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Topological phases for bound states moving in a finite volume

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We show that bound states moving in a finite periodic volume have an energy correction which is topological in origin and universal in character. The topological volume corrections contain information about the number and mass of the constituents of the bound states. These results have broad applications to lattice calculations involving nucleons, nuclei, hadronic molecules, and cold atoms. We illustrate and verify the analytical results with several numerical lattice calculations.

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Over two decades ago, Lüscher derived a relation connecting the energy levels of an interacting two-body system in a periodic cube to physical scattering phase shifts [1,2]. This finite-volume technique has become a standard tool in lattice quantum chromodynamics [3–8] and in lattice effective field theory for nucleons and cold atomic systems [9–13]. In this letter we consider finite-volume effects of composite particles in motion. We discuss corrections to the binding energies of bound states in a moving frame. We also show how the finite-volume scattering method is modified if one or both particles are composite.

We find topological phase corrections associated with the motion of bound states in a periodic box. These corrections have a universal dependence on momentum determined by the number and mass of the constituents. In asymptotically large volumes the corrections are exponentially small and can be neglected. However, it is often the case in large-scale lattice simulations that calculations are performed at volumes which are not asymptotically large. Fortunately, we find that the corrections have a simple form which can be subtracted out from the analysis.

We start with another result derived by Lüscher [14]. It describes finite-volume corrections to the binding energy of two-body dimer states for interactions with finite range. For a dimer at rest, the shift in the energy when placed in a periodic cube of volume L^3 is

$$\Delta E_{\vec{0}}(L) \approx \sum_{|\vec{n}|=1} \int d^3 r \phi_\infty^*(\vec{r}) V(\vec{r}) \phi_\infty(\vec{r} + \vec{n}L). \quad (1)$$

Here $V(\vec{r})$ is the interaction potential and ϕ_∞ is the infinite-volume wavefunction as a function of the relative separation $\vec{r}$. The summation is over integer vectors $\vec{n}$ with magnitude 1. Throughout our discussion, we assume that the energies and momenta are nonrelativistic. For finite-range interactions Eq. (1) gives a correction which scales as $e^{-\kappa L}/L$ in the large volume limit, where κ is the binding momentum.

For general N-body bound states a straightforward generalization of Lüscher's result yields

$$\Delta E_{\vec{0}}(L) \approx \sum_{\sum_j |\vec{n}_j|=1} \int \Big[\prod_i d^3 r_i\Big] \phi_\infty^*(\vec{r}_1, \cdots) V(\vec{r}_1, \cdots) \times \phi_\infty(\vec{r}_1 + \vec{n}_1 L, \cdots). \quad (2)$$

Here $\vec{r}_i$ are $N-1$ relative coordinates and $\vec{n}_i$ are again integer vectors. Although Eq. (2) clearly does not apply to relativistic quarks held by confinement within a single meson or baryon, these corrections are useful for analyzing lattice calculations of hadronic molecules, nuclei, and cold atomic bound states [15–18].

We now consider a dimer moving in the same periodic cube with momentum $2\pi\vec{k}/L$ for integer $\vec{k}$. In the dimer wavefunction we can factorize out the phase dependence due to the center-of-mass motion,

$$\psi_L(\vec{r}_1, \vec{r}_2) = e^{i2\pi\alpha\vec{k}\cdot\vec{r}_1/L} e^{i2\pi(1-\alpha)\vec{k}\cdot\vec{r}_2/L} \phi_L(\vec{r}_1 - \vec{r}_2), \quad (3)$$

where $\alpha = m_1/(m_1 + m_2)$. Since $\psi_L(\vec{r}_1, \vec{r}_2)$ is periodic in $\vec{r}_1$ and $\vec{r}_2$, ϕ_L gets a nontrivial phase for each winding around the toroidal topology of the periodic cube,

$$\phi_L(\vec{r} + \vec{n}L) = e^{-i2\pi\alpha\vec{k}\cdot\vec{n}} \phi_L(\vec{r}), \quad (4)$$

for all integer $\vec{n}$. We note that phase factors have been previously discussed in connection with finite-volume scattering in moving frames [19–21]. However, the phase factors have a qualitatively different effect on bound-state wavefunctions which simultaneously touch all wall boundaries. Each phase twist induces a measurable shift in the binding energy.

When Eq. (4) is combined with Eq. (2), we find that the finite-volume correction is a sum of sinusoidal functions of momentum. For S-wave dimers with momentum $2\pi\vec{k}/L$, the finite-volume correction has the form

$$\frac{\Delta E_{\vec{k}}(L)}{\Delta E_{\vec{0}}(L)} \approx \frac{1}{3}\sum_{l=1,2,3}\cos(2\pi\alpha k_l) \equiv \tau(\vec{k},\alpha). \quad (5)$$

Finite-volume corrections for higher angular momentum bound states at rest have recently been discussed in [22]. From the results presented there, it is straightforward to derive analogous results for $\tau(\vec{k},\alpha)$ for dimers with angular momentum.

For bound states with more than two particles, the finite-volume correction has the same general form. For an N-body bound state with all equal masses and no cluster substructure, the topological phase is

$$\phi_L(\cdots,\vec{r}_i+\vec{n}_i L,\cdots) = e^{-i2\pi\vec{k}\cdot\vec{n}_i/N}\phi_L(\cdots,\vec{r}_i,\cdots). \quad (6)$$

For S-wave bound states we get

$$\frac{\Delta E_{\vec{k}}(L)}{\Delta E_{\vec{0}}(L)} \approx \tau\left(\vec{k},\frac{1}{N}\right). \quad (7)$$

For N-body bound states with a two-cluster substructure, one can apply the two-body result, Eq. (5), with m_1 and m_2 being the masses of the two clusters. For more complicated N-body bound states with more than two clusters and/or particles with unequal masses, the same cosine functions as in Eq. (5) are also expected for $\Delta E_{\vec{k}}(L)/\Delta E_{\vec{0}}(L)$. In these cases, however, more information is needed regarding which particles or clusters occupy the tail of the bound-state wavefunction. If this is unknown, then $\Delta E_{\vec{k}}(L)/\Delta E_{\vec{0}}(L)$ can be extracted from numerical calculations, and an empirical fit to cosine functions as in Eq. (5) can yield structural information about the tail of the bound state.

Our results presented above have already been adapted by Davoudi and Savage into a general method for reducing finite-volume errors for two-body bound states such as the deuteron using boosted frames [23]. The computational advantage of this approach is that finite-volume effects can be directly removed from lattice data without extrapolating to large lattice volumes. This is especially useful for the case with more than two constituents where the analytic form for the finite-volume L-dependence is *a priori* unknown.

To illustrate the utility of the boosted-frame method, we consider lattice calculations of the triton at leading order in pionless effective field theory [24]. We use the leading-order lattice action defined in Eq. (4.6) of Ref. [10] with spatial lattice spacing 1.97 fm and temporal lattice spacing 1.32 fm/c. The two-body contact interactions, C and C_{I^2}, are set to reproduce the physical neutron-proton scattering lengths, $a_{^1S_0} = -23.7$ fm and $a_{^3S_1} = 5.4$ fm. The three-body contact interaction, D, is determined by the triton energy at infinite volume, -8.48 MeV.

Using the Lanczos algorithm for sparse-matrix eigenvector iteration [25], we have computed the triton energy as a function of periodic cube length L in spatial lattice units and momentum $2\pi\vec{k}/L$. In Table I we show a comparison of lattice results for $\Delta E_{\vec{k}}(L)/\Delta E_{\vec{0}}(L)$ for the triton versus $\tau(\vec{k},1/3)$ for lattice sizes $L = 6, 7, 8$. As seen in Table I, the lattice results approach $\tau(\vec{k},1/3)$ in the large-L limit. We note that the leading finite-volume corrections vanish for $\vec{k} = (1,1,0)$. Therefore the calculation of the triton binding energy in this boosted frame should converge much more quickly in the limit of large L. In Table II we show the triton finite-volume energy corrections $\Delta E_{\vec{k}}(L)$ in MeV versus L for $\vec{k} = (0,0,0)$ and $\vec{k} = (1,1,0)$. We see that the finite-volume errors are reduced dramatically for $\vec{k} = (1,1,0)$.

We now turn our attention to the scattering of composite states in a finite periodic cube. We consider the scattering between states A and B in the center-of-mass frame. Let μ_{AB} be the reduced mass, and let $E_{AB}(p,L)$ be the total energy of the $A-B$ scattering system with radial momentum p in a periodic cube of length L. States A and B can be point particles or composite bound states. We assume that the constituent particles comprising the states have finite-range interactions. The composite structures of A and B, however, will in general produce effective interactions with exponential tails extending to infinity.

These tails generate exponentially small finite-volume corrections to $E_{AB}(p,L)$ associated with the binding energies of A and B separately as well as the scattering of A and B together. In this analysis, we focus only on the exponential corrections to the binding energies. This will be useful in lattice simulations where the volume is not very large and the binding energy shifts may be comparable to that of the scattering process being measured. We will not be concerned with exponentially small corrections to the scattering of A and B. If the interactions between A and B are very strong, then it is theoretically possible that the finite-volume scattering corrections we neglect are comparable to the binding energy shifts. However, in such cases the part of the energy shift due to scattering which is not

TABLE I. Comparison of triton lattice results for $\Delta E_{\vec{k}}(L)/\Delta E_{\vec{0}}(L)$ and $\tau(\vec{k},1/3)$ versus L.

$\vec{k}$	$L=6$	$L=7$	$L=8$	$\tau(\vec{k},1/3)$
(1, 0, 0)	0.395	0.432	0.458	0.500
(1, 1, 0)	−0.035	−0.025	−0.016	0.000
(1, 1, 1)	−0.376	−0.413	−0.442	−0.500

TABLE II. Triton finite-volume energy corrections $\Delta E_{\vec{k}}(L)$ in MeV for $\vec{k} = (0,0,0)$ and $\vec{k} = (1,1,0)$ versus L.

$\vec{k}$	$L=5$	$L=6$	$L=7$	$L=8$
(0, 0, 0)	−0.603	−0.169	−0.049	−0.015
(1, 1, 0)	0.029	0.006	0.001	0.0002

exponentially suppressed will be much larger still, and so the loss of accuracy in the scattering analysis will be small.

In order to calculate finite-volume corrections due to the binding energy, it suffices to consider singular solutions of the free Helmholtz equation. Let $\vec{r}$ be the separation between the center of masses of the two states. In the following we assume that p is sufficiently small so that angular momentum mixing with higher-order singular solutions can be neglected. For S-wave scattering between states A and B with radial momentum p, the position-space scattering wavefunction is

$$\langle \vec{r}|\Psi_p\rangle = c\sum_{\vec{k}} \frac{e^{i(2\pi\vec{k}/L)\cdot\vec{r}}}{(2\pi\vec{k}/L)^2 - p^2} \tag{8}$$

with some normalization constant c.

We let $E^A_{\vec{k}}(L)$ and $E^B_{-\vec{k}}(L)$ be the finite-volume energies due to binding for bound states A and B with momenta $2\pi\vec{k}/L$ and $-2\pi\vec{k}/L$, respectively. For point particles without internal structure, these energies are by definition zero for all momenta. The total energy $E_{AB}(p, L)$ is then

$$\begin{aligned} E_{AB}(p, L) &= \frac{\langle\Psi_p|H|\Psi_p\rangle}{\langle\Psi_p|\Psi_p\rangle} \\ &= \frac{1}{\mathcal{N}}\sum_{\vec{k}} \frac{\frac{p^2}{2\mu_{AB}} + E^A_{\vec{k}}(L) + E^B_{-\vec{k}}(L)}{(\vec{k}^2 - \eta)^2}, \end{aligned} \tag{9}$$

where $\mathcal{N} = \sum_{\vec{k}}(\vec{k}^2 - \eta)^{-2}$ and $\eta = p^2L^2/(2\pi)^2$. The finite-volume correction can be written as

$$\begin{aligned} E_{AB}(p, L) - E_{AB}(p, \infty) &= \tau_A(\eta)\Delta E^A_{\vec{0}}(L) \\ &\quad + \tau_B(\eta)\Delta E^B_{\vec{0}}(L), \end{aligned} \tag{10}$$

where $\Delta E^A_{\vec{0}}(L)$ and $\Delta E^B_{\vec{0}}(L)$ are the finite-volume corrections for states A and B at rest, and we have defined the topological volume factor

$$\tau(\eta) = \frac{1}{\mathcal{N}}\sum_{\vec{k}} \frac{\sum_{l=1,2,3}\cos(2\pi\alpha k_l)}{3(\vec{k}^2 - \eta)^2}. \tag{11}$$

The analysis can be generalized to higher angular momentum scattering states using an extension of Lüscher's scattering relation to higher orbital angular momentum [26,27].

The finite-volume correction in Eq. (10) has nothing to do with the interaction between states A and B and should therefore be subtracted from the total energy before using Lüscher's scattering relation. This subtraction should reduce systematic errors in lattice calculations.

As an example to test the method, we consider fermion-dimer scattering for two-component fermions. The physical process which we study corresponds with spin-quartet scattering between a neutron and deuteron. In that case the two fermion components should be regarded as protons and neutrons with the same spin.

We use the same lattice Hamiltonians as in Ref. [28], except in that case the scattering length was tuned to infinity. As in Ref. [28], we consider two different lattice Hamiltonians, each of which produces a shallow dimer in the continuum limit. The first Hamiltonian, H_1, contains only a local contact interaction between fermions. The second Hamiltonian, H_2, contains a contact interaction as well as nearest-neighbor interactions. These are used to tune the binding energy of the dimer while also setting the effective range parameter to zero. Both lattice Hamiltonians reproduce the same continuum limit of fermions with attractive zero-range interactions.

We now focus on the fermion-dimer system. This corresponds with a neutron together with a deuteron in the spin-quartet channel in pionless effective field theory at leading order. Experimental measurements find a quartet scattering length ${}^4a_{nd} = 6.35(2)$ fm [29]. This can be expressed as a fraction of the spin-triplet neutron-proton scattering length, ${}^4a_{nd}/{}^3a_{np} = 1.17(1)$. A more detailed calculation including interaction range effects obtains ${}^4a_{nd} = 6.33(10)$ fm [30,31], in full agreement with experimental values.

We calculate fermion-dimer scattering on the lattice using Lüscher's finite-volume formula. Using the Lanczos algorithm we have computed the ground state energy for

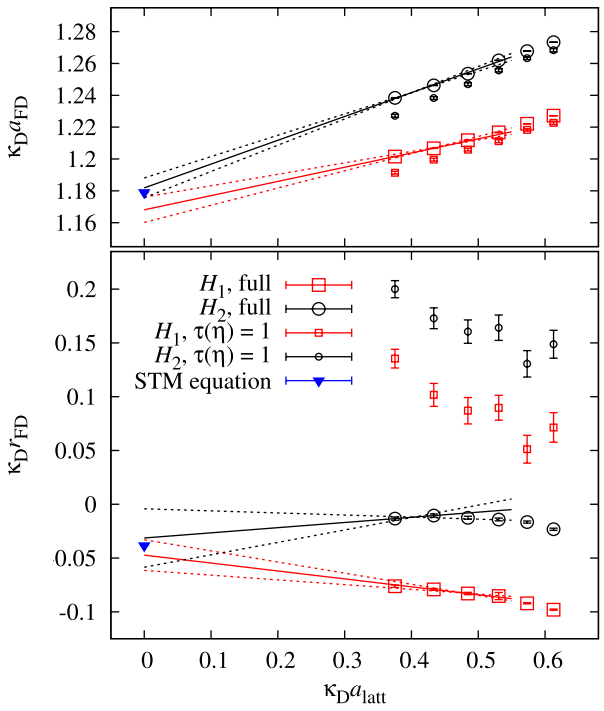

FIG. 1 (color online). Lattice results and continuum extrapolation with error estimates for the fermion-dimer scattering length (top) and effective range parameter (bottom). For comparison we show the continuum results obtained via the Skorniakov-Ter-Martirosian equation.

the fermion-dimer system on periodic cubes for six different lattice spacings a_{latt}. For each lattice spacing we consider periodic volumes L^3 ranging from $L = 6$ to $L = 17$ lattice units. From these energies we determine the low-energy parameters for fermion-dimer scattering and extrapolate to the continuum limit. The full details of this calculation will be described in a forthcoming publication, and we just summarize the results here.

Results for the fermion-dimer scattering length, a_{FD}, and the effective range parameter, r_{FD}, are shown in Fig. 1. In each case, we extrapolate to the continuum limit and write final results as dimensionless combinations multiplied by powers of the dimer binding momentum, κ_D. In the shallow binding limit κ_D equals the reciprocal of the fermion-fermion scattering length. To see the effect of the topological volume correction we have done the full calculation using the correct topological factor $\tau(\eta)$, as well as a faulty calculation which replaces $\tau(\eta)$ by 1. For comparison, we show the continuum results, $a_{\text{FD}}\kappa_D = 1.17907(1)$ and $r_{\text{FD}}\kappa_D = -0.0383(3)$, obtained via the Skorniakov-Ter-Martirosian (STM) integral equation [32,33]. We find that the small size of the effective range parameter requires a fit to low-energy scattering that includes the shape parameter, which was not done in earlier calculations of the effective range parameter [34]. We note also the agreement with the experimental value ${}^4a_{nd}/{}^3a_{np} = 1.17(1)$.

The results in Fig. 1 show that the inclusion of the topological volume factor $\tau(\eta)$ is essential for obtaining the correct continuum limit. In all cases the continuum extrapolations for H_1 and H_2 agree within error bars. However, the correct $\tau(\eta)$ factor is needed to reproduce the STM equation result. The correction is small for the scattering length, but quite large for the effective range parameter.

We expect the topological volume factor to have important effects in other lattice calculations of scattering for composite bound states. The analysis presented here should provide a simple but general method for improving the accuracy of bound-state scattering calculations. The list of possible applications is quite extensive and include lattice calculations involving the scattering of nucleons upon nuclei, the scattering of nuclei, Compton scattering and electroweak probes upon nuclei, mesonic and baryonic scattering upon hadronic molecules, and few-body scattering in cold atomic systems. An application of this method to dimer-dimer scattering is in progress.

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