\mathbf{r}'\, V(\mathbf{r} + \mathbf{n}L, \mathbf{r}' + \mathbf{n}L)\psi(\mathbf{r}') \\ &\overset{\mathbf{r}\in B\cup A}{=} \hat{H}\psi(\mathbf{r}).\end{aligned} \tag{13}$$

The exact finite-volume bound state $\psi_L(\mathbf{r})$ has an energy $-E(L)$ that depends on the size of the box. We relate the infinite and finite-volume binding energies via

$$E(L) = E_\infty + \Delta E(L), \tag{14}$$

where $\Delta E(L)$ is called the energy shift and has been investigated extensively for various systems [1,26,29,36,37]. In the derivation that follows we therefore treat $\Delta E(L)$ as a known quantity and we frequently make use of the fact that

$$\Delta E(L) = O(\mathrm{e}^{-\kappa L}). \tag{15}$$

The finite-volume wave function must be a solution to the finite-volume Schrödinger equation with energy $-E(L)$ that obeys the periodic boundary condition. In the remainder of this section, we work out an ansatz for this periodic finite-volume wave function that will form the basis for our derivation of the radius volume dependence.

Asymptotic solution. Based on the observation that the infinite and finite-volume Hamiltonians are equal in the asymptotic domain, we make the ansatz that an asymptotic solution in finite volume is of the following form (analogous to what is used in Refs. [38,39,41], based on the "linear energy method" of Ref. [42]):

$$\psi_{\mathrm{asm}}(\mathbf{r}) = \chi_A(\mathbf{r})\left[\psi_{\infty,\mathrm{asm}}(\mathbf{r}) + \Delta E(L)\frac{d}{dE}\psi_{E,\mathrm{asm}}(\mathbf{r})\Big|_{E=E_\infty}\right] + O(\Delta E(L)^2). \tag{16}$$

This means we consider the wave function as a function of the energy and relate the volume dependence to an energy dependence via $E = E(L)$, allowing us to Taylor-expand around infinite volume and keep the linear term explicitly. We include $\chi_A(\mathbf{r})$, the indicator function of A, to conveniently set the state to zero outside of the asymptotic domain. If we act on $|\psi_{\mathrm{asm}}\rangle$ with $\hat{H}_L$ in the asymptotic domain, we find

$$
\begin{aligned}
\hat{H}_L\psi_{\rm asm}(\mathbf{r}) &\overset{\mathbf{r}\in A}{=} \hat{H}\psi_{\rm asm}(\mathbf{r}) \\
&= \chi_A(\mathbf{r})\left[\hat{H}\psi_{\infty,\rm asm}(\mathbf{r}) + \Delta E(L)\frac{d}{dE}\hat{H}\psi_{E,\rm asm}(\mathbf{r})\bigg|_{E=E_\infty}\right] + O(\Delta E(L)^2) \\
&= \chi_A(\mathbf{r})\left[-E_\infty\psi_{\infty,\rm asm}(\mathbf{r}) - \Delta E(L)\frac{d}{dE}E\psi_{E,\rm asm}(\mathbf{r})\bigg|_{E=E_\infty}\right] + O(\Delta E(L)^2) \\
&= \chi_A(\mathbf{r})\left[-E_\infty\psi_{\infty,\rm asm}(\mathbf{r}) - \Delta E(L)\psi_{\infty,\rm asm}(\mathbf{r}) - \Delta E(L)E_\infty\frac{d}{dE}\psi_{E,\rm asm}(\mathbf{r})\bigg|_{E=E_\infty}\right] + O(\Delta E(L)^2) \\
&= -[E_\infty + \Delta E(L)]\chi_A(\mathbf{r})\left[\psi_{\infty,\rm asm}(\mathbf{r}) + \Delta E(L)\frac{d}{dE}\psi_{E,\rm asm}(\mathbf{r})\bigg|_{E=E_\infty}\right] + O(\Delta E(L)^2) \\
&= -E(L)\psi_{\rm asm}(\mathbf{r}) + O(\Delta E(L)^2).
\end{aligned} \tag{17}
$$

In going from the fourth to the penultimate line in this equation we have added and subtracted a term proportional to $\Delta E(L)^2$. This allows us to pull out the overall factor $E_\infty + \Delta E(L)$, and the remainder is subsequently absorbed into the $O(\Delta E(L)^2)$. Overall we have found that to leading order $|\psi_{\rm asm}\rangle$ satisfies the Schrödinger equation with energy $-E(L)$, restricted to the asymptotic domain. However, $|\psi_{\rm asm}\rangle$ does *not* satisfy the periodic boundary condition that characterizes the proper finite-volume eigenstate.

Therefore, we now proceed to construct a periodic solution based on $|\psi_{\rm asm}\rangle$. We introduce a translation operator defined via

$$\langle\mathbf{r}|\hat{T}(\mathbf{n})|\psi\rangle = \psi(\mathbf{r}+\mathbf{n}L), \tag{18}$$

from which it follows that

$$\langle\psi|\hat{T}^\dagger(\mathbf{n})|\mathbf{r}\rangle = \psi^*(\mathbf{r}+\mathbf{n}L). \tag{19}$$

It holds that

$$\hat{T}^\dagger(\mathbf{n}) = \hat{T}(-\mathbf{n}) \tag{20}$$

because

$$
\begin{aligned}
\langle\phi|\hat{T}^\dagger(\mathbf{n})|\psi\rangle &= \int d^3\mathbf{r}\,\phi^*(\mathbf{r}+\mathbf{n}L)\psi(\mathbf{r}) \\
&= \int d^3\mathbf{r}\,\phi^*(\mathbf{r})\psi(\mathbf{r}-\mathbf{n}L) \\
&= \langle\phi|\hat{T}(-\mathbf{n})|\psi\rangle.
\end{aligned} \tag{21}
$$

Translation operators also have the property

$$\hat{T}(\mathbf{n})\hat{T}(\mathbf{m}) = \hat{T}(\mathbf{n}+\mathbf{m}). \tag{22}$$

Using translation operators we can construct the asymptotic finite-volume wave function by adding shifted copies of $|\psi_{\rm asm}\rangle$ to satisfy the periodic boundary condition. This leads to

$$|\psi_{L,\rm asm}\rangle = \sum_{\mathbf{n}}\hat{T}(\mathbf{n})|\psi_{\rm asm}\rangle. \tag{23}$$

Due to the linearity of the Schrödinger equation and the fact that the finite-volume Hamiltonian commutes with our translation operators, $|\psi_{L,\rm asm}\rangle$ is a periodic solution of the finite-volume Schrödinger equation with energy $-E(L)$, to leading order, and restricted to the asymptotic domain.

Interior solution. Now that we have found an asymptotic solution, we must find a solution for $\mathbf{r}\notin A$. We need only find an appropriate form for $\mathbf{r}\in B$, since periodic copies of this set cover A^C, illustrated in Fig. 1.

By our previous discussion, we know that $\psi_\infty(\mathbf{r})$ is an approximate solution for $\mathbf{r}\in B$ up to corrections of the order $O(e^{-\kappa L})$. Specifically, by Eqs. (14) and (15) it holds that

$$\hat{H}_L\psi_\infty(\mathbf{r}) \overset{\mathbf{r}\in B}{=} \hat{H}\psi_\infty(\mathbf{r}) = -E(L)\psi_\infty(\mathbf{r}) + O(e^{-\kappa L}). \tag{24}$$

Therefore we make the ansatz that an exact finite-volume solution for $\mathbf{r}\in B$ is of the form

$$\psi_{\rm int}(\mathbf{r}) = \chi_B(\mathbf{r})[\psi_\infty(\mathbf{r}) + \phi(\mathbf{r})], \tag{25}$$

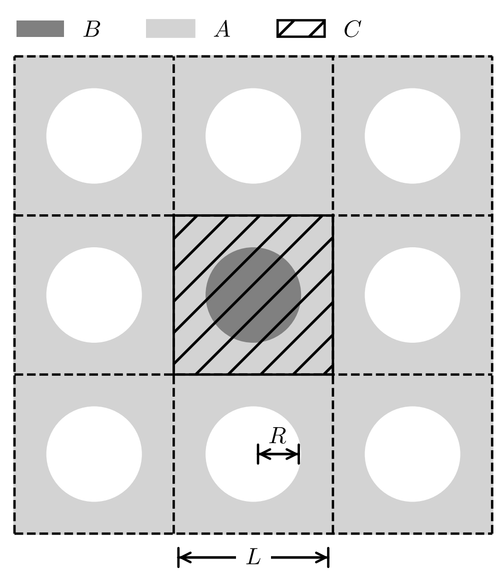

FIG. 1. Illustration showing the sets B, A, and C in a two-dimensional analogy of the three-dimensional scenario we consider. The central box C, cf. Eq. (37), is shown with neighboring periodic copies surrounding it.

where $\phi(\mathbf{r})$ is some correction of order $O(\mathrm{e}^{-\kappa L})$. We note that $\phi(\mathbf{r})$, in general, may depend on L to leading order. Now we wish to find the form of this leading-order L dependence. This state must satisfy

$$\hat{H}_L\psi_{\text{int}}(\mathbf{r}) \overset{\mathbf{r}\in B}{=} \hat{H}\psi_{\text{int}}(\mathbf{r}) = -E(L)\psi_{\text{int}}(\mathbf{r}). \tag{26}$$

Expanding the left-hand side we get

$$\hat{H}\psi_{\text{int}}(\mathbf{r}) = \chi_B(\mathbf{r})[-E_\infty\psi_\infty(\mathbf{r}) + \hat{H}\phi(\mathbf{r})]. \tag{27}$$

Expanding also the right-hand side gives

$$-E(L)\psi_{\text{int}}(\mathbf{r}) = -\chi_B(\mathbf{r})[E_\infty + \Delta E(L)][\psi_\infty(\mathbf{r}) + \phi(\mathbf{r})], \tag{28}$$

and combining the two previous equations we obtain a differential equation for $\phi(\mathbf{r})$:

$$\chi_B(\mathbf{r})\hat{H}\phi(\mathbf{r}) = -\chi_B(\mathbf{r})[E_\infty\phi(\mathbf{r}) + \Delta E(L)\psi_\infty(\mathbf{r})] + O(\mathrm{e}^{-2\kappa L}). \tag{29}$$

If we make the substitution $|\phi\rangle = \Delta E(L)|\varphi\rangle$, we get

$$\chi_B(\mathbf{r})\hat{H}\varphi(\mathbf{r}) = -\chi_B(\mathbf{r})[E_\infty\varphi(\mathbf{r}) + \psi_\infty(\mathbf{r})] + O(\mathrm{e}^{-\kappa L}). \tag{30}$$

Now we make the observation that the differential equation defining $\varphi(\mathbf{r})$ is independent of L to leading order. If the boundary conditions on $\varphi(\mathbf{r})$ are also independent of L to leading order, then we can conclude that the L dependence of $\phi(\mathbf{r})$ must be limited to the factor of $\Delta E(L)$ at this order.

We can fix two separate boundary conditions for $\varphi(\mathbf{r})$. For the first one, we use the fact that parity remains a good quantum number in finite volume, so all states will have either even or odd parity. For even-parity states, the derivative of the wave function at the origin must vanish along all three axes. For odd-parity states, the wave function must vanish at the origin. Since $\psi_{\text{int}}(\mathbf{r})$ and $\psi_\infty(\mathbf{r})$ have definite parities, $\varphi(\mathbf{r})$ must also have a definite parity by Eq. (25), and therefore we obtain that either $\varphi(\mathbf{r})$ or its derivatives must vanish at the origin, and this condition is independent of L. For the second boundary condition we impose continuity between ψ_{int} and $\psi_{L,\text{asm}}$:

$$\psi_{\text{int}}(\mathbf{r})|_{|\mathbf{r}|=R} = \psi_{L,\text{asm}}(\mathbf{r})|_{|\mathbf{r}|=R}, \tag{31a}$$

$$\psi_\infty(\mathbf{r}) + \Delta E(L)\varphi(\mathbf{r})|_{|\mathbf{r}|=R} = \sum_{\mathbf{n}} \hat{T}(\mathbf{n})\psi_{\text{asm}}(\mathbf{r})\Big|_{|\mathbf{r}|=R}, \tag{31b}$$

$$\psi_\infty(\mathbf{r}) + \Delta E(L)\varphi(\mathbf{r})|_{|\mathbf{r}|=R} = \sum_{\mathbf{n}} \hat{T}(\mathbf{n})\left\{\psi_{\infty,\text{asm}}(\mathbf{r}) + \Delta E(L)\frac{d}{dE}\psi_{E,\text{asm}}(\mathbf{r})\right\}\Big|_{E=E_\infty,|\mathbf{r}|=R}, \tag{31c}$$

$$\psi_\infty(\mathbf{r}) + \Delta E(L)\varphi(\mathbf{r})|_{|\mathbf{r}|=R} = \psi_{\infty,\text{asm}}(\mathbf{r}) + \Delta E(L)\frac{d}{dE}\psi_{E,\text{asm}}(\mathbf{r})\Big|_{E=E_\infty,|\mathbf{r}|=R} + \sum_{|\mathbf{n}|=1}\psi_{\infty,\text{asm}}(\mathbf{n}L) + O(e^{-\sqrt{2}\kappa L}), \tag{31d}$$

$$\varphi(\mathbf{r})|_{|\mathbf{r}|=R} = \frac{d}{dE}\psi_{E,\text{asm}}(\mathbf{r})\Big|_{E=E_\infty,|\mathbf{r}|=R} + \frac{1}{\Delta E(L)}\sum_{|\mathbf{n}|=1}\psi_{\infty,\text{asm}}(\mathbf{n}L) + O(\mathrm{e}^{(1-\sqrt{2})\kappa L}). \tag{31e}$$

For this boundary condition to be independent of L to leading order, it must be true that

$$\frac{1}{\Delta E(L)}\sum_{|\mathbf{n}|=1}\psi_{\infty,\text{asm}}(\mathbf{n}L) = \text{const} + O(\mathrm{e}^{(1-\sqrt{2})\kappa L}). \tag{32}$$

Although this is not true in general, it trivially holds for any odd-parity state since Eq. (32) evaluates to zero. We note that it also happens to hold for a number of even-parity states, most notably the S wave. In this paper we focus exclusively on S and P waves, for which this condition is known to hold. However, the following arguments work for any state as long as it can be shown that Eq. (32) holds.

Based on Eq. (30) and the boundary conditions, we conclude that indeed $\varphi(\mathbf{r})$ is independent of L to leading order for at least S- and P-wave states, and we write

$$\psi_{\text{int}}(\mathbf{r}) = \chi_B(\mathbf{r})[\psi_\infty(\mathbf{r}) + \Delta E(L)\varphi(\mathbf{r})] + O(e^{-\sqrt{2}\kappa L}), \tag{33}$$

where all leading-order L dependence is now explicitly accounted for. Just as before, we can make this solution periodic by adding shifted copies:

$$|\psi_{L,\text{int}}\rangle = \sum_{\mathbf{n}}\hat{T}(\mathbf{n})|\psi_{\text{int}}\rangle. \tag{34}$$

Full construction. Finally, we can join our two solutions to get the full finite-volume wave function:

$$|\psi_L\rangle = |\psi_{L,\text{asm}}\rangle + |\psi_{L,\text{int}}\rangle = \sum_{\mathbf{n}}\hat{T}(\mathbf{n})(|\psi_{\text{int}}\rangle + |\psi_{\text{asm}}\rangle). \tag{35}$$

$|\psi_{L,\text{asm}}\rangle$ and $|\psi_{L,\text{int}}\rangle$ are both periodic solutions to

$$\hat{H}_L|\psi\rangle = -E(L)|\psi\rangle \tag{36}$$

to order $O(\mathrm{e}^{-\sqrt{2}\kappa L})$. By linearity, $|\psi_L\rangle$ must also be such a solution. In addition, $|\psi_L\rangle$ is periodic and continuous.

In the next section we only need the form of $\psi_L(\mathbf{r})$ for $\mathbf{r} \in C$, where

$$C = \left(-\frac{L}{2}, \frac{L}{2}\right)^3. \tag{37}$$

Therefore, we drop the unused shifted copies of $|\psi_{\text{int}}\rangle$ and rearrange:

$$|\psi_L\rangle \overset{\mathbf{r}\in C}{=} |\psi_\infty\rangle + \Delta E(L)|\delta\rangle + \sum_{|\mathbf{n}|\neq 0} \hat{T}(\mathbf{n})|\psi_a\rangle + O(\mathrm{e}^{-2\kappa L}), \tag{38}$$

where

$$|\delta\rangle = \chi_B(\mathbf{r})|\varphi\rangle + \chi_A(\mathbf{r})\frac{d}{dE}|\psi_{E,\text{asm}}\rangle\Big|_{E=E_\infty}. \tag{39}$$

C. Radius shift

1. Definition

In general, we define the mean-squared radius of a state as the expectation value of the operator:

$$\hat{r}^2 = \frac{1}{N}\sum_{i=1}^{N}(\hat{\mathbf{r}}_i - \hat{\mathbf{R}})^2, \tag{40}$$

where N is the number of particles, $\hat{\mathbf{r}}_i$ is the position operator of the ith particle, and $\hat{\mathbf{R}}$ is the center-of-mass position operator. Since we work in coordinate representation we drop the hats for these operators in the following. For two particles, we have

$$\mathbf{r}_1 = \mathbf{R} + \tfrac{1}{2}\mathbf{r}, \tag{41a}$$

$$\mathbf{r}_2 = \mathbf{R} - \tfrac{1}{2}\mathbf{r}, \tag{41b}$$

where $\mathbf{r} = \mathbf{r}_2 - \mathbf{r}_1$ is the relative coordinate. Plugging this into Eq. (40), we find that the mean squared radius expectation value for two particles can be written in terms of their relative coordinate simply as

$$\langle r^2\rangle = \tfrac{1}{4}\langle \mathbf{r}^2\rangle. \tag{42}$$

The finite-volume radius shift $\Delta\langle r^2\rangle(L)$ is defined as

$$\Delta\langle r^2\rangle(L) = \langle r^2\rangle(L) - \langle r_\infty^2\rangle, \tag{43}$$

where $\langle r^2\rangle(L)$ is

$$\langle r^2\rangle(L) = \frac{1}{4}\frac{\langle\psi_L|\mathbf{r}^2\chi_C(\mathbf{r})|\psi_L\rangle}{\langle\psi_L|\chi_C(\mathbf{r})|\psi_L\rangle}, \tag{44}$$

so $\Delta\langle r^2\rangle(L)$ can be written as

$$\Delta\langle r^2\rangle(L) = \frac{1}{4}\frac{\langle\psi_L|\mathbf{r}^2\chi_C(\mathbf{r})|\psi_L\rangle}{\langle\psi_L|\chi_C(\mathbf{r})|\psi_L\rangle} - \langle r_\infty^2\rangle. \tag{45}$$

The matrix elements in the numerator and denominator of Eq. (45) can all be written in the form

$$\langle\psi_L|\mathbf{r}^n\chi_C(\mathbf{r})|\psi_L\rangle, \tag{46}$$

where $n = 0$ in the denominator and $n = 2$ in the numerator.

2. Expansion

Upon expanding the sums over shifted copies stemming from the definition of $|\psi_L\rangle$ in Eq. (46), we get the following terms:

$$\langle\psi_L|\mathbf{r}^n\chi_C(\mathbf{r})|\psi_L\rangle = \langle\psi_\infty|\mathbf{r}^n\chi_C(\mathbf{r})|\psi_\infty\rangle + 2\Delta E(L)\mathrm{Re}[\langle\psi_\infty|\mathbf{r}^n\chi_C(\mathbf{r})|\delta\rangle] + \sum_{|\mathbf{n}|\neq 0} 2\mathrm{Re}[\langle\psi_\infty|\mathbf{r}^n\chi_C(\mathbf{r})\hat{T}(\mathbf{n})|\psi_{\text{asm}}\rangle]$$
$$+ \sum_{\substack{|\mathbf{n}|\neq 0\\|\mathbf{m}|\neq 0}} \langle\psi_{\text{asm}}|\hat{T}(-\mathbf{n})\mathbf{r}^n\chi_C(\mathbf{r})\hat{T}(\mathbf{m})|\psi_{\text{asm}}\rangle + O(\mathrm{e}^{-2\kappa L}). \tag{47}$$

We can add zero to the first term in the form of

$$\langle\psi_\infty|\mathbf{r}^n\chi_C(\mathbf{r})|\psi_\infty\rangle = \langle\psi_\infty|\mathbf{r}^n\chi_C(\mathbf{r})|\psi_\infty\rangle + \underbrace{\sum_{|\mathbf{n}|\neq 0}\langle\psi_\infty|\mathbf{r}^n\chi_C(\mathbf{r}-\mathbf{n}L)|\psi_\infty\rangle - \sum_{|\mathbf{n}|\neq 0}\langle\psi_\infty|\mathbf{r}^n\chi_C(\mathbf{r}-\mathbf{n}L)|\psi_\infty\rangle}_{=0}, \tag{48}$$

which allows us to absorb the lone term into the first sum:

$$\langle\psi_\infty|\mathbf{r}^n\chi_C(\mathbf{r})|\psi_\infty\rangle = \sum_{\mathbf{n}}\langle\psi_\infty|\mathbf{r}^n\chi_C(\mathbf{r}-\mathbf{n}L)|\psi_\infty\rangle - \sum_{|\mathbf{n}|\neq 0}\langle\psi_\infty|\mathbf{r}^n\chi_C(\mathbf{r}-\mathbf{n}L)|\psi_\infty\rangle. \tag{49}$$

$\chi_C(\mathbf{r}-\mathbf{n}L)$ simply sums to 1 over all $\mathbf{n}$, so

$$\langle\psi_\infty|\mathbf{r}^n\chi_C(\mathbf{r})|\psi_\infty\rangle = \langle\psi_\infty|\mathbf{r}^n|\psi_\infty\rangle - \sum_{|\mathbf{n}|\neq 0}\langle\psi_\infty|\mathbf{r}^n\chi_C(\mathbf{r}-\mathbf{n}L)|\psi_\infty\rangle. \tag{50}$$

We write $\langle\psi_\infty|\mathbf{r}^n|\psi_\infty\rangle$ as $\langle\mathbf{r}_\infty^n\rangle$ and therefore we get:

$$\langle\psi_\infty|\mathbf{r}^n\chi_C(\mathbf{r})|\psi_\infty\rangle = \langle\mathbf{r}_\infty^n\rangle - \sum_{|\mathbf{n}|\neq 0}\langle\psi_\infty|\mathbf{r}^n\chi_C(\mathbf{r}-\mathbf{n}L)|\psi_\infty\rangle. \tag{51}$$

Expanding also the second term in Eq. (47), we find

$$2\Delta E(L)\,\mathrm{Re}[\langle\psi_\infty|\mathbf{r}^n\chi_C(\mathbf{r})|\delta\rangle] = 2\Delta E(L)\,\mathrm{Re}\bigg[\langle\psi_\infty|\mathbf{r}^n\chi_B(\mathbf{r})|\varphi\rangle + \langle\psi_\infty|\mathbf{r}^n\chi_{C\cap A}(\mathbf{r})\frac{d}{dE}|\psi_{E,\text{asm}}\rangle\Big|_{E=E_\infty}\bigg]. \tag{52}$$

The first term in the square brackets on the right-hand side contains no L dependence, and since we do not explicitly know the form of $\psi_\infty(\mathbf{r})$ for all $\mathbf{r}$, we choose to parametrize the entire term by a constant β_n'. Moreover, since $\psi_{E,\mathrm{asm}}(\mathbf{r})$ decays exponentially for large r, any L dependence introduced by the second term will contribute only some decaying exponential in L. Since the right-hand side overall already contains a factor of $\Delta E(L)$, the L dependence from the second term turns out to be of higher exponential order and can therefore be dropped. Altogether, neither matrix element in Eq. (52) directly contributes to the leading L dependence and so we can combine them into a single constant β_n:

$$2\Delta E(L)\,\mathrm{Re}\langle\psi_\infty|\mathbf{r}^n\chi_C(\mathbf{r})|\delta\rangle = \beta_n\Delta E(L) + O(e^{-\sqrt{2}\kappa L}). \quad (53)$$

Turning to the third term in Eq. (47), since $\psi_{\mathrm{asm}}(\mathbf{r})$ is always evaluated shifted by at least a distance L, and because the second term in the definition of $\psi_{\mathrm{asm}}(\mathbf{r})$, Eq. (16), is already suppressed by a factor $\Delta E(L)$, that part is overall beyond leading exponential order and can be dropped. Effectively, we may replace $\psi_{\mathrm{asm}}(\mathbf{r})$ with $\psi_{\infty,\mathrm{asm}}(\mathbf{r})$, and we can furthermore replace $\psi_\infty(\mathbf{r})$ with the asymptotic form because it will only ever be evaluated in the asymptotic region. We therefore arrive at

$$\sum_{|\mathbf{n}|\neq 0} 2\mathrm{Re}\langle\psi_\infty|\mathbf{r}^n\chi_C(\mathbf{r})\hat{T}(\mathbf{n})|\psi_{\mathrm{asm}}\rangle = \sum_{|\mathbf{n}|=1} 2\mathrm{Re}\langle\psi_{\infty,\mathrm{asm}}|\mathbf{r}^n\chi_C(\mathbf{r})\hat{T}(\mathbf{n})\chi_A(\mathbf{r})|\psi_{\infty,\mathrm{asm}}\rangle + O(e^{-\sqrt{2}\kappa L}), \quad (54)$$

where we have also made use of the fact that only $|\mathbf{n}| = 1$ terms contribute to leading exponential order.

Finally, for the fourth term in Eq. (47), we can again note that the second term of $\psi_{\mathrm{asm}}(\mathbf{r})$ will contribute only beyond leading exponential order since it is shifted by at least L and suppressed by $\Delta E(L)$. Therefore, we can replace $\psi_{\mathrm{asm}}(\mathbf{r})$ with $\chi_A(\mathbf{r})\psi_{\infty,\mathrm{asm}}(\mathbf{r})$ and obtain

$$\sum_{\substack{|\mathbf{n}|\neq 0\\|\mathbf{m}|\neq 0}} \langle\psi_{\mathrm{asm}}|\hat{T}(-\mathbf{n})\mathbf{r}^n\chi_C(\mathbf{r})\hat{T}(\mathbf{m})|\psi_{\mathrm{asm}}\rangle = \sum_{\substack{|\mathbf{n}|\neq 0\\|\mathbf{m}|\neq 0}} \langle\psi_{\infty,\mathrm{asm}}|\hat{T}(-\mathbf{n})\mathbf{r}^n\chi_{C\cap A}(\mathbf{r})\hat{T}(\mathbf{m})|\psi_{\infty,\mathrm{asm}}\rangle + O(e^{-\sqrt{2}\kappa L}). \quad (55)$$

Commuting the $\hat{T}(-\mathbf{n})$ operator to the right furthermore gives

$$\sum_{\substack{|\mathbf{n}|\neq 0\\|\mathbf{m}|\neq 0}} \langle\psi_{\mathrm{asm}}|\hat{T}(-\mathbf{n})\mathbf{r}^n\chi_C(\mathbf{r})\hat{T}(\mathbf{m})|\psi_{\mathrm{asm}}\rangle = \sum_{\substack{|\mathbf{n}|\neq 0\\|\mathbf{m}|\neq 0}} \langle\psi_{\infty,\mathrm{asm}}|(\mathbf{r}-\mathbf{n}L)^n\chi_{C\cap A}(\mathbf{r}-\mathbf{n}L)\hat{T}(\mathbf{m}-\mathbf{n})|\psi_{\infty,\mathrm{asm}}\rangle + O(e^{-\sqrt{2}\kappa L}). \quad (56)$$

The only case in which this is of leading exponential order is when $\mathbf{n} = \mathbf{m}$ and when their magnitude is equal to one, so

$$\sum_{\substack{|\mathbf{n}|\neq 0\\|\mathbf{m}|\neq 0}} \langle\psi_{\mathrm{asm}}|\hat{T}(-\mathbf{n})\mathbf{r}^n\chi_C(\mathbf{r})\hat{T}(\mathbf{m})|\psi_{\mathrm{asm}}\rangle = \sum_{|\mathbf{n}|=1} \langle\psi_{\infty,\mathrm{asm}}|(\mathbf{r}-\mathbf{n}L)^n\chi_{C\cap A}(\mathbf{r}-\mathbf{n}L)|\psi_{\infty,\mathrm{asm}}\rangle + O(e^{-\sqrt{2}\kappa L}). \quad (57)$$

We can make the substitution $\chi_{C\cap A}(\mathbf{r}-\mathbf{n}L) \to \chi_C(\mathbf{r}-\mathbf{n}L)$ since including the shifted B in the integration domain only makes a less-than-leading-order difference over the product of shifted wave functions:

$$\sum_{\substack{|\mathbf{n}|\neq 0\\|\mathbf{m}|\neq 0}} \langle\psi_{\mathrm{asm}}|\hat{T}(-\mathbf{n})\mathbf{r}^n\chi_C(\mathbf{r})\hat{T}(\mathbf{m})|\psi_{\mathrm{asm}}\rangle = \sum_{|\mathbf{n}|=1} \langle\psi_{\infty,\mathrm{asm}}|(\mathbf{r}-\mathbf{n}L)^n\chi_C(\mathbf{r}-\mathbf{n}L)|\psi_{\infty,\mathrm{asm}}\rangle + O(e^{-\sqrt{2}\kappa L}). \quad (58)$$

Reassembling all the simplified terms back into Eq. (47), we get

$$\begin{aligned}\langle\psi_L|\mathbf{r}^n\chi_C(\mathbf{r})|\psi_L\rangle = \langle\mathbf{r}_\infty^n\rangle + \beta_n\Delta E(L) + \sum_{|\mathbf{n}|=1}\{&\langle\psi_{\infty,\mathrm{asm}}|((\mathbf{r}-\mathbf{n}L)^n - \mathbf{r}^n)\chi_C(\mathbf{r}-\mathbf{n}L)|\psi_{\infty,\mathrm{asm}}\rangle\\ &+ 2\mathrm{Re}[\langle\psi_{\infty,\mathrm{asm}}|\mathbf{r}^n\chi_{C\cap A}(\mathbf{r})\hat{T}(\mathbf{n})|\psi_{\infty,\mathrm{asm}}\rangle]\} + O(e^{-\sqrt{2}\kappa L}).\end{aligned} \quad (59)$$

Plugging this then into Eq. (45) and expanding to leading exponential order, we arrive at

$$\begin{aligned}\Delta\langle r^2\rangle(L) = \alpha\Delta E(L) + \sum_{|\mathbf{n}|=1}\Bigg[&\langle\psi_{\infty,\mathrm{asm}}|\frac{1}{4}(L^2 - 2\mathbf{r}\cdot\mathbf{n}L)\chi_C(\mathbf{r}-\mathbf{n}L)|\psi_{\infty,\mathrm{asm}}\rangle\\ &+ \mathrm{Re}\left\{\langle\psi_{\infty,\mathrm{asm}}|\frac{1}{2}\left(\mathbf{r}^2 - 4\langle r_\infty^2\rangle\right)\chi_{C\cap A}(\mathbf{r})\hat{T}(\mathbf{n})|\psi_{\infty,\mathrm{asm}}\rangle\right\}\Bigg] + O(e^{-\sqrt{2}\kappa L}),\end{aligned} \quad (60)$$

where $\alpha = \frac{1}{4}\beta_2 - \langle r_\infty^2\rangle\beta_0$ is a parameter that must be fit to numerical data.

3. Simplification

We now focus on simplifying both terms. To that end, we write Eq. (60) in shorthand notation as

$$\Delta\langle r^2\rangle(L) = \alpha\,\Delta E(L) + \mathrm{Re}\langle\psi_{\infty,\mathrm{asm}}|\hat{\eta}|\psi_{\infty,\mathrm{asm}}\rangle + O(e^{-\sqrt{2}\kappa L}), \tag{61}$$

where

$$\hat{\eta} = \sum_{|\mathbf{n}|=1}\bigg\{\frac{1}{4}(L^2 - 2\mathbf{r}\cdot\mathbf{n}L)\chi_C(\mathbf{r}-\mathbf{n}L) + \frac{1}{2}\big[\mathbf{r}^2 - 4\langle r_\infty^2\rangle\big]\chi_{C\cap A}(\mathbf{r})\hat{T}(\mathbf{n})\bigg\}. \tag{62}$$

Note that we define $\hat{\eta}$ as an operator, but choose to write it explicitly in terms of $\mathbf{r}$, with the understanding that this is equivalent to writing $\hat{\mathbf{r}}$ when we specify that $\hat{\eta}$ is local in coordinate space, $\langle\mathbf{r}'|\hat{\eta}|\mathbf{r}\rangle = \eta(\mathbf{r})\delta^{(3)}(\mathbf{r}-\mathbf{r}')$. Also note that the following manipulations of $\hat{\eta}$ are done with the understanding that $\hat{\eta}$ will be evaluated between wave functions as in Eq. (61). All matrix elements are computed in configuration space, which is what we refer to as "integration" in the following.

We define the rotation operator $\hat{R}(\mathbf{n})$ that maps the vector $\mathbf{n}$ onto the direction of $\hat{\mathbf{z}}$. This definition does not uniquely describe a particular rotation, however, the ambiguity does not matter for our purposes. For example, we say that

$$\hat{R}(\mathbf{n})\hat{T}(\mathbf{n})\hat{R}^\dagger(\mathbf{n}) = \hat{T}(\hat{\mathbf{z}}). \tag{63}$$

We note that

$$\hat{R}^\dagger(\mathbf{n}) = \hat{R}^{-1}(\mathbf{n}). \tag{64}$$

Because of this we can insert the identity $\hat{R}^\dagger(\mathbf{n})\hat{R}(\mathbf{n})$ anywhere we would like. Inserting this identity into $\hat{\eta}$ and commuting the operators to opposite sides, we get

$$\hat{\eta} = \sum_{|\mathbf{n}|=1}\hat{R}^\dagger(\mathbf{n})\bigg\{\frac{1}{4}(L^2 - 2zL)\chi_C(\mathbf{r}-\hat{\mathbf{z}}L) + \frac{1}{2}\big[\mathbf{r}^2 - 4\langle r_\infty^2\rangle\big]\chi_{C\cap A}(\mathbf{r})\hat{T}(\hat{\mathbf{z}})\bigg\}\hat{R}(\mathbf{n}). \tag{65}$$

Since the real part will be taken at the end as per our previous manipulations, we take the Hermitian conjugate of the second term and then commute the translation operator back to the right, leading to

$$\hat{\eta} = \sum_{|\mathbf{n}|=1}\hat{R}^\dagger(\mathbf{n})\bigg\{\frac{1}{4}(L^2 - 2zL)\chi_C(\mathbf{r}-\hat{\mathbf{z}}L) + \frac{1}{2}\big[(\mathbf{r}-\hat{\mathbf{z}}L)^2 - 4\langle r_\infty^2\rangle\big]\chi_{C\cap A}(\mathbf{r}-\hat{\mathbf{z}}L)\hat{T}(-\hat{\mathbf{z}})\bigg\}\hat{R}(\mathbf{n}). \tag{66}$$

We can make the substitution $\chi_C(\mathbf{r}-\hat{\mathbf{z}}L) \to \chi_P(\mathbf{r})$, where

$$P = \{\mathbf{x}\in\mathbb{R}^3 : \mathbf{x}\cdot\hat{\mathbf{z}} > L/2\}, \tag{67}$$

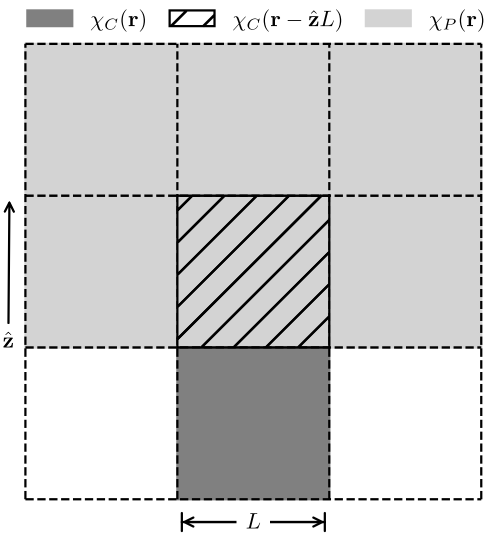

FIG. 2. Illustration showing the indicator functions of the sets C and P in a 2D analogy. The central box is shown at the bottom with neighboring periodic copies surrounding it. Note that P extends infinitely from the edges of the figure.

illustrated in Fig. 2. This substitution does not cause a leading-order change, so we write

$$\hat{\eta} = \sum_{|\mathbf{n}|=1}\hat{R}^\dagger(\mathbf{n})\bigg\{\frac{1}{4}(L^2 - 2zL)\chi_P(\mathbf{r}) + \frac{1}{2}\big[(\mathbf{r}-\hat{\mathbf{z}}L)^2 - 4\langle r_\infty^2\rangle\big]\chi_{P\cap A}(\mathbf{r})\hat{T}(-\hat{\mathbf{z}})\bigg\}\hat{R}(\mathbf{n}). \tag{68}$$

We may furthermore insert the function $\chi_A(\mathbf{r})$ into the first term without introducing a leading-order change. This makes the indicator function conveniently identical for both terms:

$$\hat{\eta} = \sum_{|\mathbf{n}|=1}\hat{R}^\dagger(\mathbf{n})\chi_{P\cap A}(\mathbf{r})\bigg\{\frac{1}{4}(L^2 - 2zL) + \frac{1}{2}\big[(\mathbf{r}-\hat{\mathbf{z}}L)^2 - 4\langle r_\infty^2\rangle\big]\hat{T}(-\hat{\mathbf{z}})\bigg\}\hat{R}(\mathbf{n}). \tag{69}$$

We can write this now as

$$\hat{\eta} = \sum_{|\mathbf{n}|=1}\hat{R}^\dagger(\mathbf{n})\hat{\xi}\hat{R}(\mathbf{n}), \tag{70}$$

where

$$\hat{\xi} = \chi_{P\cap A}(\mathbf{r})\big\{\tfrac{1}{4}(L^2 - 2zL) + \tfrac{1}{2}\big((\mathbf{r}-\hat{\mathbf{z}}L)^2 - 4\langle r_\infty^2\rangle\big)\hat{T}(-\hat{\mathbf{z}})\big\}. \tag{71}$$

Finally, we arrive at the final simplified form:

$$\Delta\langle r^2\rangle(L) = \alpha\,\Delta E(L) + \mathrm{Re}\left(\sum_{|\mathbf{n}|=1}\langle\hat{R}(\mathbf{n})\psi_{\infty,\mathrm{asm}}|\hat{\xi}|\hat{R}(\mathbf{n})\psi_{\infty,\mathrm{asm}}\rangle\right) + O(e^{-\sqrt{2}\kappa L}). \tag{72}$$

Depending on the actual (cubic) symmetry properties of $|\psi_{\infty,\mathrm{asm}}\rangle$, some of the terms in the sum may not need to be computed. For example, for the finite-volume analog of an S-wave state (discussed in more detail below), $\hat{R}(\mathbf{n})\psi_{\infty,\mathrm{asm}}(\mathbf{r}) = \psi_{\infty,\mathrm{asm}}(\mathbf{r})$ for all rotations $\hat{R}(\mathbf{n})$, so all the terms in the sum are identical and only one needs to be evaluated explicitly.

4. Coordinate transformation

Now we present a coordinate system in which the quantity $\langle\psi|\hat{\xi}|\psi\rangle$ is relatively straightforward to compute in closed form. We use a two-center bispherical coordinate system parametrized by r, u, and ϕ, where r is the distance from the origin, u is the distance from the origin of the neighboring periodic box in the $\hat{\mathbf{z}}$ direction, and ϕ is the azimuthal angle about the z axis. The valid set of coordinates is given by

$$\{(r,u,\phi)\in[0,\infty)\times[0,\infty)\times[0,2\pi): r+u\geqslant L\}. \tag{73}$$

For reference, we note that the transformation to Cartesian coordinates is provided by

$$x = \sqrt{r^2 - \frac{(L^2+r^2-u^2)^2}{4L^2}}\cos\phi, \tag{74}$$

$$y = \sqrt{r^2 - \frac{(L^2+r^2-u^2)^2}{4L^2}}\sin\phi, \tag{75}$$

$$z = \frac{L^2+r^2-u^2}{2L}. \tag{76}$$

The volume element in the (r,u,ϕ) coordinate system has the simple form

$$d^3\mathbf{r} = \frac{ru}{L}\mathrm{d}r\mathrm{d}u\mathrm{d}\phi. \tag{77}$$

The main advantage of using this coordinate system is that

$$\hat{T}(-\hat{\mathbf{z}})r = |\mathbf{r}-\hat{\mathbf{z}}L| = u, \tag{78}$$

so integrals over shifted radial functions are just as simple as integrals over unshifted radial functions. The trade-off, however, is that the bounds of the integration domain become more complicated, especially given that not all coordinate values are valid. With this in mind, the bounds of integration with the indicator function $\chi_{P\cap A}(\mathbf{r})$ become

$$\int\chi_{P\cap A}(\mathbf{r})\ldots d^3\mathbf{r} = \int_R^{L/2}\int_{L-u}^{L+u}\int_0^{2\pi}\cdots\frac{ru}{L}\mathrm{d}\phi\mathrm{d}r\mathrm{d}u + \int_{L/2}^{\infty}\int_u^{\infty}\int_0^{2\pi}\cdots\frac{ru}{L}\mathrm{d}\phi\mathrm{d}r\mathrm{d}u. \tag{79}$$

In the (r,u,ϕ) coordinate system, $\hat{\xi}$ has the form

$$\hat{\xi} = \chi_{P\cap A}(\mathbf{r})\left\{\tfrac{1}{4}(u^2-r^2) + \tfrac{1}{2}\left(u^2 - 4\langle r_\infty^2\rangle\right)\hat{T}(-\hat{\mathbf{z}})\right\}. \tag{80}$$

The coordinate system described above allows us to obtain closed-form expressions for the finite-volume radius shift for certain important cases, which we present in the following section. We use this formalism to derive explicit analytical expressions for the radius shift for S- and P-wave states shown in Sec. III B, with details of the calculation presented in the Appendix.

III. RESULTS

A. Broken spherical symmetry

As already alluded to before, spherical symmetry is broken by confining the system to a periodic cubic box, and as a consequence angular momentum ℓ is not a good quantum number anymore. The relevant spatial symmetry is instead described by the group of rotations that leave a cube invariant. The structure of this group is well known and has been discussed, for example, in Ref. [43]. Angular-momentum multiplets in general break up into irreducible representations of the cubic group, of which there are overall five different ones, denoted $\Gamma = A_1, A_2, E, T_1, T_2$, with dimensions 1, 1, 2, 3, 3, respectively. It is typically a good assumption to identify S-wave ($\ell = 0$) states in infinite volume with A_1^+ cubic states, and P-wave states with the T_1^- representation, where the superscript indicates positive or negative parity.[1]

B. Explicit formulas

We present here analytic forms of the radius shift for $\ell = 0$ and $\ell = 1$ contributions to the A_1^+ and T_1^- cubic representations, respectively. After calculating the radius shift for S-wave and P-wave states using the method presented above, we find that

$$\Delta\langle r^2\rangle_0^{A_1^+}(L) = |\gamma|^2\mathrm{e}^{-\kappa L}\left(\frac{L^2}{4\kappa} + \frac{3\left(1-8\kappa^2\langle r_\infty^2\rangle\right)}{8\kappa^3} + \frac{a}{\kappa^4 L}\right) + \frac{3}{16}|\gamma|^2L^3\mathrm{Ei}(-\kappa L) + O(e^{-\sqrt{2}\kappa L}), \tag{81}$$

and

$$\Delta\langle r^2\rangle_1^{T_1^-}(L) = |\gamma|^2\mathrm{e}^{-\kappa L}\left(-\frac{L^2}{4\kappa} + \frac{3\left(5+8\kappa^2\langle r_\infty^2\rangle\right)}{8\kappa^3} + \frac{a}{\kappa^4 L}\right) + \frac{3}{16\kappa^2}|\gamma|^2L(8-\kappa^2L^2)\mathrm{Ei}(-\kappa L) + O(e^{-\sqrt{2}\kappa L}), \tag{82}$$

where a is a dimensionless fit parameter. The details of how we arrived at these expressions are given in the Appendix. We make the following observations:

(1) S-wave representations are one dimensional, and the same is true for A_1^+. All three basis states for $\ell = 1$ (and therefore for $\Gamma = T_1^-$ in the P-wave approximation) have the same radius shift since they are all just different rotations of essentially the same degenerate state.

(2) In general, the radius-shift formula will have at least two additional fit parameters compared with the energy shift. The first of these is the α introduced in Eq. (60), while the second is R, the upper bound of the

[1] Higher angular momenta ℓ contribute to both cubic multiplets, but there are significant gaps. As discussed in Ref. [43], A_1^+ receives contributions from $\ell = 0, 4, 6, 8, \ldots$, while for T_1^- the sequence is $\ell = 1, 3, 4, 5, \ldots$.

interior integration domain that enters via the indicator function $\chi_{P\cap A}$ in Eq. (80), which is in general unknown if the interaction does not have a strict finite range. Remarkably, however, the S- and P-wave radius shift formulas still feature only *one* additional fit parameter compared with the energy shift since we were able to absorb all R and α dependence into a single constant a, as shown in the Appendix.

(3) We also note that the S- and P-wave radius shifts are exactly negatives of each other up to order $O(\mathrm{e}^{-\kappa L} \times L^0) = O(\mathrm{e}^{-\kappa L})$. That is, the S- and P-wave radius shifts are

$$\Delta\langle r^2\rangle_0^{A_1^+}(L) = \frac{|\gamma|^2\mathrm{e}^{-\kappa L}}{16\kappa^2}[\kappa L^2 + 3L + O(L^0)],$$
$$\Delta\langle r^2\rangle_1^{T_1^-}(L) = -\frac{|\gamma|^2\mathrm{e}^{-\kappa L}}{16\kappa^2}[\kappa L^2 + 3L + O(L^0)].$$

This finding is similar to what has been found for the finite-volume energy shifts [37].

(4) From the correlation between binding energies and mean-squared radii, which in infinite-volume usually implies that more deeply bound states become more compact, combined with the known volume dependence of the binding energy [36,37], one might naively expect the leading radius corrections to have exactly the opposite signs of what we found here. S-wave bound states become more deeply bound in finite volume, so the naive intuition would be that their radii would *decrease*, and vice versa for P-wave states. However, the behavior we derived here can in fact be related to how the finite volume affects the wave functions, similar to the intuitive argument that explains the sign of the energy shift [36,37]: Since A_1^+ S-wave states have even parity, the derivative of the wave function across the boundary of the box must be zero. This means that the finite-volume wave function can have a larger-magnitude tail near the boundary of the box than the corresponding infinite-volume wave function at the same distance. Since the mean-squared radius, defined as the expectation value of r^2, relatively emphasizes contributions from large distances, overall the radius can increase in finite volume. For T_1^- P-wave states on the other hand, odd-parity forces the wave function to zero at the boundary, compressing the wave-function profile and therefore leading to a smaller radius compared with infinite volume.

C. Numerical checks

Part of this work is determining the optimal strategy for using the shift formulae for practical radius extrapolations. For this purpose, we assume that we are dealing with a finite-volume simulation that provides both energies and wave functions for the states of interest, such as a straightforward lattice discretization of the Hamiltonian or a discrete variable representation (DVR) based on plane-wave states, an efficient few-body implementation of which has been discussed in Refs. [44–46]. Since we have access to the energy data, it makes sense to use that first to extract the binding momentum κ and the ANC γ. Once κ and γ have been determined, they can be used as fixed parameters in the radius volume dependence, leaving only two parameters still to be fit, $\langle r_\infty^2\rangle$ and a.

Determining a particular "best" fitting algorithm is difficult due to the unknown higher-order terms and the exponential form of the volume dependence. One option, employed in much of the FV bound-state literature cited previously, is to fit the data on a logarithmic scale and focus on the large-volume region where the higher-order corrections are smaller. However, fitting on a logarithmic scale introduces several complications. First, in order to obtain a simple form, one generally needs to subtract the infinite-volume value from the data. While this can be done relatively easily for the binding energy in some cases,[2] in general the infinite-volume value is one of the fit parameters, so we do not know its value before performing the fit. Even after getting past that problem, logarithmic scales can make it very difficult to determine constant terms, such as $\langle r_\infty^2\rangle$ in

$$\langle r^2\rangle(L) = \langle r_\infty^2\rangle + \Delta\langle r^2\rangle(L), \tag{83}$$

cf. Eq. (60), because the logarithm of the right-hand side diverges near the correct value, i.e., when the fit is near optimal. Since the residuals may not reflect the true quality of the fit, this fitting method tends to be unstable.

The method we propose assumes that the only source of uncertainty comes from the unknown higher-order terms. Therefore, it makes sense to simply minimize the residuals on a linear scale, weighted by the inverse absolute value of those higher-order terms. Since of course we do not know the exact form of the higher-order terms, we merely assume that they scale appropriately as $\mathrm{e}^{-\sqrt{2}\kappa L}$. To illustrate this method with concrete examples, we perform fits using a weighted least-squares algorithm where the weights are assigned as described above. Specifically, we apply this procedure to perform fits of the form

$$E(L) = \Delta E(L) + E_\infty \tag{84}$$

for the energy, and as in Eq. (83) for the radius.

For our numerical simulation we use the DVR framework of Ref. [44], and as concrete interaction we use attractive local Gaussian potentials of the form

$$V(r) = V_0 \exp\left[-\left(\frac{r}{R_0}\right)^2\right], \tag{85}$$

with parameters $V_0 < 0$ and $R_0 > 0$. This interaction does not have a strict finite range R as assumed for convenience in the derivation of the radius volume dependence, but corrections stemming from the Gaussian tails of the potential can generally be neglected.

[2]For A_1^+ and T_1^- states without Coulomb interaction, the leading volume dependence is a pure exponential, so one can determine the infinite-volume energy by demanding that the volume dependence is linear on an appropriately scaled logarithmic scale, as done for example in Ref. [26].

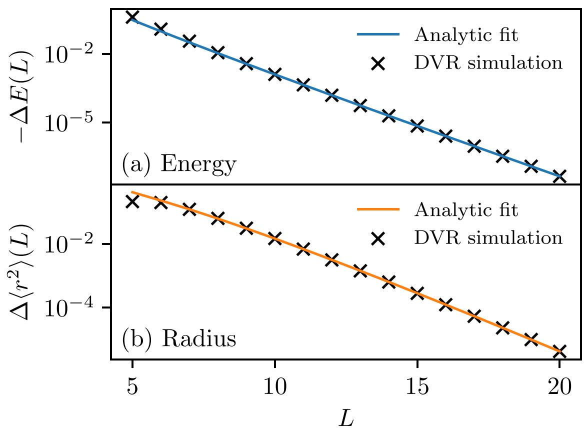

FIG. 3. Volume dependence for the energy and mean squared radius of an S-wave state using a Gaussian potential ($R = 2, V_0 = -3$). Quantities are reported in natural units with the particle mass set to one. The energy and radius shifts from a numerical simulation and the analytic fit are plotted in the upper and lower panels, respectively.

Example fits for S- and P-wave states are shown in Figs. 3 and 4, respectively. Even though the fits were performed on a linear scale, as described above, they look excellent on the logarithmic scale that we chose to improve the display and highlight the excellent agreement of the numerical simulation with our predictions. This is because of the exponential weighting.

The quality of the fit for the radius is particularly good given that κ and γ were predetermined by the energy fit and the fit parameter a has very little influence on the shape of the curve. We see the analytic fit significantly deviating from the simulation data only in very small volumes due to the higher-order terms and due to violating of the condition $L \gg R$. The latter is most likely the dominant reason because we observe that the deviation occurs over approximately the same volume range for both the energy and the radius, with comparable magnitude.

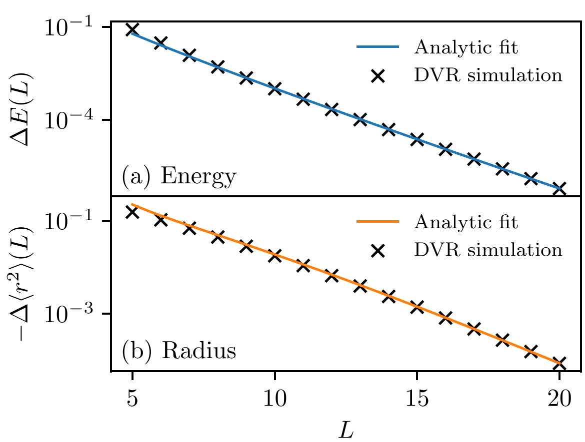

FIG. 4. Volume dependence for the energy and mean squared radius of a P-wave state using a Gaussian potential ($R = 1, V_0 = -14$). Quantities are reported in natural units with the particle mass set to one. The energy and radius shifts from a numerical simulation and the analytic fit are plotted in the upper and lower panels, respectively.

TABLE I. Fit results for $\langle r^2_\infty\rangle$ over different volume ranges for an S-wave state ($R = 2, V_0 = -3$) compared with the mean squared radius at the largest volume in the fit region. Quantities are reported in natural units with the particle mass set to one.

Fit range: $L = 6, \ldots, L_{\max}$		
$L_{\max}$	$\langle r^2\rangle(L_{\max})$	$\langle r^2_\infty\rangle_{\text{fit}}$
10	0.774 577 868 318 02	0.7625(3)
12	0.763 023 468 936 72	0.760 22(3)
14	0.760 516 853 247 93	0.759 917(3)
16	0.760 004 146 206 13	0.759 883 9(3)
18	0.759 903 663 511 78	0.759 880 64(2)
20	0.759 884 610 244 28	0.759 880 344(2)
Continuum: 0.759 880 31		

A quantitative overview of the radius extrapolations we can get using this method is shown in Tables I and II. For comparison, continuum results were calculated as reference by numerically solving the radial equation for the system via the shooting method and evaluating the mean squared radius using the wave functions obtained in that manner. The radius extrapolations perform well over a variety of volume ranges and the extrapolated radius is consistently more accurate (compared with the reference results) than the radius from the largest simulated volume. We note that the uncertainty in the extrapolated radius extracted from the fits is only a lower bound for the true theoretical uncertainties. A more sophisticated approach would propagate the uncertainties in κ and γ from the energy fits and include also the systematic uncertainty stemming from omitted higher-order terms in the radius volume dependence.

IV. SUMMARY AND OUTLOOK

We have studied the leading volume dependence for the mean squared radius of bound states of two point particles in a finite periodic box. Using an ansatz for the wave function in finite volume and a sequence of systematic simplifications, we derived a general formula for the finite-volume correction to the radius expectation value. With the help of a carefully

TABLE II. Fit results for $\langle r^2_\infty\rangle$ over different volume ranges for a P-wave state ($R = 1, V_0 = -14$) compared with the mean squared radius at the largest volume in the fit region. Quantities are reported in natural units with the particle mass set to one.

Fit range: $L = 6, \ldots, L_{\max}$		
$L_{\max}$	$\langle r^2\rangle(L_{\max})$	$\langle r^2_\infty\rangle_{\text{fit}}$
10	0.578 866 122 009 667	0.5927(3)
12	0.589 849 429 592 643	0.595 27(8)
14	0.594 046 766 392 319	0.596 07(2)
16	0.595 575 413 626 522	0.596 305(5)
18	0.596 112 250 896 048	0.596 366(1)
20	0.596 295 400 058 964	0.596 381 4(2)
Continuum: 0.596 385 7		

constructed coordinate system, we were able to evaluate this general expression and obtain closed-form expressions for the important cases of S- and P-wave states falling within the A_1^+ and T_1^- irreducible representations of the cubic group in finite volume. These expressions are to a large extent informed by the volume dependence of the energy and involve a surprisingly small number of additional parameters that need to be fit to numerical simulation data. As part of this work we have performed such numerical simulation using Gaussian model potentials and found excellent agreement of our analytic results with calculations.

Our results constitute important progress towards obtaining precise predictions from finite-volume simulations for observables beyond binding energies for quantum systems such as atomic nuclei. While we have studied here explicitly the mean squared radius, our method of constructing an ansatz for the periodic finite-volume wave function without explicit knowledge of the short-distance behavior, and subsequently evaluating matrix elements based on this ansatz, provides a recipe for deriving the volume dependence of other static properties, such as, for example, quadrupole moments.

An important next step towards implementing radius extrapolations in practical applications will be the extension of our findings to bound states comprised of more than two particles. Guidance for such work can be provided by the formalism that derived the binding-energy volume dependence for arbitrary cluster states [26]. Moreover, recent work that studies charged-particle bound states in periodic boxes [29] can inform the extension of our method to such systems.

Finally, it is worth noting that radii of atomic nuclei are typically measured using electromagnetic scattering processes. Specifically, charge radii can be inferred from the slope of the so-called charge form factor $F_C(\mathbf{q}^2)$, where $\mathbf{q}$ is the momentum transferred to the nucleus by virtual-photon exchange, in the limit $\mathbf{q}^2 \to 0$. Matter radii can then be further estimated from the measured charge radii. For theory, it is desirable to follow an analogous procedure, which compared with evaluating the expectation value of r^2 can ensure consistency with the experimental determination and in particular take into account a systematic expansion of the electromagnetic current operator. Following this approach in finite volume requires understanding the volume dependence of $F_C(\mathbf{q}^2)$, which can be informed by the results presented in this paper. These developments are most conveniently to be pursued within the framework of a nonrelativistic effective-field theory formulated in finite volume, as used, for example, in Refs. [47,48].

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APPENDIX: DETAILED DERIVATION OF THE FINAL RADIUS-SHIFT EXPRESSIONS

We calculate here the explicit final expressions for the finite-volume radius shifts given in the main text.

1. *S*-wave evaluation

For an S-wave state, the infinite-volume wave function has the form

$$\psi_{\infty,\mathrm{asm}}(r,\theta,\phi) = \frac{\gamma}{\sqrt{4\pi}}\frac{\mathrm{e}^{-\kappa r}}{r} \tag{A1}$$

for large r. Since the S-wave state is rotationally symmetric and can be chosen to be real, we can simplify Eq. (72) to

$$\Delta\langle r^2\rangle_0^{A_1^+}(L) = \alpha\Delta E(L) + 6\,\langle\psi_{\infty,\mathrm{asm}}|\hat{\xi}|\psi_{\infty,\mathrm{asm}}\rangle + O(e^{-\sqrt{2}\kappa L}). \tag{A2}$$

We can also insert the known form of the S-wave energy shift to get

$$\Delta\langle r^2\rangle_0^{A_1^+}(L) = -\frac{3|\gamma|^2\alpha}{\mu L}\mathrm{e}^{-\kappa L} + 6\,\langle\psi_{\infty,\mathrm{asm}}|\hat{\xi}|\psi_{\infty,\mathrm{asm}}\rangle + O(e^{-\sqrt{2}\kappa L}). \tag{A3}$$

Writing out the integrand that appears in the evaluation of the matrix element, we get

$$\begin{aligned}\psi^*_{\infty,\mathrm{asm}}(\mathbf{r})\hat{\xi}\psi_{\infty,\mathrm{asm}}(\mathbf{r}) &= \chi_{P\cap A}(\mathbf{r})\frac{|\gamma|^2\mathrm{e}^{-\kappa(r+u)}}{16\pi r^2 u}\big(2r\big(u^2-4\langle r_\infty^2\rangle\big)\\ &\quad + u(u-r)(r+u)\mathrm{e}^{\kappa(u-r)}\big),\end{aligned} \tag{A4}$$

noting that both u and r will be integrated over as described in the main text. We now perform the integrals in Eq. (79) with this integrand and drop higher-order terms:

$$\begin{aligned}\langle\psi_{\infty,\mathrm{asm}}|\hat{\xi}|\psi_{\infty,\mathrm{asm}}\rangle &= \frac{|\gamma|^2}{32}L^3\mathrm{Ei}(-\kappa L) + |\gamma|^2\mathrm{e}^{-\kappa L}\Bigg(\frac{L^2}{24\kappa} + \frac{\big(1-8\kappa^2\langle r_\infty^2\rangle\big)}{16\kappa^3}\\ &\quad - \frac{\mathrm{e}^{-2\kappa R}\big(\mathrm{e}^{2\kappa R}\{4\kappa^2[\kappa R^3 + 2\langle r_\infty^2\rangle(3-6\kappa R)] - 3\} + 6\kappa\big(\kappa R^2 + R - 4\kappa\langle r_\infty^2\rangle\big) + 3\big)}{48\kappa^4 L}\Bigg) + O(e^{-\sqrt{2}\kappa L}).\end{aligned} \tag{A5}$$

Putting everything back together we get

$$\Delta\langle r^2\rangle_0^{A_1^+}(L) = \frac{3}{16}|\gamma|^2L^3\mathrm{Ei}(-\kappa L) + |\gamma|^2\mathrm{e}^{-\kappa L}\bigg(\frac{L^2}{4\kappa} + \frac{3\big(1-8\kappa^2\langle r_\infty^2\rangle\big)}{8\kappa^3} - \frac{3\alpha}{\mu L} - \frac{\mathrm{e}^{-2\kappa R}\big(\mathrm{e}^{2\kappa R}\big\{4\kappa^2\big[\kappa R^3 + 2\langle r_\infty^2\rangle(3-6\kappa R)\big] - 3\big\} + 6\kappa\big(\kappa R^2 + R - 4\kappa\langle r_\infty^2\rangle\big) + 3\big)}{8\kappa^4 L}\bigg) + O(e^{-\sqrt{2}\kappa L}). \tag{A6}$$

We can absorb many of the constants that appear in this expression into a single constant a. Doing that, we arrive at Eq. (81) in the main text.

2. *P*-wave evaluation

As stated in the main text, all three basis states for $\ell = 1$ and $\Gamma = T_1^-$ have the same radius shift since they are all just different rotations of essentially the same degenerate state. It therefore suffices to consider just one of the wave functions in the multiplet, the asymptotic form of which we can write as

$$\psi_{\infty,\mathrm{asm}}(r,\theta,\phi) = \sqrt{\frac{3}{4\pi}}\frac{\gamma\mathrm{e}^{-\kappa r}(\kappa r+1)\cos\theta}{\kappa r^2}. \tag{A7}$$

We begin again with Eq. (72). Expanding the sum and plugging in the known form of the *P*-wave energy shift, we get

$$\begin{aligned}\Delta\langle r^2\rangle_1^{T_1^-}(L) = {}& \frac{3|\gamma|^2\alpha}{\mu L}\mathrm{e}^{-\kappa L} + \mathrm{Re}[\langle\hat{R}(\hat{\mathbf{x}})\psi_{\infty,\mathrm{asm}}|\hat{\xi}|\hat{R}(\hat{\mathbf{x}})\psi_{\infty,\mathrm{asm}}\rangle + \langle\hat{R}(\hat{\mathbf{y}})\psi_{\infty,\mathrm{asm}}|\hat{\xi}|\hat{R}(\hat{\mathbf{y}})\psi_{\infty,\mathrm{asm}}\rangle \\ & + \langle\hat{R}(\hat{\mathbf{z}})\psi_{\infty,\mathrm{asm}}|\hat{\xi}|\hat{R}(\hat{\mathbf{z}})\psi_{\infty,\mathrm{asm}}\rangle + \langle\hat{R}(-\hat{\mathbf{y}})\psi_{\infty,\mathrm{asm}}|\hat{\xi}|\hat{R}(-\hat{\mathbf{y}})\psi_{\infty,\mathrm{asm}}\rangle + \langle\hat{R}(-\hat{\mathbf{x}})\psi_{\infty,\mathrm{asm}}|\hat{\xi}|\hat{R}(-\hat{\mathbf{x}})\psi_{\infty,\mathrm{asm}}\rangle \\ & + \langle\hat{R}(-\hat{\mathbf{z}})\psi_{\infty,\mathrm{asm}}|\hat{\xi}|\hat{R}(-\hat{\mathbf{z}})\psi_{\infty,\mathrm{asm}}\rangle] + O(e^{-\sqrt{2}\kappa L}).\end{aligned} \tag{A8}$$

For the *P*-wave state we have chosen in Eq. (A7) it holds that

$$\hat{R}(-\mathbf{n})|\psi_{\infty,\mathrm{asm}}\rangle = -\hat{R}(\mathbf{n})|\psi_{\infty,\mathrm{asm}}\rangle. \tag{A9}$$

Moreover, $\hat{R}(\hat{\mathbf{z}})$ is simply the identity operator. Using this to simplify the expression, we get

$$\begin{aligned}\Delta\langle r^2\rangle_1^{T_1^-}(L) = {}& \frac{3|\gamma|^2\alpha}{\mu L}\mathrm{e}^{-\kappa L} + 2\mathrm{Re}[\langle\psi_{\infty,\mathrm{asm}}|\hat{\xi}|\psi_{\infty,\mathrm{asm}}\rangle + \langle\hat{R}(\hat{\mathbf{x}})\psi_{\infty,\mathrm{asm}}|\hat{\xi}|\hat{R}(\hat{\mathbf{x}})\psi_{\infty,\mathrm{asm}}\rangle \\ & + \langle\hat{R}(\hat{\mathbf{y}})\psi_{\infty,\mathrm{asm}}|\hat{\xi}|\hat{R}(\hat{\mathbf{y}})\psi_{\infty,\mathrm{asm}}\rangle] + O(e^{-\sqrt{2}\kappa L}).\end{aligned} \tag{A10}$$

Writing out the integrand that appears in the evaluation of the matrix elements leads to

$$\begin{aligned}&\psi_{\infty,\mathrm{asm}}^*(\mathbf{r})\hat{\xi}\psi_{\infty,\mathrm{asm}}(\mathbf{r}) + [\hat{R}(\hat{\mathbf{x}})\psi_{\infty,\mathrm{asm}}(\mathbf{r})]^*\hat{\xi}[\hat{R}(\hat{\mathbf{x}})\psi_{\infty,\mathrm{asm}}(\mathbf{r})] + [\hat{R}(\hat{\mathbf{y}})\psi_{\infty,\mathrm{asm}}(\mathbf{r})]^*\hat{\xi}[\hat{R}(\hat{\mathbf{y}})\psi_{\infty,\mathrm{asm}}(\mathbf{r})] \\ &= \chi_{P\cap A}(\mathbf{r})\frac{3|\gamma|^2(\kappa r+1)\mathrm{e}^{-\kappa(2r+u)}}{64\pi\kappa^2L^3r^6u^2}\Bigg\{4L^2r^2\left|1-\frac{(L^2+r^2-u^2)^2}{4L^2r^2}\right|\big(Lu^2(\kappa r+1)(u-r)(r+u)e^{\kappa u} \\ &\quad + 2r^4\mathrm{e}^{\kappa r}\big(u^2-4\langle r_\infty^2\rangle\big)(\kappa u+1)\big) + (L^2+r^2-u^2)(Lu^2(\kappa r+1)(u-r)(r+u)e^{\kappa u}(L^2+r^2-u^2) \\ &\quad + 2r^4e^{\kappa r}\big(u^2-4\langle r_\infty^2\rangle\big)(\kappa u+1)(r^2-u^2-L^2))\Bigg\},\end{aligned} \tag{A11}$$

noting that both u and r will be integrated over as described in the main text. We now perform the integrals in Eq. (79) with this integrand and drop higher-order terms:

$$\begin{aligned}&\langle\psi_{\infty,\mathrm{asm}}|\hat{\xi}|\psi_{\infty,\mathrm{asm}}\rangle + \langle\hat{R}(\hat{\mathbf{x}})\psi_{\infty,\mathrm{asm}}|\hat{\xi}|\hat{R}(\hat{\mathbf{x}})\psi_{\infty,\mathrm{asm}}\rangle + \langle\hat{R}(\hat{\mathbf{y}})\psi_{\infty,\mathrm{asm}}|\hat{\xi}|\hat{R}(\hat{\mathbf{y}})\psi_{\infty,\mathrm{asm}}\rangle \\ &= \frac{3}{32\kappa^2}|\gamma|^2L(8-\kappa^2L^2)\mathrm{Ei}(-\kappa L) + |\gamma|^2\mathrm{e}^{-\kappa L}\Bigg[-\frac{L^2}{8\kappa} + \frac{3\big(5+8\kappa^2\langle r_\infty^2\rangle\big)}{16\kappa^3} \\ &\quad + \frac{\mathrm{e}^{-2\kappa R}}{16\kappa^4LR}\big(\mathrm{e}^{2\kappa R}\big(4\kappa^3R^4 - 12R^2\big(\kappa+4\kappa^3\langle r_\infty^2\rangle\big) + 3R\big(8\kappa^2\langle r_\infty^2\rangle + 5\big) \\ &\quad - 24\kappa\langle r_\infty^2\rangle\big) - 3\big[2\kappa^2R^3 + 6\kappa R^2 + R\big(5-8\kappa^2\langle r_\infty^2\rangle\big) - 16\kappa\langle r_\infty^2\rangle\big]\big)\Bigg] + O(e^{-\sqrt{2}\kappa L}).\end{aligned} \tag{A12}$$

Putting everything back together, we get

$$\Delta\langle r^2\rangle_1^{T_1^-}(L) = \frac{3}{16\kappa^2}|\gamma|^2 L(8-\kappa^2L^2)\mathrm{Ei}(-\kappa L) + |\gamma|^2 \mathrm{e}^{-\kappa L}\bigg[-\frac{L^2}{4\kappa} + \frac{3\big(5+8\kappa^2\langle r_\infty^2\rangle\big)}{8\kappa^3} + \frac{\mathrm{e}^{-2\kappa R}}{8\kappa^4 LR}\big(\mathrm{e}^{2\kappa R}\big[4\kappa^3R^4 - 12R^2\big(\kappa+4\kappa^3\langle r_\infty^2\rangle\big) + 3R\big(8\kappa^2\langle r_\infty^2\rangle+5\big) - 48\kappa\langle r_\infty^2\rangle\big] - 3\big[2\kappa^2R^3 + 6\kappa R^2 + R\big(5-8\kappa^2\langle r_\infty^2\rangle\big) - 16\kappa\langle r_\infty^2\rangle\big]\big) + \frac{3\alpha}{\mu L}\bigg] + O(e^{-\sqrt{2}\kappa L}). \tag{A13}$$

As for A_1^+ S-wave states, we can absorb the constants that appear in this expression into a single constant a that needs to be fitted. Doing that, we arrive at Eq. (82) in the main text.

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