PHYSICAL REVIEW C **87**, 067001 (2013)

Examining potential shortcomings in using phase shifts as a link between experiment and QCD

A. Švarc*
Rudjer Bošković Institute, Bijenička c. 54, 10 000 Zagreb, Croatia
(Received 27 November 2012; published 20 June 2013)

Lüscher [M. Lscher, Commun. Math. Phys. **105**, 153 (1986); Nucl. Phys. B **354**, 531 (1991)] has shown that in the single-channel problem (where the elastic region is below the first inelastic threshold) there exists a direct link between the discrete value of the energy in a finite QCD volume and the scattering phase shift at the same energy. However, when the theorem is extended to the baryon resonance sector (multichannel situation in the inelastic region above first inelastic threshold), eigenphases (diagonal multichannel quantities) replace phase shifts (single-channel quantities). It is necessary to stress that the renowned $\pi/2$ resonance criterion is formulated for eigenphases and not for phase shifts, so the resonance extracting procedure has to be applied with utmost care. The potential instability of extracting eigenphases from experimental data that occurs if an insufficient number of channels is used can be reduced if a trace function that explicitly takes the multichannel aspect of the problem into account is used instead of single-channel phase shifts.

DOI: 10.1103/PhysRevC.87.067001 PACS number(s): 12.38.−t, 13.75.−n, 13.85.Fb, 25.80.Ek

Because a central task of baryon spectroscopy is to establish a connection between resonant states predicted by QCD and hadron scattering observables, the discovery that QCD can produce a "scattering theory" quantity—the scattering phase shift—has attracted a lot of attention, particularly among experimental physicists. Lüscher's theorem [1,2] provided this possibility. It is well known that resonances do not correspond to isolated energy levels in the (discrete) spectrum of the QCD Hamiltonian measured on the lattice, so an additional effort is needed to extract resonance parameters (mass, width, residua/branching fractions) from the lattice data. In the single-channel case, i.e., in the case of elastic scattering, the pertinent procedure is well known as the Lüscher framework [1,2]. In this framework, for a system described by a given quantum-mechanical Hamiltonian, one relates the measured discrete value of the energy in a finite volume to the scattering phase shift at the same energy for the same system in the infinite volume. Consequently, studying the volume dependence of the discrete spectrum of the lattice QCD gives the energy dependence of the elastic scattering phase shift and eventually enables one to locate the resonance pole positions.

However, because the original Lüscher's derivation has been carried out for energies below the first inelastic threshold, it is not directly applicable for scrutinizing the baryon spectrum. To overcome this problem, this formalism has recently been generalized to multichannel scattering and the required baryon resonance energy range. This was first done in Ref. [3] on the basis of potential scattering theory, while later on in Refs. [4–10] nonrelativistic effective field theory (EFT) was used for this purpose. Finally, even more general extensions of the theorem beyond a single-channel theory have been very recently reported [11,12]. In all cases the conclusions remained very similar to those for the single-channel case, but with one very important difference. Eigenphases replaced phase shifts. And it is very important to emphasize that this seemingly minor change represents a fundamental difference between Lüscher's approach in the elastic situation and its generalization to the inelastic situation: whereas in the former, one aims at the extraction of a single-channel quantity (the scattering phase shift), which is in principle obtainable from the single-channel measurement, the latter case is a multichannel problem. Not one, but several scattering phases have to be extracted, and scattering matrix diagonalization has to be performed in order to obtain eigenphases. Hence, one has to be very careful to apply resonance criteria properly and correctly.

The intention of this Brief Report is to stress the difference between using phase shifts and eigenphases and to discuss interrelations among phase shifts, eigenphases, K-matrix poles, and T-matrix poles as potential resonance criteria for quantifying resonance parameters (mass, width, and residua/branching fractions). The main purpose is to avoid confusion and misunderstandings by using physical phase shifts instead of eigenphases. The secondary task is to restore awareness about the importance of a trace function as a tool to remove the instabilities in the resonance extraction procedure with eigenphases and K-matrix poles by manifestly imposing multichannel features. I believe that this paper is important because it stresses the principal features of Lüscher's approach and its generalization to the inelastic domain with the motive to avoid unjustified simplifications in identifying resonances as has been done in recent, renowned experimental work by Dürr *et al.* [13]. In Dürr *et al.* [13], it has been explicitly stated that "*The $\pi\pi$ scattering phase $\delta_{11}(k)$ in the isospin $I = 1$, spin $J = 1$ channel passes through $\pi/2$ at the resonance energy*...," so the well-known $\pi/2$ criterion to obtain the resonance mass has been used directly on phase shifts. This is, however, incorrect. The scattering *eigenphase*, and not the *scattering phase,* passes through $\pi/2$ at the resonance energy. Single-channel measurement of only one phase shift is simply not enough, and this assumption, even when being fairly reasonable as in the mentioned case, is not generally true. Instead, one should either use eigenshifts, eigenshift traces, or standard pole determination methods to extract T-matrix poles from the

*alfred.svarc@irb.hr

energy-dependent phase shifts, and not phase shifts directly. Using phase shifts only is erroneous. Therefore, I strongly encourage the use of approaches like those in Refs. [4–10], where Lüscher's formalism has been used to obtain phase shifts and an accurate determination of the resonance pole positions in the multichannel scattering has been made.

Beginning to fulfill the outlined task first brings us to the well-known issue of defining what a resonance actually is in scattering theory. A precise definition of a resonance is in principle a nontrivial, and even ill-defined, mathematical problem [14], but for practical purposes it is sufficient to discuss only two alternative definitions as has been suggested by Exner and Lipovský [15]: we may either define resonances via scattering resonances, which are characterized by the prolonged time two particles spend together with respect to the standard scattering process,[1] or through resolvent resonances, which are characterized by the existence of a pole of the scattering matrix. However, even when these two definitions definitely differ, Exner and Lipovsky [15] stress that they do coincide for most physical situations. So, this allows us to restrict our discussion to only one of them: we use the existence of scattering matrix poles as a fairly robust criteria for identifying the resonant state.[2]

In the context of discussing scattering matrix poles, Dalitz and Moorhouse [16] have also introduced *scattering matrix eigenphases* and extensively discussed the concept that the behavior of the resonance eigenphase can be taken as a resonance signal. I quote: "…Dalitz (1963)[3] and Dalitz & Moorhouse (1965)[4] considered the eigenphases δ_α and eigenstates ϕ_α of the unitary matrix S, as is certainly always permissible. It then appeared plausible that the (real) *resonance energy* E_0 corresponded to one of these *eigenphases* increasing rapidly through $\pi/2$."

The most important point is that $\pi/2$ resonance criteria for phases is introduced for *eigenphases*, and not for physical channel *phase shifts*.

In addition to introducing eigenphases as a concept, Dalitz and Moorhouse in further analysis also illustrated how this simple $\pi/2$ criterion actually works in reality for a multichannel theory. They have shown that a multichannel character and a no-crossing theorem strongly predetermine the delicate behavior of eigenshifts in the vicinity of resonance energy. A simple three-channel model with constant background phases has been used to show that $\pi/2$ criterion combined with a no-crossing theorem causes all channels to have a rapid variation near the resonance, but only one of them traverses through $\pi/2$. When the energy of the system approaches the resonance value, the first eigenphase experiences a rapid change and approaches the second one. But, instead of crossing it and continuing through $\pi/2$, because of the no-crossing theorem it just "bumps" into it, "repels" transferring the "momentum" to the second phase shift, and continues smoothly on towards the constant background value of the second phase shift. The second one, however, takes over the rapid energy variation and keeps on changing fast. A similar event happens when the second eigenphase "meets" the next one. Thus, near the resonance energy all three eigenphases are required to undergo rapid energy variations over energy ranges that are small compared with the width r of the resonance at energy E_0, but actually only one traverses through $\pi/2$.

This behavior has also been examined in detail by Goebel and McVoy [19] and by McVoy [20], who show that these rapid energy variations are due to the existence of branch cuts in all channel eigenphases $\delta_\alpha(E)$ and corresponding eigenvectors ϕ_α on the unphysical sheet of the E plane, and lying much closer to the physical axis than does the resonance pole. It is important to notice that these branch cuts do not occur in the complete S matrix $S = \sum_\alpha \phi_\alpha e^{2i\delta_\alpha} \tilde{\phi}_\alpha$, but only in channel eigenphases separately, and therefore do not have any physical significance. And the way out has been found by realizing that the only way this can happen is that the occurrence of these branch cuts in the ϕ_α and δ_α must be just such that all these branch cuts exactly cancel out in the full S-matrix combination. Because of that Goebel and McVoy [19,20] conclude that, with such a complexity of branch cuts without physical significance, the eigenphase representation for the S matrix is not generally a useful representation for the scattering in the neighborhood of a resonance.

Now we are faced with a situation where we have to consider both poles and eigenphases.

I believe that four major facts in relating poles and eigenpahses should be stressed:

(i) eigenphase $\pi/2$ criterion is equivalent to K matrices having poles at resonant energies (the rapid increase of the eigenphase through $\pi/2$ is equivalent to the fact that the corresponding eigenvalue of the reaction matrix $K = i(S-1)/(S+1)$ has a pole at this energy, see Ref. [21]);

(ii) resonance parameters obtained from K and T matrix poles are quantitatively different (despite being interrelated at least for a meromorphic type of background—see Ref. [22]);

(iii) as a direct corollary of (i) and (ii) we have to conclude that resonance parameters obtained from eigenphases and from T matrix poles *must be* quantitatively different; and

(iv) while the T-matrix poles are, in principle, single-channel quantities (it is sufficient to measure observables between only one initial channel and only one final channel to reconstruct the T-matrix between these channels), K-matrix poles and consequently eigenphases are multichannel quantities (one needs to know reactions between all channels to reliably reconstruct single-channel K-matrix elements like the full coupled-channel T-matrix inverse has to be done).[5]

[1] The lifetime of the particle-target system in the region of interaction is larger than the collision time in a direct collision process causing a time delay.

[2] For further reading I recommend Dalitz and Moorhouse [16], where these issues have been extensively elaborated.

[3] See Ref. [17]

[4] See Ref. [18].

[5] An illustration: one needs to measure all observables only for the $\pi N \to \eta N$ reaction to obtain the $\pi N \to \eta N$ T matrix, but one

In literature we usually find three resonance quantification criteria for resolvent resonances: a pole of the scattering matrix, a pole of the K matrix, and the energy when the eigenphase increases rapidly through $\pi/2$. However, it is rarely said that the second criterion and the third criterion *are identical* but *different* from the first one, and very rarely said that the second criterion and the third criterion tend to be unstable if too small a number of channels is analyzed.

Let me now pay some attention to K-matrix poles, phase shifts, eigenphases, and eigenphase instability, to its origin and its implications.

In the case of elastic scattering (single-channel theory), like in the original Lüscher approach, the physical channel phase shift is identical to the S-matrix eigenshift, and single-channel measurement suffices. However, for the inelastic region, a multichannel theory is needed to obtain all phase shifts, and the physical scattering matrix has to be diagonalized to get eigenphases. So, eigenchannels and physical channels differ, and to obtain one or all eigenphases one has to know all physical channels at the same time.

This seems to be a good moment to illustrate this interplay of physical phase shifts and eigenphases in a simple, two-channel toy model.

Let us introduce a two-channel model where processes in channels $1 \to 1$ and $1 \to 2$ are described by a single, inelastic resonance and the $2 \to 2$ process is described by a constant phase shift. Following Goebel and McVoy [19], Eq. (3), we can write down the manifestly unitary scattering matrix $S(w)$ in terms of the physical channel phase shifts $\delta_1(w)$ and $\delta_2(w)$ as

$$S(w) = \begin{pmatrix} \eta\, e^{2\imath\,\delta_1(w)} & \imath\,\sqrt{1-\eta^2}\, e^{\imath\,[\delta_1(w)+\delta_2(w)]} \\ \imath\,\sqrt{1-\eta^2}\, e^{\imath\,[\delta_1(w)+\delta_2(w)]} & \eta\, e^{2\imath\,\delta_2(w)} \end{pmatrix}.$$

Let us observe that matrix elements of $S(w)$ are directly obtainable from experiment, so $\delta_1(w)$ and $\delta_2(w)$ are experimentally obtainable phase shifts. However, to obtain eigenphases we have to diagonalize this matrix:

$$S^E(w) = U^\dagger \cdot S(w) \cdot U = \begin{pmatrix} e^{2\imath\,\delta_1^E(w)} & 0 \\ 0 & e^{2\imath\,\delta_2^E(w)} \end{pmatrix}.$$

For the following choice of input parameters,

$$\delta_1(w) = \mathrm{Arg}\left(1 + 2\imath\,\frac{\frac{\Gamma}{2}}{M - w - \imath\,\frac{\Gamma}{2}}\right),$$
$$\delta_2(w) = \alpha = 1,$$
$$M = 1.5, \qquad \frac{\Gamma}{2} = 0.2\,, \qquad \eta = 0.7,$$

the results for physical phase shifts and eigenphases are shown in Fig. 1.

In Fig. 1(a) we see the physical phase shifts directly obtainable from single-channel $1 \to 1$, $1 \to 2$, and $2 \to 2$

needs to measure observables for all $\pi N \to X\,Y$ processes to obtain the $\pi N \to \eta N$ K matrix (inversion of the full coupled-channel T matrix is needed). Inverting only the $\pi N \to \eta N$ T matrix gives an incorrect result.

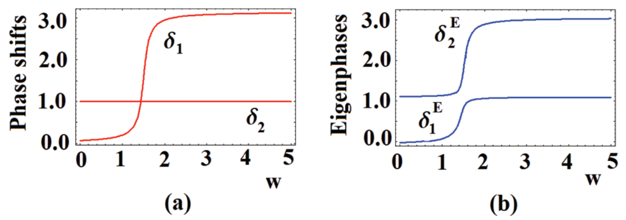

FIG. 1. (Color online) Phase shifts and eigenphases for two-channel toy model.

processes, and in Fig. 1(b) we see eigenshifts obtained by diagonalizing the scattering matrix $S(w)$ and at the same time obtainable from lattice QCD.[6]

So, experiments measure Fig. 1(a), and lattice QCD is used to calculate Fig. 1(b). To obtain directly comparable quantity, we *first* have to measure Fig. 1(a) and *then diagonalize it*. And, to do this, we need *all* the channels.

So, nature cannot be cheated. If knowing all channels is needed in one approach, knowing them all in any other approach is needed as well.

As a direct consequence of these considerations, all criteria formulated on K matrices and eigenphases tend to be unstable if only one channel or too few channels are measured. In other words, while small changes of single-channel data can result only in small changes of T-matrix poles (T-matrix poles being a single-channel quantity), small changes of single-channel data can indeed produce big changes of K-matrix poles and eigenphases, because other nonobserved, hence not controlled, channels can be drastically different. So, in the matrix inversion procedure for obtaining the K matrix or in the diagonalization procedure to obtain eigenshifts, notable changes in individual members can be introduced even when one channel is kept almost fixed.

Let me illustrate this fact in our toy model. If we measure the physical phase $\delta_1(w)$ only, we will *never* be able to reliably predict the eigenphase $\delta_1^E(w)$ which is to be compared with Lüscher's lattice QCD prediction, because it is obtained by diagonalization of $S(w)$ with the *completely unknown* physical phase $\delta_2(w)$. So, if we take something else instead of a constant for $\delta_2(w)$ (a resonance for instance), Fig. 1(b) will look drastically different, and without measuring the $2 \to 2$ channel we will not be able to say anything at all.

This instability, and the multichannel feature of eigenphases, was the main reason why a trace function (in this particular case eigenphase trace) has been introduced. Namely, as it has previously been stated, Goebel and McVoy [19] and McVoy [20] have demonstrated that the individual branch cuts in each channel eigenphase must exactly cancel out in the full S matrix, so a trace of eigenphases being a sum of eigenphases must also be free of these individual branch cuts. Following an old idea of Macek's [23], Hazi [24] has explicitly shown that for an isolated resonance in a multichannel problem the sum of the eigenphases δ_α (eigenphase trace), and not individual eigenphases, satisfies the usual formula appropriate for the

[6]Observe that eigenshifts respect the Von Neumann-Wigner no-crossing theorem as was to be expected.

elastic phase shift: $\mathrm{tr}(\delta_\alpha) = \Delta_0 + \tan^{-1}[r/2(E_0 - E)]$, where Δ_0 is the sum of the background phases. This sum (the trace) explicitly enforces the multichannel character of the problem, so standard techniques used for phase shifts in a single-channel theory can be explicitly used for eigentrace in a multichannel theory. This feature has also been explicitly discussed recently by Ceci. *et al.* [25] who demonstrated that a K-matrix trace can be used to relate K-matrix poles and standard T-channel Breit-Wigner parameters in a background-independent way. These issues have been recently recognized by several groups, and each of them has offered their own way to overcome the problem.

One of them is the GWU group [26] where the authors have analyzed the influence of different K-matrix parametrizations on eigenphases and T-matrix poles. They have shown that, regardless of whether the Chew-Mandelstam K-matrix is parametrized either in the form of a polynomial or in the form of poles with nonsingular background, T matrices are very similar. However, they show that eigenphases are very different. It is very important that they are able to relate the origin of this difference to the fact that they fit only πN-elastic and η-production channels, so uncertainties in other channels cause eigenphases (and K-matrix poles consequently) to vary. They also introduce the trace function (but not for eigenphases but for their derivatives) and demonstrate its advantages over individual channel quantities.

The second group is the Bonn-Jülich-Valencia Collaboration, where they have used a framework based on unitarized chiral perturbation theory (UCHPT) for the extraction of the scalar resonance parameters. This model was very successful with regard to the infinite volume considerations and reproduced well the $\pi\pi/\pi\eta$ and $K\bar{K}$ data up to 1200 MeV [5]. Later on it was also extended to the finite volume considerations [9] with considerable success. The most important point of all is that they recognize the fact that $\pi/2$ resonance criteria cannot be used to extract pole positions, but they extract them directly from the T-matrix poles. They address two main issues. The first one is the use of fully relativistic propagators in the effective field theory framework in a finite volume, and the second one is to discuss in detail the analysis of "raw" lattice data for the multichannel scattering. They supplement lattice data with a piece of the well-established prior phenomenological knowledge that stems from UCHPT, in order to facilitate the extraction of the resonance parameters. In particular, they show that, with such prior input, the extraction of the pole position from the data corresponding only to the periodic boundary conditions is indeed possible. To verify the above statements, they analyze "synthetic" lattice data. To this end, they produce energy levels by using UCHPT in a finite volume, assume Gaussian errors for each data point, and then consider these as the lattice data, forgetting how they were produced (e.g., forgetting the parameters of the effective chiral potential and the value of the cutoff). In the analysis of such synthetic data, they test their approach, trying to establish resonance masses and widths as scattering matrix poles from the fit to the data.

As only two two-body channels are nowadays fairly well known (πN elastic scattering and η production), the use of trace formalism is unfortunately practically impossible. Consequently, using trace function is rather neglected, and single-channel K matrices or single-channel eigenphases are very often erroneously used instead of K-matrices and eigenphase traces. This, however, only stresses the critical lack of experimental data in inelastic channels and shows that new measurements of all possible hadronic reactions in the baryon resonance energy range 1.5 GeV $\leqslant E \leqslant$ 2.5 GeV are badly needed. So I strongly endorse a new proposal for the J-PARC experiment at the 50-GeV Proton Synchrotron [27].

As a summary I would just like to remind the physics community that using Lüscher's theorem to establish a connection between QCD and experiment via phase shifts has to be done with care in the real baryon resonance energy range. Eigenphases (diagonal multichannel and not single-channel quantities) replace phase shifts, so the well-known $\pi/2$ criterion to obtain the resonance mass cannot be used directly on phase shifts as has been suggested in a well-known Dürr *et al.* paper [13]. I would also like to stress the importance of using traces instead of using single-channel quantities when K matrices or eigenphases are analyzed, as delicate cancellations are needed to remove the influence of individual branch cuts in each channel separately [16]. Single-channel analysis for K-matrix elements or eigenphases should be by all means avoided, and a trace function (basically a multichannel quantity) should be used instead.

[1] M. Lüscher, Commun. Math. Phys. **105**, 153 (1986).
[2] M. Lüscher, Nucl. Phys. B **354**, 531 (1991).
[3] C. Liu, X. Feng, and S. He, Int. J. Mod. Phys. A **21**, 847 (2006).
[4] M. Lage, U.-G. Meissner, and A. Rusetsky, Phys. Lett. B **681**, 439 (2009).
[5] V. Bernard, M. Lage, U.-G. Meissner, and A. Rusetsky, J. High Energy Phys. 01 (2011) 019.
[6] M. Döring, U.-G. Meissner, E. Oset, and A. Rusetsky, Eur. Phys. J. A **48**, 114 (2012).
[7] M. Döring and U.-G. Meissner, J. High Energy Phys. 01 (2012) 009.
[8] M. Döring, J. Haidenbauer, U.-G. Meissner, and A. Rusetsky, Eur. Phys. J. A **47**, 163 (2011).
[9] M. Döring, U.-G. Meissner, E. Oset, and A. Rusetsky, Eur. Phys. J. A **47**, 139 (2011).
[10] E. Oset, M. Döring, U. G. Meissner, A. Rusetsky, Proceeding of the XIV International Conference on Hadron Spectroscopy Hadron 2011, edited by B. Grube, S. Paul, and N. Brambilla (2011), p. 261, arXiv:1108.3923.
[11] N. Ishii, Lattice field theory. Proceedings, 28th International Symposium, Lattice 2010, Villasimius, Italy, June 14–19, 2010, PoS(Lattice 2010)145, arXiv:1102.5408.
[12] M. T. Hansen and S. R. Sharpe, Phys. Rev. D **86**, 016007 (2012).
[13] S. Dürr, Z. Fodor, J. Frison, C. Hoelbling, R. Hoffmann, S. D. Katz, S. Krieg, T. Kurth, L. Lellouch, T. Lippert, K. K. Szabo, and G. Vulvert, supporting online material for Science **322**, 1224 (2008).

[14] B. Simon, Int. J. Quantum Chem. **14**, 529 (1978).
[15] P. Exner and J. Lipovský, in *Adventures in Mathematical Physics*, AMS Contemporary Mathematics Series Vol. 447, edited by François Germinet and Peter D. Hislop (American Mathematical Society, Providence, RI, 2007), pp. 73–81.
[16] R. H. Dalitz and R. G. Moorhouse, Proc. R. Soc. London, Ser. A **318**, 279 (1970).
[17] R. H. Dalitz, Annu. Rev. Nucl. Sci. **13**, 339 (1963).
[18] R. H. Dalitz and R. G. Moorhouse, Phys. Lett. **14**, 159 (1965).
[19] C. J. Goebel and K. W. McVoy, Phys. Rev. **164**, 1932 (1967).
[20] K. W. McVoy, in *Fundamentals in Nuclear Theory*, edited by A. De-Shalit and C. Villi (International Atomic Energy Agency, (1967), p. 419
[21] R. H. Dalitz, Rev. Mod. Phys. **33**, 471 (1961).
[22] A. Švarc, arXiv:1202.3045.
[23] J. Macek, Phys. Rev. A **2**, 1101 (1970).
[24] A. U. Hazi, Phys. Rev. A **19**, 920 (1979).
[25] S. Ceci, A. Švarc, B. Zauner, D. M. Manley, and S. Capstick, Phys. Lett. B **659**, 228 (2008).
[26] R. L. Workman, R. A. Arndt, W. J. Briscoe, M. W. Paris, and I. I. Strakovsky, Phys. Rev. C **86**, 035202 (2012).
[27] K. H. Hicks *et al.*, "3-Body Hadronic Reactions for New Aspects of Baryon Spectroscopy," proposal for the J-PARC 50 GeV Proton Synchrotron, 2012, http://j-parc.jp/researcher/Hadron/en/pac_1207/pdf/P45_2012-3.pdf.