

## Pushing the periodic boundaries

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I express my gratitude as the recipient of the 2021 Kenneth G. Wilson award. I then briefly summarize the work leading to the award: the development and application of methods that use the finite system size of lattice calculations, the finite volume, as a useful probe of multi-hadron interactions.

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\*Speaker.

## 1. Kenneth G. Wilson Award

It is a great honor to receive the *Kenneth G. Wilson award for Excellence in Lattice Field Theory*. Indeed it is already a huge honor just to be a part of the vibrant, positive and forward-thinking research community surrounding lattice field theory. I am consistently impressed by the rapid progress that our field is making and by the range of expertise that comes together to make modern lattice calculations possible. I am acutely aware that my contributions have been to one very specific part of the broad landscape of ideas and methods driving our field. I would like to thank the community and the selection committee for acknowledging my contribution.

I would also like to thank my many collaborators. I will refrain from listing everyone here, but to the incredible group of scientists with whom I have worked and continue to work: Thanks for your patience, for the opportunity to learn from your expertise, for inspiring and motivating, and for making scientific collaboration such a thoroughly enjoyable experience. I will single out two of you: First, Steve Sharpe, you were an exceptional PhD advisor and continue to be an exceptional collaborator. Thank you for helping me to hit the ground running and for setting a standard of mentorship and advising that I will strive to emulate in the years to come. Second, Raúl Briceño, you introduced me to your vision of inexhaustible research directions at a time when I really needed that sort of kick, and you would not give up on convincing me to collaborate with you. Working with you over the past near-decade has been a blast. I would further like to acknowledge the phenomenal work environments of the University of Washington (Seattle), the University of Mainz, CERN and the University of Edinburgh.

In the following, I give a (likely somewhat personally biased) overview of the finite-volume methods being developed and applied in lattice calculations of multi-hadron processes. I have decided not to worry about explicitly stating where I was involved, allowing the references to give credit to my work and the work of many others. The message I hope to convey is that finite-volume effects give a remarkable handle on a wide range of scattering and transition amplitudes, and that our knowledge of these relations as well as our ability to apply them in lattice calculations has matured dramatically in recent decades. This is due to an enormous number of contributions from a significant fraction of this community.

## 2. The finite volume

Numerical lattice QCD calculations are necessarily performed in a finite Euclidean spacetime. Often one designs the calculation in a finite four-dimensional spacetime geometry of type  $T \times L^3$ , where the temporal extent  $T$  is longer than the three equal spatial extents  $L$ . The most common set-up is to apply periodic boundary conditions on the quarks and gluons in the three spatial directions and anti-periodic (periodic) boundary conditions on the quarks (gluons) in the Euclidean time direction. Important exceptions exist to this approach, including non-cubic spatial volumes and anti-periodic or twisted boundary conditions.

### 2.1 History and status of the formalism

The role of the Euclidean signature and the finite volume depends on the observable. In the case of quantities such as masses and decay constants, expressible as matrix elements involving

local currents and single-hadron states, one can define a useful fit to a Euclidean correlation function that gives a  $T \times L^3$ -estimator of the desired observable, also depending on the lattice spacing and the quark masses of the calculation. Then, just as one aims to extrapolate to the continuum limit and to the physical quark-mass values, one must also extrapolate  $T, L \rightarrow \infty$  to reach the physical prediction. For such single-hadron observables, the difference between the  $T \times L^3$ -estimator and the targeted infinite-volume observable is exponentially suppressed, often falling as  $e^{-M_\pi T}$  and  $e^{-M_\pi L}$  where  $M_\pi$  is the physical pion mass. In this case, the finite-volume effects are often a percent-level source of systematic uncertainty and, in many cases, are a subdominant contribution to the error budget. The formal understanding of such exponentially suppressed volume effects in lattice QCD was pioneered by Lüscher [1] and has since been re-visited and extended by many authors [2–25]. Many quantities considered by the Flavo(u)r Lattice Averaging Group (FLAG) have exponentially suppressed volume effects and the FLAG report [26] also contains specific standards on the rigorous treatment of these effects.

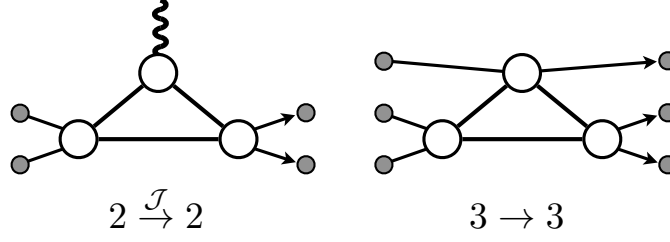
The situation is quite different for observables defined with multi-hadron states, including scattering amplitudes such as  $\pi\pi \rightarrow \pi\pi$  and decay and transition amplitudes such as  $K \rightarrow \pi\pi$  and  $\pi\gamma \rightarrow \pi\pi$ . For these quantities, a direct extraction of a useful finite-volume estimator from the Euclidean correlator is very challenging [27].<sup>1</sup> With this limitation in mind, the community has made great progress by using the finite volume as a tool rather than an unwanted artifact. In particular, the finite spatial volume discretizes the spectrum such that one can define a set of energies  $E_n(L)$  (for  $n = 0, 1, 2, \dots$ ) and matrix elements of local currents  $\langle n, L | \mathcal{J} | n', L \rangle$ . It is possible to relate this non-perturbative low-energy information describing QCD in a box to the non-perturbative low-energy information that is extracted experimentally: multi-hadron amplitudes.

This program was initiated in the context of lattice QCD by Lüscher,<sup>2</sup> who developed a general formalism for extracting elastic  $\pi\pi \rightarrow \pi\pi$  scattering amplitudes from  $\pi\pi$  finite-volume energies (assuming the scattering energy is below the four-pion threshold) [38–41] and by Lellouch and Lüscher, who developed the closely related formalism for extracting the  $K \rightarrow \pi\pi$  decay amplitudes from finite-volume matrix elements [42]. The original formulas have since been extended to more general systems. On the side of relating energies to scattering amplitudes this has included extensions to describe multiple two-particle channels of both identical and non-identical, potentially non-degenerate particles with any intrinsic spin, and to accommodate a range of geometries and boundary conditions as well as non-zero spatial momentum in the finite-volume frame [43–64]. Examples covered by these extensions include  $\pi K \rightarrow \eta K$ ,  $\pi\pi \rightarrow K\bar{K}$ ,  $N\pi \rightarrow N\pi$  and  $\rho\rho \rightarrow \rho\rho$  where in the final case the quark masses must be taken sufficiently heavy that the  $\rho$  becomes a stable particle. In these extensions, the formulas only rigorously hold at energies for which no three- or four-particle channels are open, and only up to neglected, exponentially suppressed volume effects.

The situation is similar for  $0 \xrightarrow{\mathcal{J}} 2$  and  $1 \xrightarrow{\mathcal{J}} 2$  transition amplitudes. Here the inputs are both finite-volume energies and matrix elements and the formalism accommodates the same types of two-particle systems as described above, together with generic local currents that may inject energy and momentum into the system [56–58, 65–69]. Example processes covered by this formalism

<sup>1</sup>See, however, Refs. [28–36] and the discussion in the final section here.

<sup>2</sup>See also early work by Huang and Yang in which the two-particle scattering length arises in coefficients of the large-volume expansion of the finite-volume multi-boson ground-state energy [37].



**Figure 1:** Triangle diagrams contributing to both  $2 \xrightarrow{\mathcal{J}} 2$  transition amplitudes (left) and  $3 \rightarrow 3$  scattering amplitudes (right). In both cases the external grey discs as well as the lines forming the triangles represent low-energy degrees of freedom, e.g. pions in QCD. The vertical wavy line in the left panel represents the external current and the white circles represent vertex functions. In both cases, the internal kinematics can be chosen such that the integral over the loop momentum includes contributions where the three internal legs are arbitrarily close to the mass shell. This leads to new types of singularities in the physical amplitudes and these must also be addressed in the finite-volume formulae for extracting these observables [72, 99–107].

include  $\gamma^* \rightarrow \pi\pi$ ,  $\pi\gamma^* \rightarrow \pi\pi$ ,  $K\gamma^* \rightarrow K\pi$ ,  $B \rightarrow \rho\ell^+\ell^- \rightarrow \pi\pi\ell^+\ell^-$  and  $N\gamma^* \rightarrow N\pi$ , where  $\gamma^*$  is a virtual photon and  $\ell^+\ell^-$  a pair of leptons.

Important progress has also been made in cases where a third effective degree of freedom is present. This falls into two categories:  $2 \xrightarrow{\mathcal{J}} 2$  matrix elements and  $2 \rightarrow 3$  and  $3 \rightarrow 3$  scattering amplitudes. Similarities exist between the two types of processes because both contain triangle-diagram contributions as shown in Fig. 1. For the case of  $2 \xrightarrow{\mathcal{J}} 2$ , the method to extract the amplitudes from finite-volume information has been developed for identical scalar particles [57, 70–75]. This specifically applies to the  $\pi\pi \rightarrow \gamma\pi\pi$  amplitude as well as the form factor  $\rho\gamma^* \rightarrow \rho$  in which the non-stable nature of the  $\rho$  resonance is rigorously accommodated. For the case of  $2 \rightarrow 3$  and  $3 \rightarrow 3$  amplitudes the formal methods have been extended to nearly all types of non-degenerate and non-identical scalar channels [76–95]. Accessible channels today include  $\pi^+\pi^+\pi^+ \rightarrow \pi^+\pi^+\pi^+$ ,  $(\pi\pi\pi)_{I=0} \rightarrow (\rho\pi)_{I=0} \rightarrow \omega \rightarrow (\rho\pi)_{I=0} \rightarrow (\pi\pi\pi)_{I=0}$  and  $\pi\pi K \rightarrow \pi\pi K$ .<sup>3</sup> The generalization for coupled channels and spinning particles is still outstanding.

Three additional classes of observables deserve mention: First,  $1 \xrightarrow{\mathcal{J}} 3$  transitions such as  $K \rightarrow \pi\pi\pi$  or  $\mathcal{J} \rightarrow \pi\pi\pi$  where  $\mathcal{J}$  is a generic local operator, e.g. an axial or vector current. The formal methods to extract these types of observables from finite-volume energies and matrix elements have also been developed, only last year, and already by two competing groups [108, 109]. Second, methods have been presented to extract long-range matrix elements relevant for the neutral kaon mass difference and long-distance contributions to  $K \rightarrow \pi\ell^+\ell^-$ , as well as Compton scattering of the pion ( $\pi\gamma^* \rightarrow [\pi\pi, K\bar{K}] \rightarrow \pi\gamma^*$ ) and nucleon ( $N\gamma^* \rightarrow N\pi \rightarrow N\gamma^*$ ), and double- $\beta$  decays of QCD-stable hadrons [110–118]. Third, and finally, the increased precision of lattice QCD calculations has recently lead to the inclusion of isospin-breaking effects including QED. This introduces extensive finite-volume complications related to the fact that the photon is a massless low-energy degree of freedom. The field is already much too extensive to survey in a few sentences but, in the spirit of this overview, I would be remiss to not mention work focusing on QED corrections to

<sup>3</sup>In the context of three-particle effects it is useful to note that three frameworks have been presented by competing groups. These are equivalent where comparable in the sense that the same infinite-volume scattering amplitudes predict the same finite-volume energies. They differ in the intermediate quantities that are used and in the framework of the derivation. See Refs. [92, 96–98] for detailed comparisons.

multi-hadron process, see Refs. [119–121].

At this stage it seems safe to expect that a general framework for  $n \rightarrow n'$  and  $n \xrightarrow{\mathcal{L}} n'$ , for  $n, n' \leq 3$  should be available soon, where generic coupled channels of two- and three-particle states are understood. In fact, taking a slightly more optimistic stance, a fully general framework for any number of channels with any number of particles does not seem unreasonable. With such a methodology in place, it will be possible to quantitatively assess the feasibility of a given multi-hadron lattice calculation. To give a bit more substance to these speculations, in the next section I give a summary of the general derivation strategy used to develop many of these relations and also comment on recent applications of the formulae.

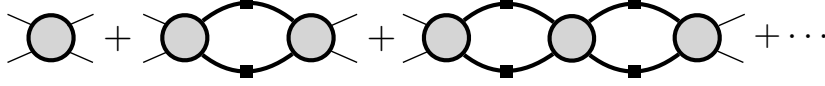
## 2.2 Derivations and applications

Here I completely focus on the types of finite-volume formalism that I have been involved in developing and extending. The majority of the work follows a basic paradigm established in Ref. [38] and emphasized more explicitly in subsequent work, e.g. Refs. [45, 67, 69, 71, 79].

The first step is to represent the process of interest in a skeleton expansion of Feynman diagrams. In particular, one can give a diagrammatic representation of both the physical infinite-volume observable and a closely related finite-volume quantity. In the case of  $2 \rightarrow 2$  scattering the finite-volume object is any two-point function built from operators with the same internal quantum numbers as the two-hadron states. The details of the operators are irrelevant as only the finite-volume pole positions are of interest. These give the energies  $E_n(L)$ , which can then be related to the scattering amplitude. A similar approach is applied for  $2 \rightarrow 3$  and  $3 \rightarrow 3$  scattering amplitudes. For  $1 \xrightarrow{\mathcal{L}} 2$  and  $2 \xrightarrow{\mathcal{L}} 2$  transition amplitudes one considers three-point functions. These lead to formal expressions for the finite-volume matrix elements that can be related to the infinite-volume amplitudes.

The propagators in both the finite- and infinite-volume Feynman diagrams correspond to the low-energy degrees of freedom, the hadrons in QCD. One envisions a generic effective field theory including all interactions allowed by the symmetries, but the construction is agnostic to any details of couplings or power-counting schemes. Instead, the diagrams are formally grouped into a skeleton expansion of irreducible vertex functions (for example Bethe-Salpeter kernels) and fully dressed propagators. The defining approach here is to identify diagrammatic building blocks that have only exponentially suppressed  $L$  dependence, which is neglected in the derivation. To this end, one naturally makes use of the different Feynman rules for finite-volume vs. infinite-volume quantities. In momentum space, the only distinction is in the treatment of loop momenta. While these are integrated over all real values in infinite volume, the finite-volume boundary conditions restrict the spatial modes to a discrete set: all integer-vector multiples of  $(2\pi/L)$ . Thus the business of studying finite-volume effects amounts to comparing the results of summing and integrating the loops for various types of diagrams. One can show that the power-like  $L$  dependence of interest only arises from the parts of Feynman diagrams that can “go on shell”. For the case of  $2 \rightarrow 2$  scattering, for example, the center-of-mass energy is restricted to values for which only two-particle states can propagate. Then the relevant skeleton expansion takes the form shown in Fig. 2.

The final step is to express the finite-volume Feynman diagrams in terms of infinite-volume diagrams together with residues. These separations consistently lead to geometric series that can



**Figure 2:** Example of the skeleton expansion entering the finite-volume derivations here for the case of  $2 \rightarrow 2$  scattering. The internal lines with black squares are fully dressed propagators corresponding to low-energy degrees of freedom, e.g. pions or more generally hadrons in QCD. The grey circles represent Bethe-Salpeter kernels which are defined such that the geometric series shown includes all possible underlying Feynman diagrams with four external legs. The utility of this expansion is that, in the low-energy regime for which only two-particle states can propagate, the Bethe-Salpeter kernels have exponentially suppressed  $L$  dependence. Thus the power-like volume-effects are identified from the two-particle loops shown explicitly.

be summed into a closed form, and the result is an expression relating the relevant finite-volume quantities (either energies or matrix elements) to infinite-volume observables, via known geometric functions. In the case of  $2 \xrightarrow{\mathcal{L}} 2$  and  $3 \rightarrow 3$  amplitudes, these relations rely on an intermediate infinite-volume quantity, in which the triangle singularities of Fig. 1 are removed. An inherent ambiguity arises in how such singularities are separated so that the relation between the finite-volume energies and the intermediate quantity (as well as the intermediate quantities themselves) are scheme dependent. However the formalism also provides the scheme-dependent relation to the final physical scattering amplitude, which is again unambiguous.

It is important to stress that there is an underlying physical principle that makes it highly plausible, at the very least, that these types of derivations should generally work for all types of physical amplitudes. The dominant finite-volume effects arise from those intermediate states within diagrams that can propagate arbitrarily far through the periodic boundaries. These are long-lived intermediate states, and in the heuristic spirit of the time-energy uncertainty principle, this translates to states built from nearly on-shell particles, particles with four-momenta satisfying  $p^2 = m^2$ . This can be made rigorous by studying the differences between finite-volume momentum sums and infinite-volume momentum integrals within Feynman diagrams. Only singularities associated with on-shell particles generate power-like  $L$  dependence in these differences and, expanding about the singular point, one finds that only the on-shell Feynman diagrams contribute in the final results.

Note that, from this argument, one expects the power-like  $L$  dependence to be determined by some combination of on-shell Feynman diagrams, but it is not immediately obvious that one should obtain the unique combination defining the physical scattering amplitude. Again this is addressed by explicitly working through all contributions, but from a high-level perspective one can argue that any other result would be quite surprising. Since the finite-volume energies  $E_n(L)$  are physical observables of the underlying theory, their value cannot be sensitive to any details of the generic low-energy effective theory. Generally speaking, a non-standard combination of diagrams would introduce an unphysical dependence on exactly these details.

Two important caveats to the discussion above should be mentioned. First, as already stressed, for  $2 \xrightarrow{\mathcal{L}} 2$  and  $3 \rightarrow 3$  amplitudes, the finite-volume information is most directly related to an intermediate quantity. The difference between this and the physical amplitude depends on physically observable sub-processes. In the case of the two-to-two transition amplitude one obtains form-factor dependence ( $1 \xrightarrow{\mathcal{L}} 1$  as a subprocess of  $2 \xrightarrow{\mathcal{L}} 2$ ) and in the case of three-to-three scattering the sub-process is the two-particle amplitude ( $2 \rightarrow 2$  as a subprocess of  $3 \rightarrow 3$ ). Second, there is

no obvious reason why the finite-volume energies should only depend on scattering observables for physical scattering energies, i.e. those realized in experiment. In fact, Ref. [1] already showed that the  $2 \rightarrow 2$  scattering amplitude, analytically continued to the complex plane, dictates the exponentially suppressed  $L$ -dependence of the pion mass. The separation between experimentally accessible quantities in the power-like  $L$  dependence and non-accessible quantities in  $e^{-M_\pi L}$  dependence is blurred in the formalism for more complicated amplitudes. In particular, the  $3 \rightarrow 3$  formalism requires knowledge of the  $2 \rightarrow 2$  scattering amplitude below the two-particle threshold. For two-pion channels, one can rely on knowledge of the sub-threshold amplitude from chiral perturbation theory and dispersion theory as discussed, for example, in Refs. [122–128].

Turning to applications, it cannot be stressed enough that the extensive formal progress would be close to meaningless if it were not matched by state-of-the-art lattice QCD calculations using these relations. Also here the progress is overwhelming and reviewing the field has become a daunting task. For example, placing a cut on works dated on or after 2019 still yields over sixty articles concerning the extraction of scattering, decay and transition amplitudes using finite-volume methods [105, 107, 120, 128–185].

Much of this work considers the case of a single two-particle flavor channel, e.g. two-pions with definite isospin. Even with this restriction, one formally has an infinite number of unknown scattering amplitudes at each center-of-mass energy, corresponding to an infinite tower of angular-momentum components that contribute to a given finite-volume energy. This is the price to pay for reducing the symmetry from the infinite group of continuous spatial rotations to the finite symmetries of the cube. In practice, the effect of higher partial waves on a given value of  $E_n(L)$  are suppressed, due to the angular-momentum-barrier suppression of the amplitudes themselves, so that one can truncate to a maximum angular momentum and reduce to a finite number of unknowns at each energy. The truncation to only one angular-momentum component is special here as it reduces the finite-volume formula to a one-to-one mapping with each lattice-determined energy giving the value of the scattering amplitude at that energy.

In all cases where multiple angular momenta contribute, as well as the case of multiple two-particle flavor channels, this one-to-one relation no longer applies. The same is true for all formulas involving decay and transition amplitudes, e.g.  $1 \xrightarrow{\mathcal{L}} 2$  and  $2 \xrightarrow{\mathcal{L}} 2$ , as well as the formalism for three particles. These relations therefore require one to parametrize the infinite-volume scattering observables and to simultaneously fit to as many energies and matrix elements as possible. The approach has been effectively pursued by the HADSPEC collaboration and more recently by other collaborations in the context of  $2 \rightarrow 2$  coupled-channel scattering [137, 160, 164, 177, 186–194]. An instructive exploration of the analogous method for coupled channel  $1 \xrightarrow{\mathcal{L}} 2$  transition amplitudes was also recently presented in Ref. [195]. Finally, such parameterizations are inherent in the recent work on three-particle scattering [105, 107, 128, 142, 148, 158, 163, 168, 173].

Given the need to parametrize more complicated systems, one might ask whether the general formulas are necessary, e.g. whether one could just identify a particular low-energy effective field theory (EFT) and constrain the low-energy coefficients by calculating finite-volume quantities and fitting these to lattice data. This is certainly a viable and productive approach but cannot be seen as a complete alternative to general methods. One reason is that EFTs necessarily have a limited range of applicability dictated by the separation of scales defining the theory and by the targeted precision.

For example, for coupled-channel systems involving strange and charm quarks, for certain baryon scattering channels and for certain beyond-the-Standard-Model or other non-QCD theories, it is often more reliable to use the analytic properties of the scattering amplitude rather than commit to a particular EFT description. Also the singularities arising in  $3 \rightarrow 3$  scattering can persist to many-loop extensions of the triangle diagram shown in Fig. 1 and this can present additional issues in a given EFT that are automatically addressed in the general formalism. Finally, the general formalism allows one to separate features specific to the EFT from those that are generically true for a certain type scattering amplitude. Either way, we do not have to choose as both tools have been developed and can be applied as desired.

### 3. Closing remarks

In this note, I have given a brief summary of finite-volume methods and their applications in lattice QCD. In addition to the original publications, a number of review articles are available [96, 98, 196–200], providing more detailed discussion on various aspects of the work cited above. I emphasize two take-home messages: First, finite-volume effects provide a useful and surprisingly powerful probe of multi-hadron physics, and second, there is no apparent stumbling block to pushing the established methods to a generic formalism for multi-hadron amplitudes, for any number of channels with any number of particles, including transitions mediated by an external current.

Once the methodology is established, it will be possible to assess, on a case by case basis, what sort of finite-volume information is required (and at which precision) in order to constrain the observable of interest. For the case of a future relation accommodating any number and type of channels, it is clear that the set of unknown functions (the scattering amplitudes across all open channels) will proliferate and so practical utility may quickly become limited. At the same time, having the formal relations in place may make it possible to estimate the systematic uncertainties of neglecting certain multi-particle channels in a given calculation.

It is also useful to have an eye on alternative methods that do not follow this paradigm. One approach that has received much attention recently is the idea that quantum computers could allow for real-time field theoretic simulations, providing a more direct extraction of the scattering amplitude [201–210]. However, also here the system will unavoidably be constrained to a finite volume and, as described in Refs. [211, 212], the issues associated with this can be significant. On the flip side, our knowledge of finite-volume effects motivated by lattice QCD can also guide us in developing strategies to assess the same effects in such real-time quantities.

Another interesting direction is to overcome the Euclidean signature of the lattice calculation by systematically regulating the inverse Laplace transform [28, 31]. This would formally allow an extraction of both inclusive rates [29, 33] and scattering and decay amplitudes [30, 35] at all energies, without the need to treat all open channels explicitly. Such methods potentially require spatial volumes significantly larger than those typically used today, as well as high-precision determinations of the Euclidean correlators. The master-field paradigm, considered recently in Refs. [213–217], may play a useful role here. While this approach may seem far reaching, its recent application in the two-dimensional  $O(3)$  non-linear  $\sigma$ -model is encouraging [36].



Given the progress over the last years, its easy to see an optimistic future for this field: Lattice QCD will continue to identify cutting-edge multi-hadron observables for many years to come, and to transition these from formal methods, to pilot calculations, to systematic precision extractions, driving our understanding of the strong force and the search for new physics beyond the Standard Model.

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