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Volume dependence of N-body bound states

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ABSTRACT

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.

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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].

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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,

$$V_{1\cdots N}(\mathbf{r}_1, \cdots \mathbf{r}_N; \mathbf{r}'_1, \cdots \mathbf{r}'_N) = \sum_{i<j} W_{i,j}(\mathbf{r}_i, \mathbf{r}_j; \mathbf{r}'_i, \mathbf{r}'_j) 1_{\not{i},\not{j}} + \sum_{i<j<k} W_{i,j,k}(\mathbf{r}_i, \mathbf{r}_j, \mathbf{r}_k; \mathbf{r}'_i, \mathbf{r}'_j, \mathbf{r}'_k) 1_{\not{i},\not{j},\not{k}} + \cdots\,, \tag{2}$$

where we use the shorthand notation

$$1_{\not{i}_1,\cdots \not{i}_k} = \prod_{j \neq i_1,\cdots i_k} \delta^d(\mathbf{r}_j - \mathbf{r}'_j) \tag{3}$$

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

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

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

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

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 $\hat{K}^{\mathrm{rel}}_{1|N-1}$ 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 $\hat{K}^{\mathrm{rel}}_{1|N-1}$.

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 $\psi^B_{N-1}(\mathbf{r}_2, \cdots \mathbf{r}_N)$. 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

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

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

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

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.

[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.

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