



Testing a new method for scattering in finite volume in the ϕ^4 theory

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Abstract We test an alternative proposal by Bruno and Hansen (J High Energy Phys 2021(6), [https://doi.org/10.1007/JHEP06\(2021\)043](https://doi.org/10.1007/JHEP06(2021)043), 2021) to extract the scattering length from lattice simulations in a finite volume. For this, we use a scalar ϕ^4 theory with two mass nondegenerate particles and explore various strategies to implement this new method. We find that the results are comparable to those obtained from the Lüscher method, with somewhat smaller statistical uncertainties at larger volumes.

1 Introduction

Lattice QCD has been shown to be a powerful tool to determine scattering quantities from first principles. The standard approach is the Lüscher method [2], which relates the finite-volume spectrum obtained from the lattice to the infinite-volume scattering amplitude. It has been applied to many physical systems, including results at the physical point—see Ref. [3] for a review. The formalism has also been recently extended to three particles with three different but conceptually equivalent formulations available in the literature at present [4–8], see Refs. [9, 10] for recent reviews.

In Ref. [1], the authors propose a new strategy to extract scattering quantities. Henceforth, this will be referred to as the BH method. This approach is based on the usage of four-point functions rather than energy levels. The hope is that this approach can be generalised more easily to multi-hadron processes.

As pointed out by the authors, the case of threshold kinematics is particularly favourable as it allows for a direct extraction of the scattering length, with the πN channel being one concrete example.

In this letter we test this novel approach in a scalar ϕ^4 theory. Using this theory has proven to be an excellent test bed for novel scattering studies, as shown in Refs. [11–13]. In order to mimic the πN case, we consider two mass nondegenerate real scalar particles. We explore the necessary techniques, and the optimal approach to use the BH method at threshold. Moreover, we compare to the standard Lüscher approach and find good agreement.

2 Description of the Model

The Euclidean model used here is composed by two real scalar fields ϕ_i , $i = 0, 1$ with the Lagrangian

$$\mathcal{L} = \sum_{i=0,1} \left(\frac{1}{2} \partial_\mu \phi_i \partial_\mu \phi_i + \frac{1}{2} m_i \phi_i^2 + \lambda_i \phi_i^4 \right) + \mu \phi_0^2 \phi_1^2, \quad (1)$$

with nondegenerate (bare) masses $m_0 < m_1$. The Lagrangian has a $Z_2 \otimes Z_2$ symmetry $\phi_0 \rightarrow -\phi_0 \otimes \phi_1 \rightarrow -\phi_1$, which prevents sectors with even and odd number of particles to mix.

To study the problem numerically, we define the theory on a finite hypercubic lattice with lattice spacing a and a volume $T \cdot L^3$, where T denotes the Euclidean time length and L the spatial length. We define the derivatives of the Lagrangian (Eq. 1) on a finite lattice as the finite differences $\partial_\mu \phi(x) = \frac{1}{a} (\phi(x + a\mu) - \phi(x))$. In addition, periodic boundary conditions are assumed in all directions. The discrete action is given in Ref. [12] for the complex scalar theory, but it is trivial to adapt to this case. We set $a = 1$ in the following for convenience.

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3 Observables

In Ref. [1], Bruno and Hansen derived a relation between the scattering length a_0 and the following combination of Euclidean four-point and two-point correlation functions at the two-particle threshold:

$$C_4^{\text{BH}}(t_f, t, t_i) \equiv \frac{\langle \tilde{\phi}_0(t_f) \tilde{\phi}_1(t) \tilde{\phi}_1(t_i) \tilde{\phi}_0(0) \rangle}{\langle \tilde{\phi}_0(t_f) \tilde{\phi}_0(0) \rangle \langle \tilde{\phi}_1(t) \tilde{\phi}_1(t_i) \rangle} - 1, \quad (2)$$

with the time ordering $t_f > t > t_i > 0$, and $\tilde{\phi}_i(t) = \sum_{\mathbf{x}} \phi_i(t, \mathbf{x})$ being field projected to zero spatial momentum. The relation of C_4^{BH} to the scattering length reads

$$C_4^{\text{BH}}(t_f, t, t_i) \xrightarrow[t \gg t_i \gg 0]{T \gg t_f \gg t} \frac{2}{L^3} \left[\pi \frac{a_0}{\mu_{01}} (t - t_i) - 2a_0^2 \sqrt{\frac{2(t - t_i)}{\mu_{01}}} + O((t - t_i)^0) \right], \quad (3)$$

where $\mu_{01} = (M_0 M_1)/(M_0 + M_1)$ is the reduced mass. It is defined in terms of the renormalized masses M_0 and M_1 of the two particles. These masses can be extracted as usual from an exponential fit at large time distances of the two-point correlation functions $\langle \tilde{\phi}_i(t) \tilde{\phi}_i(0) \rangle \approx A_{1,i} (e^{-M_i t} + e^{-M_i(T-t)})$ for $i = 0, 1$. To reduce the statistical error we average over all points with the same source sink separation.

4 Numerical result

4.1 BH method

We generate ensembles using the Metropolis-Hastings algorithm with bare masses $m_0 = -4.925$ and $m_1 = -4.85$, and for simplicity we choose $\lambda_0 = \lambda_1 = 2\mu = 2.5$. The list of ensembles generated in this work with their corresponding measured values of the masses M_0 and M_1 are compiled in Table 1. In this model, as observed in previous investigations of the scalar theory [13], we do not see relevant effects of excited states in the two-point correlators, i.e., they are dominated by the ground state from the first time slice.

In the following we discuss three different strategies to extract the scattering length:

1. We attempt a direct fit of Eq. (3) the the data.
2. We include an overall constant in the fit to account for the $O((t - t_i)^0)$ effect.
3. We make use of a shifted function at fixed t_i and t_f , $\Delta_t C_4^{\text{BH}}(t_f, t, t_i) = C_4^{\text{BH}}(t_f, t + 1, t_i) - C_4^{\text{BH}}(t_f, t, t_i)$, which cancels the constant term. We then determine a_0 by fitting to

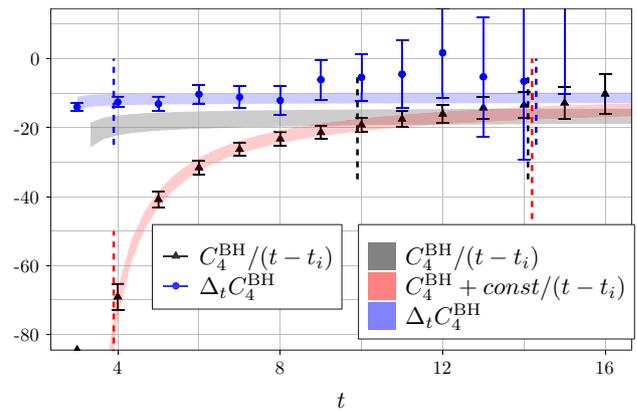


Fig. 1 Four-point function of Eq. (3) multiplied by $L^3/2$, for $L = 22$ and $T = 96$ with $t_i = 3$ and $t_f = 16$ divided by $(t - t_i)$ black triangles. the dashed vertical lines represent the fit interval, the black band represent the result of the fit Eq. (3) and the red band is the same fit with an extra constant term. The blue circles and band represent the discrete derivative of the correlator Eq. (4) and the corresponding fit

$$\Delta_t C_4^{\text{BH}}(t_f, t, t_i) \approx \frac{2}{L^3} \left[\pi \frac{a_0}{\mu_{01}} - 2a_0^2 \sqrt{\frac{2}{\mu_{01}}} \times \left(\sqrt{t + 1 - t_i} - \sqrt{t - t_i} \right) \right]. \quad (4)$$

The three methods are compared in Fig. 1 for one of our ensembles. The black triangles represent the correlator of Eq. (3) divided by $(t - t_i)$ with $t_i = 3$ and $t_f = 16$. This representation is convenient, as it converges towards a constant when $(t - t_i) \rightarrow \infty$. From the monotonic increase of the data points, it is clear that the effect of the $((t - t_i)^0)$ term in Eq. (3) is still sizeable even at large time separations. A fit in the time region $[10, 14]$ —the black band—is reasonable ($\chi^2/d.o.f \sim 0.7$) but results in large uncertainties. The quality of the fit deteriorates very quickly if the fit range is extended: a fit in the time region $[6, 14]$ yields a $\chi^2/dof \sim 5$.

With the second strategy—the red band in Fig. 1—one is able to start fitting at significantly smaller t -values. The data are well described with a $\chi^2/dof \sim 0.2$.

For the third approach, we study $\Delta_t C_4^{\text{BH}}(t)$. This is shown in Fig. 1 as blue circles, and the blue band represents the best fit result with error. The main advantage of the last strategy is that it allows us to extract the physical information at smaller t without introducing extra parameters in the fit. Indeed, the data looks almost constant over the complete t -range available. Only very close to t_i the square root term might become visible.

For this third strategy, which looks most promising from a systematic point of view, we also investigate the dependence on the choice for t_i and t_f . This is shown in Fig. 2 for the same ensemble as in Fig. 1. We do not observe any significant systematic effect stemming from excited state contributions

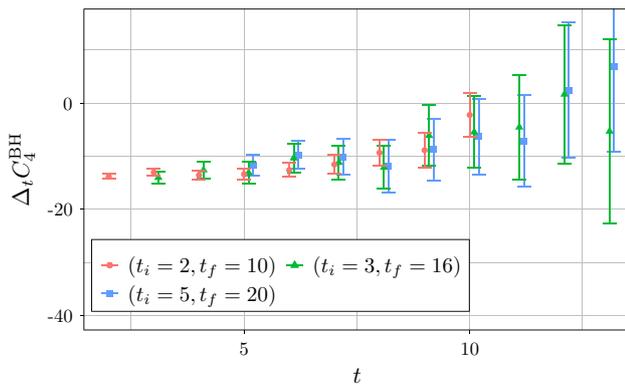


Fig. 2 Plot of the discrete derivative of the correlator Eq. (4) for different values of t_i and t_f . We do not observe any systematic shift and all correlators are compatible. The points with smaller t_i and t_f tend to have smaller error

when changing t_i or t_f . However, we clearly see significantly smaller statistical uncertainties with smaller t_i and t_f values.

4.2 Comparison to the Lüscher method

In this section we compare the BH method described above with the Lüscher threshold expansion [14, 15]. The latter relates the two-particle energy shift, defined as $\Delta E_2 = E_2 - M_0 - M_1$, to the scattering length a_0 via

$$\Delta E_2 = -\frac{2\pi a_0}{\mu_{01} L^3} \left[1 + c_1 \frac{a_0}{L} + c_2 \left(\frac{a_0}{L} \right)^2 \right] + O(L^{-6}), \quad (5)$$

with $c_1 = -2.837297$, $c_2 = 6.375183$ and E_2 being the interacting two-particle energy. E_2 can be extracted from $C_2(t) = \langle \tilde{\phi}_1(t) \tilde{\phi}_0(t) \tilde{\phi}_1(0) \tilde{\phi}_0(0) \rangle$, whose large- t behaviour is

$$C_2(t) \xrightarrow[T \rightarrow \infty]{t \gg 0} A_2 e^{-E_2 \frac{T}{2}} \cosh \left(E_2 \left(t - \frac{T}{2} \right) \right) + B_2 e^{-(M_0 + M_1) \frac{T}{2}} \cosh \left((M_1 - M_0) \left(t - \frac{T}{2} \right) \right). \quad (6)$$

Note that the last term is a known thermal pollution due to finite T in the presence of periodic boundary conditions. Using M_0 and M_1 as input determined from the corresponding two-point functions, the only additional parameter is B_2 .

Alternatively, it is possible to eliminate the second term defining

$$\tilde{C}_2(t) = C_2(t) / \cosh \left((M_1 - M_0) \left(t - \frac{T}{2} \right) \right), \quad (7)$$

and then taking the finite derivative

$$\Delta_t \tilde{C}_2(t) = \tilde{C}_2(t + 1) - \tilde{C}_2(t). \quad (8)$$

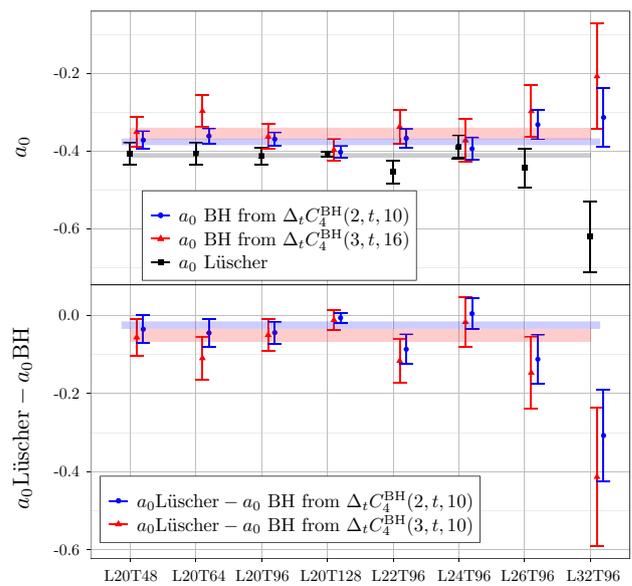


Fig. 3 Comparison of a_0 computed with BH method Eq. (4) with $t_i = 2$ and $t_f = 10$ (blue circles), with $t_i = 3$ and $t_f = 16$ (red triangles) and Lüscher method Eq. (5) (black squares) in the top panel. In the bottom panel we plot the correlated difference between Lüscher method and BH method. The horizontal bands correspond to the weighted average of each method

The two-particle energies obtained from Eq. (6) are compatible to those from Eq. (8). The results are reported in Table 1, along with the values for the scattering length a_0 computed from E_2 using Eq. (5). We have calculated the correlated difference between our two estimates of a_0 obtained within the Lüscher method, column 7 and 8 of Table 1. We find that the difference is always compatible with zero within one sigma, with the exception of the ensembles L20T48 and L32T96 where it is within two sigma.

A comparison between the BH and the Lüscher method is depicted in Fig. 3 for all our ensembles. The values are compatible with each other, however the BH method gives systematically larger values for a_0 . We do not observe a clear statistical correlation or anti correlation between the BH and the Lüscher method. We find that the correlation coefficient varies within the range $[-0.25, 0.6]$ in all ensembles. We notice that exponentially suppressed finite-volume errors are in principle a source of systematic error. However, in Fig. 3, the determination of a_0 does not show any systematic effect varying L from 20 to 32.

5 Conclusion

In this letter, we have investigated the BH method, proposed in Ref. [1], using a scalar theory on the lattice. We have indeed verified that it is a viable method to obtain the scattering length, and that it produces results that are compatible with

Table 1 Values of a_0 , M_0 , M_1 and E_2 measured. The column $\Delta_r C_4^{\text{BH}}$ corresponds to the value of a_0 fitted with Eq. (4) fixing $t_i = 3$ and $t_f = 16$ or $t_i = 2$ and $t_f = 10$, the column $C_{\text{BH}} + c$ is the result of the fit Eq. (3) adding a constant term. The two-particle energy E_2 is computed from C_2 with the fit of Eq. (6) and from $\Delta_r \tilde{C}_2$ with Eq. (8). The corresponding value of a_0 computed with the Lüscher method is reported in the corresponding columns. We used $2 \cdot 10^7$ configurations

for each ensemble, generated from 200 replicas each of 10^5 thermalized configurations, we bin the configurations in blocks of 10^5 (the entirely replica) and we resample the resulting 200 configurations with jackknife. For the light mass M_0 we measured the integrated autocorrelation time $\tau_{\text{int}} \sim 1.5$, while $\tau_{\text{int}} \sim 0.5$ for M_1 , we skip 1000 configurations in each replica for thermalization

T	L	M_0	M_1	E_2		a_0 Lüscher		a_0 BH		
				C_2	$\Delta_r \tilde{C}_2$	C_2	$\Delta_r \tilde{C}_2$	$\Delta_r C_4^{\text{BH}}(3,t,16)$	$C_4^{\text{BH}} + c$	$\Delta_r C_4^{\text{BH}}(2,t,10)$
48	20	0.14675(5)	0.27487(5)	0.4252(3)	0.4253(3)	-0.41(3)	-0.42(3)	-0.35(4)	-0.35(6)	-0.37(2)
64	20	0.14659(5)	0.27480(5)	0.4249(3)	0.4250(3)	-0.41(3)	-0.41(4)	-0.30(4)	-0.29(6)	-0.38(2)
96	20	0.14662(4)	0.27487(4)	0.4251(2)	0.4251(3)	-0.41(2)	-0.41(3)	-0.36(3)	-0.36(4)	-0.38(1)
96	22	0.14604(3)	0.27470(4)	0.4237(2)	0.4237(3)	-0.45(3)	-0.45(5)	-0.34(4)	-0.31(6)	-0.37(2)
96	24	0.14574(4)	0.27458(4)	0.4223(2)	0.4221(3)	-0.39(3)	-0.36(6)	-0.36(5)	-0.41(7)	-0.39(2)
96	26	0.14547(4)	0.27455(3)	0.4218(2)	0.4219(3)	-0.44(5)	-0.47(8)	-0.30(7)	-0.3(1)	-0.36(3)
96	32	0.14521(4)	0.27449(4)	0.4210(2)	0.4213(3)	-0.62(9)	-0.7(1)	-0.2(1)	-0.1(2)	-0.35(5)
128	20	0.14668(3)	0.27484(3)	0.42509(7)	0.4251(3)	-0.409(7)	-0.41(3)	-0.40(3)	-0.39(3)	-0.40(1)

those of the Lüscher method [14]. The most reliable strategy to analyse the four-point function is found to be the use of finite differences in time to remove an overall constant term.

We observe a systematic difference between the Lüscher and BH method. Interestingly, for each ensemble separately both determinations appear compatible. The systematic trend becomes evident only after averaging over all runs, as shown in the bands of Fig. 3. This might be attributed to different lattice artefacts, since both methods represent different estimators for a_0 . We are not able to check this hypothesis here, because we cannot take the continuum limit. However, the different systematics of the two methods offer in general a useful opportunity for cross checks.

The statistical error is similar in both approaches. Also the scaling in L appears to be similar, with maybe a slight advantage for the BH method. However, any advantage of one method compared to another one will in general depend on the theory considered. We conclude that it seems promising to use the BH method in lattice QCD for instance for πN scattering, where also the lattice spacing dependence could be investigated.

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[16] and the open source software packages R [17] have been used. We thank B. Kostrzewa for useful discussions on Kokkos.

Data Availability Statement This manuscript has no associated data or the data will not be deposited. [Authors’ comment: The data generated for this letter is available in form of correlation function upon request.]

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