

## Partial-wave correlations with uncertainties in the two-nucleon system

Adolfo Guevara Escalante<sup>1,\*</sup>, Rodrigo Navarro Pérez,<sup>2,†</sup> and Enrique Ruiz Arriola<sup>1,‡</sup>

<sup>1</sup>*Departamento de Física Atómica, Molecular y Nuclear and Instituto Carlos I de Física Teórica y Computacional, Universidad de Granada, E-18071 Granada, Spain*

<sup>2</sup>*Department of Physics, San Diego State University, 5500 Campanile Drive, San Diego, California 02182-1233, USA*



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The nucleon-nucleon scattering problem is usually analyzed in terms of partial waves and the corresponding coupled-channel phase shifts and mixing angles, but the available experiments induce correlations among the corresponding channels with different quantum numbers. Based on the Granada 2013 database we analyze the meaning and impact of those correlations, taking into account both the purely statistical ones reflecting the primary experimental data uncertainties as well as the systematic ones exhibiting the ambiguities in the form of the potential representing the unknown nuclear force for distances below 3 fm. We find that the combined uncertainties not only display a dominance of systematic over statistical effects, but also show that these correlations are almost compatible with zero. These findings support the frequent practice of determining potentials from separated channel-by-channel direct fits to phase shifts with the combined systematic and statistical effects without the full-fledged partial wave analysis inferred from experimental data but *only* with much larger uncertainties.

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### I. INTRODUCTION

The determination of the nucleon-nucleon ( $NN$ ) scattering amplitude [1] has traditionally been done in terms of a partial wave expansion [2] and the corresponding phase shifts constrained by unitarity, particularly in the elastic energy regime located below the pion production threshold. Early attempts used the phase shifts *directly* as fitting parameters at fixed energies for differential cross sections and polarization observables [3] (see, e.g., Refs. [4,5] for reviews up until the late 1950s). Such a procedure proves crucial to unveil the most general  $NN$  potential [6] which is of concern to nuclear physics calculations, but also induces correlations among the phase shifts which need to be taken into account for a faithful representation of the data within their given *uncertainties*. The issue of correlations in this regard is rather old, and within a phase-shift context it goes back to the mid 1950s (see, e.g., Refs. [7,8]). With some important modifications, this is essentially the same procedure implemented over the years by a countless number of attempts and is still followed nowadays. A historical overview up to 1989 was reported [9] and the series of Refs. [10–19] describes statistically satisfactory descriptions of the data since 1993 using phenomenological potentials. This includes in particular some of the most up to date versions of the modern chiral potentials [20,21], which are routinely used in *ab initio* calculations including three-body chiral interactions. (For recent and comprehensive

reviews, see, e.g., Refs. [22–24] and references therein). In this paper we undertake a detailed study of these statistical correlations where from a large set of 8000 proton-proton ( $pp$ ) and neutron-proton ( $np$ ) scattering data below 350 MeV laboratory energy a subset of 6713 of  $3\sigma$  self-consistent data (the Granada 2013 database) is selected and fitted [15], and we explore the multidimensional parameter space taking into account *correlation uncertainties* which have been overlooked to the best of our knowledge.

One common practice of nuclear theoreticians has been to propose  $NN$  potentials and fitting to phase shifts *separately* [25–34] so that one could avoid undergoing a full partial wave analysis (PWA). This is a rather convenient shortcut from a computational point of view, and a good starting point to undertake a finer PWA, but such a scheme is at odds with the existence of correlations. Actually, as it has been long known [35,36] (see also Ref. [27] for an early discussion) and we have emphasized in previous works [18] a good fit to phase shifts with an acceptable confidence level does not imply a satisfactory description of the complete scattering amplitude and casts doubts about the portability of the partial wave analysis itself without explicitly quoting the correlations. When such correlations are reported [8] correlated fits become possible [37–39]. However, these correlations are subjected to uncertainties themselves. Therefore, by undertaking the present correlation study we hope to give a specific answer to the question of under what conditions is the independent phase-shifts fit a faithful description of the original scattering data including all sorts of uncertainties.

Before embarking on the issue of correlations and their uncertainties, let us review the nature of the problem in order to motivate our study. Much of the current information about any

\*adguevara@ugr.es

†rnavarroperez@sdsu.edu

‡earriola@ugr.es

theoretical analysis of  $NN$  scattering data is often presented in terms of the corresponding coupled-channel phase shifts and mixing angles which are determined by the conventional least squares minimization method against the existing scattering data. The fitting method acquires statistical meaning under certain conditions which can be checked *a posteriori* [17,40]. Typically these statistical methods allow for a determination and propagation of the uncertainties and correlations of the fitting parameters and hence of the corresponding phase shifts. The net result stressed in previous works [18,41,42] has been that these statistical uncertainties turn out to be about an order of magnitude smaller than the standard deviation between all the (statistically equivalent, i.e., similar reduced  $\chi^2$  values) PWAs carried out in the past. The reason may be attributed to the details of the statistically equivalent interactions in the region below a relative separation of 3 fm. This is particularly significant; while phase shifts are not experimental observables themselves, they are regarded as model-independent quantities which can be extracted from data. However, as we remind below, they turn out to be statistically dependent objects as inferred from data uncertainties and model dependent due to the different statistically equivalent fits based on different  $NN$  potentials.<sup>1</sup> The existence of correlations exhibits a level of redundancy and is quite natural within a potential model approach to nuclear forces. It simply reflects the fact that there are more phase shifts than independent potential components according to general symmetry principles as long as nucleons and pions are regarded as elementary particles. Of course, one should not forget, on a more fundamental level, the fact that QCD, the underlying theory of strong interactions in terms of quarks and gluons for the two lightest  $u, d$  flavors, essentially depends solely on two parameters which, in the isospin limit, can be mapped at the hadronic level onto the pion weak decay  $f_\pi$  and the pion mass  $m_\pi$  suggests that all correlations should be traced from the underlying  $f_\pi, m_\pi$  dependence. At the current experimental accuracy those fundamental correlations are, however, practically invisible. The same is true at the fundamental level, despite encouraging progress at a fundamental level within the lattice QCD approach to the  $NN$  problem [44,45] (see also, e.g., Refs. [46,47] for recent studies and references therein and Ref. [48] for an overview). Thus we are left, for the time being, with the phenomenological analysis.

The paper is structured as follows. In Sec. II we review the essential difference of the phase shifts as primary or secondary parameters and the corresponding fitting strategies as well as the implications for statistical and systematic uncertainties.

<sup>1</sup>For  $NN$  potentials deduced from quantum field theory at the hadronic level this model dependence also covers finite cutoff regularization scheme dependence or equivalently strong form factors due to short distance singularities inherent in the perturbative evaluation of Feynman diagrams involving a meson exchange picture (see, e.g., Ref. [9] for a review). Modern effective field theory (EFT) approaches with suitable counterterms based on chiral symmetry (see, e.g., Refs. [20,21] for recent reviews) also display a scheme dependence which may be larger than nominally expected due to the need for a finite regularization scheme [43].

The necessary definitions of the statistics of correlations are introduced in Sec. III and particularized for our case. Our main numerical results are presented in Sec. IV where we separate the study for both statistical and systematic uncertainties at different confidence levels. Finally, in Sec. V we come to the conclusions and provide an outlook.

## II. PHASE SHIFTS AS PRIMARY OR DERIVED QUANTITIES

While a procedure based on taking the phase shifts as primary fitting quantities facilitates enormously the direct evaluation of statistical correlations through the corresponding covariance matrix at *fixed* energy values, alternative procedures using  $NN$  potentials may be competitive enough in terms of goodness of fit at *arbitrary* energy values but complicate the uncertainty analysis of correlations. Thus, we find it appropriate to ponder the need for taking the phase shifts as secondary quantities, as it has become customary for the past 50 years (see, e.g., Ref. [49] and the discussion below). The reader familiar with these issues may skip this section.

### A. Statement of the problem

From a mathematical point of view the path from scattering data to the scattering amplitude proves to be an unambiguous procedure [50] provided a complete set of measurements encompassing differential cross sections and polarization observables at a particular energy value are available [51] (see Ref. [52] for an analytical solution). From the scattering amplitudes the corresponding partial wave amplitudes and hence the phase shifts may be obtained. While the situation of planning experiments this way in a significant sample of measured energies would be the ideal one, it has seldom been applied in the region below the pion production threshold of most importance for theoretical nuclear physics in *ab initio* calculations of binding energies of light nuclei. Instead rather fragmentary intervals of energies, angles, and measured observables carried out at different laboratories are more frequently available to undertake large scale analysis encompassing as many compatible data as possible.

The formalism of  $NN$  PWA was comprehensively reviewed in Refs. [23,24] with an emphasis put on the verification vs falsification of statistical tests and the possibility of uncertainty quantification and propagation. We refer to these papers for further details and specific formulas in the general case corresponding to the scattering of two spin-1/2 particles and the relation to experimental cross sections and polarization observables as well as the modifications due to the tensor force and the inclusion of determinant long range effects such as Coulomb, vacuum polarization, and relativistic corrections as well as charge-dependent (CD) one-pion-exchange potentials. For our purposes of illustrating the discussion here, we may summarize the situation for the much simpler spinless spherical local potential,  $V(r)$ , case where the only measurable observable would be the differential cross section  $\sigma(\theta, E) = |f(\theta, E)|^2$  with  $\theta$  the scattering angle and  $E$  the scattering center-of-mass (c.m.) energy. The scattering amplitude can be

expanded in the conventional partial wave expansion as

$$f(\theta, E) = \sum_{l=0}^{\infty} (2l+1) \frac{e^{2i\delta_l(p)} - 1}{2ip} P_l(\cos \theta). \quad (1)$$

Here,  $P_l(z)$  are Legendre polynomials and  $\delta_l(p)$  are the phase shifts depending on the c.m. momentum  $p = \sqrt{2\mu E}$  with  $\mu$  the reduced mass. For the spherical potential case the total wave function can be factorized as usual,  $\Psi(\vec{x}) = (u_l(r)/r)Y_{l,m}(\theta, \phi)$  with  $Y_{l,m}(\theta, \phi)$  the spherical harmonics, and the phase shifts  $\delta_l(p)$  are computed by solving the reduced Schrödinger equation for the reduced wave function  $u_l(r)$  where

$$-u_l''(r) + \left[ \frac{l(l+1)}{r^2} + 2\mu V(r) \right] u_l(r) = p^2 u_l(r), \quad (2)$$

with the asymptotic conditions (we assume nonsingular potentials  $r^2 V(r) \rightarrow 0$  as  $r \rightarrow 0$ )

$$u_l(r) \underset{r \rightarrow 0}{\sim} r^{l+1}, \quad u_l(r) \underset{r \rightarrow \infty}{\sim} \sin \left( pr - \frac{l\pi}{2} + \delta_l \right). \quad (3)$$

For a potential with finite range  $a$ , the partial wave expansion is truncated at about  $l_{\max} \approx p_{\max} a$ .

### B. Energy-independent analysis

The simplest situation corresponds to having complete data in a *single* energy  $E$  (or momentum  $p$ ), namely,  $(\sigma(\theta_1, E), \dots, \sigma(\theta_N, E))$ . In this case one can determine the  $l_{\max} \sim pa$  phase shifts *directly* from the data as fitting parameters  $(\delta_0(E), \dots, \delta_{l_{\max}}(E))$  by minimizing

$$\chi^2(\delta_1(E), \dots, \delta_{l_{\max}}(E), Z) = \left( \frac{1-Z}{\Delta Z} \right)^2 + \sum_{i=1}^N \left[ \frac{\sigma^{\text{expt}}(\theta_i, E) - Z\sigma^{\text{th}}(\theta_i, \delta_1(E), \dots, \delta_{l_{\max}}(E))}{\Delta\sigma(\theta_i, E)} \right]^2. \quad (4)$$

Here the normalization  $Z$  with estimated uncertainty  $\Delta Z$  (provided by the experimentalists) is *common* for *one* energy. Moreover, the matrix error deduced as a second derivative with respect to the fitting parameters allows to determine both the error and the correlations of different partial waves at this same energy. Thus, phase shifts become “experimental” and *model-independent* observables,  $\delta_l^{\text{expt}}(E) \pm \Delta\delta_l^{\text{expt}}(E)$  for  $l = 0, \dots, l_{\max}$  at this particular energy.

The energy-independent analysis, despite being direct for extraction of uncertainties and correlations, suffers from some undesirable deficiencies. First, the number of active phase shifts increases with the energy, since the maximal orbital angular momentum in the partial wave expansion is typically  $l_{\max} \sim 2p_{\text{c.m.}}/m_{\pi}$ . Second, phase shifts at different energies may display trigonometric and unpleasant ambiguities, although for nearby energies data may be extrapolated to a fixed energy. Finally, every energy is treated independently, so that if we have fewer experimental measurements than the number of necessary phase shifts,  $N \leq l_{\max}$ , a PWA becomes unfeasible. Although the energy-independent analysis is the only way to make a model-independent PWA, it is no longer an active

strategy in part because of how the available experimental data have been accumulated over the years.

### C. Energy-dependent analysis

If one has incomplete data for a fixed energy but a set of measurements at several energies and angles  $(\sigma(\theta_1, E_1), \dots, \sigma(\theta_N, E_N))$  one cannot generally determine phase shifts  $\delta_l(E_i)$  at those energies because of lack of data. Instead, a *model-dependent* interpolation with fitting parameters  $\mathbf{p}$  in the energy is needed, so that one has  $\delta_l(E; \mathbf{p})$ ; i.e., the phase shifts become secondary or derived quantities.<sup>2</sup> Thus, one minimizes

$$\chi^2(\mathbf{p}, Z) = \sum_{i=1}^N \left[ \frac{\sigma(\theta_i, E_i)^{\text{expt}} - Z\sigma^{\text{th}}(\theta_i, E_i, \mathbf{p})}{\Delta\sigma(\theta_i, E_i)} \right]^2 + \left( \frac{1-Z}{\Delta Z} \right)^2. \quad (5)$$

Different experiments have different normalization constants  $Z$  so that generally

$$\chi^2(\mathbf{p}, Z_1, \dots, Z_E) = \sum_{i=1}^E \chi_i^2(\mathbf{p}, Z_i). \quad (6)$$

The outcome of this multienergy analysis would be an error matrix for the parameters  $\mathbf{p}$  whereby errors could be propagated to compute the error matrix for the phase shifts, using the standard covariance matrix approach.

The analysis pioneered by the Nijmegen group in the mid-1990s [10] was the first example of a large scale PWA of  $NN$  data which had a statistically significant fit due to the inclusion of long range fine effects and a meticulous selection of mutually consistent scattering data. This work was partly followed by the Granada group and has allowed to pin down the  $NN$  phase shifts up to pion production threshold rather accurately [53]. In the spinless case the Granada approach corresponds to a separation of the potential into a well-known quantum field theoretical piece  $V_{\text{QFT}}(r)$  for the long range tail and an unknown short distance piece.  $V_{\text{QFT}}(r)$  can be calculated by evaluating the corresponding Feynman diagrams in perturbation theory. The short distance piece can be determined by a PWA and is coarse grained on “thick” sampling points  $r_n$  suitably located by Dirac delta shells as

$$V_{\text{Short}}(r) = \sum_n \Delta r V(r_n) \delta(r - r_n), \quad (7)$$

where  $r_n = n\Delta r$ . Here  $\Delta r \sim 1/p_{\max} \approx 0.6$  fm, the shortest de Broglie wavelength. From the error matrix in the fitting parameters  $V(r_i)$  one may propagate to the error matrix of phase shifts.

In the general case with spin-1/2 particles, one has instead a set of potential functions  $V_i(r)$  associated to the general decomposition of the potential in a given operator base

<sup>2</sup>A typical example is to take a rational representation of the  $K$  matrix,  $p \cot \delta_l = \sum_{n=0}^K a_n p^n / \sum_{n=0}^M b_n p^n$ , where the corresponding coefficients build the vector of fitting parameters  $\mathbf{p} = (a_0, \dots, a_K; b_0, \dots, b_M)$ .

$V(\vec{x}) = \sum_i O_i V_i(r)$  (see, e.g., Refs. [23,24]) and as a consequence the fitting parameters are given by  $V_i(r_n)$ . The upshot of the whole scheme is the best fit of the Granada 2013 database with  $N_{\text{Dat}} = 6741$   $pp + np$  selected scattering data below 350 MeV laboratory energy with a total  $\chi^2 = 6855.50$  and  $N_{\text{Par}} = 55$  fitting parameters, which corresponds to a reduced  $\chi^2$  per degrees of freedom (DOF) of  $\chi^2/\text{DOF} = 1.025$  [19]. On the statistical level *most* phases are determined by a 1 per mile or less accuracy, the main reason being the strong constraints imposed by CD-one-pion-exchange interaction. For recent reviews on uncertainties in the  $NN$  problem see, e.g., Refs. [23,24].

While the model dependence due to the inclusion of suitable potentials is generated by the need to intertwine fragmentary scattering measurements, it has the further benefit that one can, in principle, use the fitted potentials in *ab initio* nuclear structure calculations. As we will see, it also provides an additional source of uncertainty for those calculations, a subject which has become in the last decade the cornerstone of the predictive power in nuclear physics.

#### D. Systematic and statistical uncertainties

The decomposition of the potential into an unknown short range part and a well-known long range part complies with expected analytical properties of the scattering amplitude in the absence of long distance electromagnetic effects [54] and provides a universal representation for  $V_{\text{QFT}}(r)$ . However, the representation of the short range part is generally ambiguous, and the coarse grained representation, Eq. (7), while quite convenient and computationally cheap, is not unique and several other functions have been proposed which are statistically acceptable; i.e., they have  $\chi^2/\text{DOF} \sim 1$ . They are seven pre-Granada analyses starting with the Nijmegen benchmarking study [10–14] the primary Granada 2013  $\chi^2$  analysis [15] and the subsequent five Granada potentials [15–18].<sup>3</sup> The differences in the phase shifts are mainly attributed to a systematic uncertainty in  $V_{\text{short}}(r)$ . In previous work [18,23,24,41,42] we estimated systematic uncertainties taken over a total of  $N = 13$  analyses which have provided a satisfactory  $\chi^2/\text{DOF}$  at the time of their fit. One important consequence of the Granada energy-dependent analysis corresponds to the out-coming uncertainty structure, where it was found that the statistical uncertainties are about an order of magnitude *smaller* than the systematic uncertainties [18,23,24,41,42]. This observation will be highly relevant for our determination of systematic uncertainties of correlations.

So far, the dominance of systematic vs statistical uncertainties is a very important but purely empirical observation based on combining the available statistically equivalent PWA. We try to give here some rationale of the situation. One may wonder how is it possible that statistically equivalent model fits may yield different phase shifts. To understand this let

us consider a situation where we could compare the energy-independent strategy, where phase shifts are taken as primary fitting parameters with the energy-dependent one where the phase shifts are obtained from the minimizing potential parameters.

The corresponding phase shifts will be denoted as  $\delta_\alpha$  where  $\alpha = (E_n, l)$  runs over all the available energies and relevant angular momenta. Thus, written in compact form, we have

$$\min_{\delta} \chi^2(\delta) \equiv \chi^2(\delta^*), \quad (8)$$

where  $\delta_\alpha^*$  are the minimizing phase shifts whose statistical uncertainties,  $\Delta\delta_\alpha$ , and correlation matrix can be obtained from the standard covariance matrix.

In the energy-dependent strategy we use a potential with parameters, which we denote for short as  $V_i$ , and we actually have that effectively the phase shifts become functions of the potential parameters  $\delta_\alpha(V) \equiv \delta_\alpha(V_1, \dots, V_M)$  so that

$$\chi^2(V) = \chi^2(\delta(V)). \quad (9)$$

Thus, from a variational point of view, the minimization with respect to the potential parameters operates in general as a *restriction*. Of course, the introduction of arbitrarily many parameters in the potential may produce overfitting which as we will see below is in fact not necessary. Hence minimization means

$$\min_V \chi^2(\delta(V)) \equiv \chi^2(\delta(V^*)) \geq \min_{\delta} \chi^2(\delta) \equiv \chi^2(\delta^*). \quad (10)$$

Now, in the limit of small deviations we set

$$\delta_\alpha(V^*) = \delta_\alpha^* + \epsilon_\alpha, \quad (11)$$

and because of the stationary condition we get that the accuracy in the minimum is quadratic in the small deviation:

$$\chi^2(\delta(V^*)) - \chi^2(\delta^*) = \chi^2(\delta^* + \epsilon) - \chi^2(\delta^*) = \mathcal{O}(\epsilon^2). \quad (12)$$

Thus, by construction we expect the energy-dependent strategy to provide  $\mathcal{O}(\epsilon)$  phase shifts for  $\mathcal{O}(\epsilon^2)$  values of  $\chi^2$ . In other words, using a potential we can get rather good fits with not so precise phase shifts. Any potential taken as a basis for the PWA will induce a bias and we can only hope that, by using different potentials with different biases, the global bias will be removed on average.

In the above notation, the findings of our previous work correspond to the fact that, if we take *different* potentials, say  $V^{(1)}, V^{(2)}, \dots$ , on average  $\langle \epsilon_\alpha \rangle = 0$  but their mean squared standard deviation  $\text{Std}(\epsilon_\alpha)$ , which we call the systematic uncertainty, is much larger than the statistical uncertainty,  $\Delta\delta_\alpha$ , i.e.,

$$\text{Std}(\epsilon_\alpha) \gg \Delta\delta_\alpha. \quad (13)$$

The underlying reason of *why* there is such a big increase remains, to our knowledge, a mystery. Nonetheless, as we will see later in this paper, all these simple considerations have implications in the short-cut approach of fitting nuclear potentials directly to phase shifts extracted without passing through the rather cumbersome approach of the PWA.

<sup>3</sup>Our selection, based on comparison with measurable data, excludes several often used important potentials such as the extended soft core (see, e.g., Ref. [55]) and might appear too strict in cases where sometimes a qualitative agreement suffices.

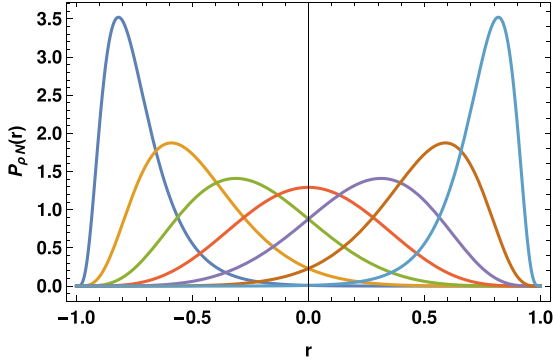


FIG. 1. Theoretical distribution function of the correlation coefficient  $r$  for a sample of size  $N = 13$  generated from a bivariate Gaussian population with theoretical correlation coefficients (from left to right)  $\rho = -0.75, -0.5, -0.25, 0, 0.25, 0.50, 0.75$ .

### III. STATISTICAL DEFINITIONS FOR CORRELATIONS

To assess numerically these correlations and their uncertainties we rely on a few definitions from statistics. We briefly introduce here the main statistical quantities necessary to directly present our results. However, we encourage the reader to review the Appendix for a more in-depth discussion of the theory on the uncertainty estimate of the correlation coefficient. The Appendix takes a pedagogical approach since the theory, although a century old, does not usually appear comprehensively in standard statistics textbooks (we take Refs. [56–58]).

Our purpose in this work will be to estimate a confidence interval for the population correlation  $\rho$  among the different  $N$  partial waves at different laboratory energies. In practice we only have access to a finite sample of pairs  $(x_1, y_1) \dots (x_N, y_N)$  of size  $N$  extracted from a bivariate distribution  $P(x, y)$ . We define then standardized variables

$$\hat{x}_i = \frac{x_i - \bar{x}}{s_x} \sqrt{\frac{N}{N-1}}, \quad (14)$$

where the bar notation indicates the conventional sample mean and  $s^2$  corresponds to the unbiased sample variance [see Eqs. (A4) and (A5) for specific definitions]. The linear correlation coefficient  $r$ , which is an estimator for  $\rho$ , is given by the sample mean of the variable  $\xi_i = \hat{x}_i \hat{y}_i$ :

$$r \equiv \mathcal{C}(\hat{x}, \hat{y}) = \bar{\xi} = \overline{\hat{x}\hat{y}} = \frac{1}{N} \sum_{i=1}^N \hat{x}_i \hat{y}_i, \quad (15)$$

which fulfills the inequality  $-1 \leq \mathcal{C} \leq 1$  with  $\mathcal{C} = -1, 0, 1$  corresponding to full anticorrelation, full independence, and full correlation, respectively, of the sets  $\{\hat{x}_1, \dots, \hat{x}_N\}$  and  $\{\hat{y}_1, \dots, \hat{y}_N\}$ . Of course, the correlation coefficient depends on the sample of size  $N$  and hence different extractions will produce different values of  $r$  so that it will eventually provide a distribution  $P_{\rho,N}(r)$  due to the finite sample size.

For the particular case of a bivariate Gaussian distribution the resulting  $P_{\rho,N}(r)$  was derived long ago and can be found in Eq. (A16). Figure 1 shows the corresponding distribution  $P_{\rho,N}(r)$  for a few values of the correlation coefficient and in

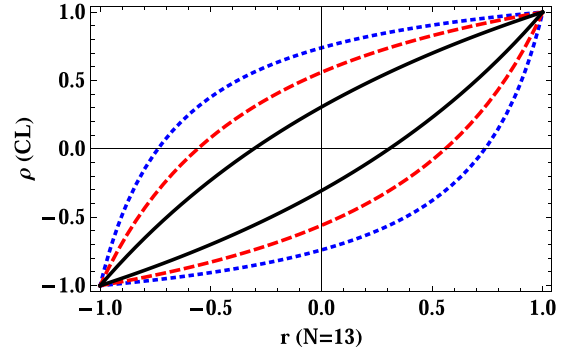


FIG. 2. Estimated confidence limits for the correlation  $\rho$  as a function of the empirical correlation coefficient of a sample of size  $N = 13$  for one, two, and three standard deviations corresponding to 68%, 95%, and 99% confidence levels, respectively.

the particular case  $N = 13$  which will be our main interest here. As we can clearly see, rather large empirical values,  $|r| \geq 0.5$ , would be needed if one claims that  $\rho \neq 0$  significantly.

According to a naive application of the central limit theorem, for  $N \gg 1$ , the distribution becomes a Gaussian with mean  $\rho$  and standard deviation  $\sqrt{(1 + \rho^2)/N}$ . In that case the formula involving the sample variance can be used directly:

$$\rho = \overline{\hat{x}\hat{y}} \pm \frac{1}{\sqrt{N}} [(\overline{\hat{x}\hat{y}} - \overline{\hat{x}\hat{y}})^2], \quad (16)$$

which for our case  $N = 13$  works rather well for  $|\rho| \ll 1$ , but fails for sizable correlations due to the asymmetric shape of the distribution. Equation (16) can erroneously give estimates of  $r$  which fall outside the interval  $[-1, 1]$ . A way to address the general asymmetric situation is by recurring to the central limit theorem, in terms of the Fisher transform, which for large  $N$  behaves as a Gaussian variable,

$$z = \frac{1}{2} \ln \frac{1+r}{1-r} = \frac{1}{2} \ln \frac{1+\rho}{1-\rho} + \frac{\xi}{\sqrt{N-3}}, \quad (17)$$

with  $\xi \in N[0, 1]$ . Thus  $z$  has a mean  $\mu_z = \tanh^{-1} \rho$  and variance  $\sigma_z = 1/\sqrt{N-3}$ . For our  $N = 13$  case this formula works well enough (it can hardly be distinguished in Fig. 1 so we do not plot it) for the asymmetric case and higher order corrections may be found in Ref. [59]. Therefore we have the ranges

$$\rho = \tanh \left\{ \tanh^{-1}(r) \pm \frac{z}{\sqrt{N-3}} \right\}, \quad (18)$$

where  $z = 1, 2, 3$  correspond to 68%, 95%, and 99% confidence levels (CLs), respectively. These three CL bands are displayed for illustration purposes in Fig. 2.

### IV. NN PARTIAL WAVE CORRELATIONS

We may now proceed directly to evaluate the corresponding linear correlation coefficients. For any pair of partial waves, say  $\delta_\alpha$  and  $\delta_\beta$ , and for a given laboratory energy we proceed by computing the sample correlation  $\mathcal{C}(\hat{\delta}_\alpha, \hat{\delta}_\beta)$  from Eq. (15) and assign the error according to Eq. (18) for  $z = 1, 2$

corresponding to 68% and 95% confidence levels. As already mentioned we will address separately both the correlations due to purely statistical origin, i.e., directly stemming from the experimental measurements, and our estimates of systematic origin corresponding to the different representations and parametrizations of the interaction and reflecting inherent ambiguities in the scattering problem.

In our study of the 13 PWA fits we will segregate the six Granada potentials from the remaining seven previous phenomenological approaches. While all the potentials share the necessary long range effects to provide statistically significant fits at their time, this separation makes sense for a variety of reasons. First, all the Granada analyses are explicitly provided in published form with statistical error bars, a practice which only applies to the original and benchmarking Nijmegen analysis (but unfortunately not to their subsequent high-quality potentials). Second, the selected database is the same. A third reason is that the strict separation between  $V_{\text{OFT}}(r)$  and  $V_{\text{Short}}(r)$  is applied in all six Granada cases. Finally, it is encouraging that from grouping the Granada potentials separately, there seems to be no particular bias as compared to the precedent and quite diverse PWA using the original and 40% smaller 1993 Nijmegen database.

We consider correlations among all partial waves with total angular momentum  $J \leq 3$ , corresponding to waves from  $^1S_0$  to  $^3G_3$ . Our results for the linear correlation coefficients among different partial waves are shown in Fig. 3, where we show the  $1\sigma$  and  $2\sigma$  confidence levels according to the Fisher transformation mapping specified in Eq. (18). For a better comparison we display them in a block form resembling the (symmetric) correlation matrix and splitting the upper diagonal involving the central phases, which have a total angular momentum  $J \leq 1$  and the peripheral phases  $J \geq 2$ . In this representation the off-diagonal block corresponds to the correlation between central and peripheral waves. The thin band corresponds to the purely statistical correlations of the Granada 2013 partial wave analysis whereas the thicker bands represent the 13 high-quality potentials developed since the Nijmegen analysis (left panels) as well as the 6 Granada interactions (right panels). In all cases we take as the  $x$  axis the nucleon laboratory energies for  $0 \leq T_{\text{laboratory}} \leq 350$  MeV (ticks represent each multiples of 50 MeV) and the  $y$  axis as the correlation coefficient in the range  $-1 \leq r \leq 1$ .

### A. Statistical correlations

Correlations are generated using the bootstrap method, where the 6713  $np + pp$  experimental results corresponding to 6173 scattering data containing differential cross sections and polarization asymmetries are replicated  $N = 1000$  times following Ref. [60] by performing a Gaussian fluctuation on the existing data and taking the CD one-pion exchange (OPE) with delta shells and the pion-nucleon-nucleon coupling constants as fitting parameters and minimizing the  $\chi^2$  for each of the  $N = 1000$  replicas. This approach produces a nonparametric multidimensional distribution of parameters which is not necessarily Gaussian (see Ref. [60] for illustrations) but also an  $N = 1000$  sample of population of phase shifts at any single laboratory energy value whereby their mutual correla-

tions and the corresponding uncertainties using the formulas in the previous section can be obtained.

For a finite range potential with a sharp boundary, the partial wave expansion has a cutoff in the maximal angular momentum  $J_{\text{max}}$  which roughly and in a semiclassical picture corresponds to the maximal impact parameter consistent with the occurrence of a collision, namely,  $b \lesssim r_c$ . The exponential falloff of the OPE potential above a certain cutoff radius implies that larger angular momenta than this  $J_{\text{max}}$  are mainly determined by the OPE potential tail.

According to the Granada analysis, the partial waves may roughly be divided into active and passive channels corresponding to the low partial waves actually involving the fitting parameters and the higher partial waves mainly, but not fully, determined by the CD OPE potential. We naturally expect the peripheral partial waves to be strongly correlated because they behave approximately in a perturbative manner and are determined by a unique Yukawa-like function.

### B. Systematic correlations

Our way of handling systematic correlations is to regard the very choice of the short range potential as random and treat them as a sample of a population of possible potential choices. This regards a total of  $N = 13$  PWAs carried out in the past 25 years and which have been successful within a statistical point of view, namely, the pioneering Nijmegen analysis and a total of six Granada potentials. One common feature of all the fitting potentials is that they contain exactly the same CD OPE potential starting at distances larger than 3 fm and all other EM corrections such as relativistic, magnetic moments, and vacuum polarization.

The results are depicted in Fig. 3 and, consistent with previous studies, systematic uncertainties are much larger than statistical uncertainties. Most remarkable is the fact that many of the apparently significant statistical correlations turn into lack of correlations within uncertainties. Thus, if we accept the spread of phase shifts of the  $N = 13$  potentials as a lower bound on the current uncertainty, one may take most of the partial waves as *uncorrelated* and one may proceed to fit different partial wave channels independently of each other.

## V. CONCLUSIONS

In this paper we analyzed the correlations and their uncertainties among the different partial waves in  $NN$  scattering below 350 MeV stemming either from statistical data uncertainties or a lack of knowledge on the interaction at short distances.

One of the direct applications of the results found here is that the naive approach of fitting  $NN$  phase shifts to fix nuclear forces in potential models without undertaking a large scale partial wave analysis to experimental data may, to some extent, be justified. The reason is that, regarding the largest source of uncertainty which corresponds to our current deficient representation of the  $NN$  interaction below 3 fm, phase shifts in different partial waves are *uncorrelated* in the entire energy range and within the corresponding uncertainties. The

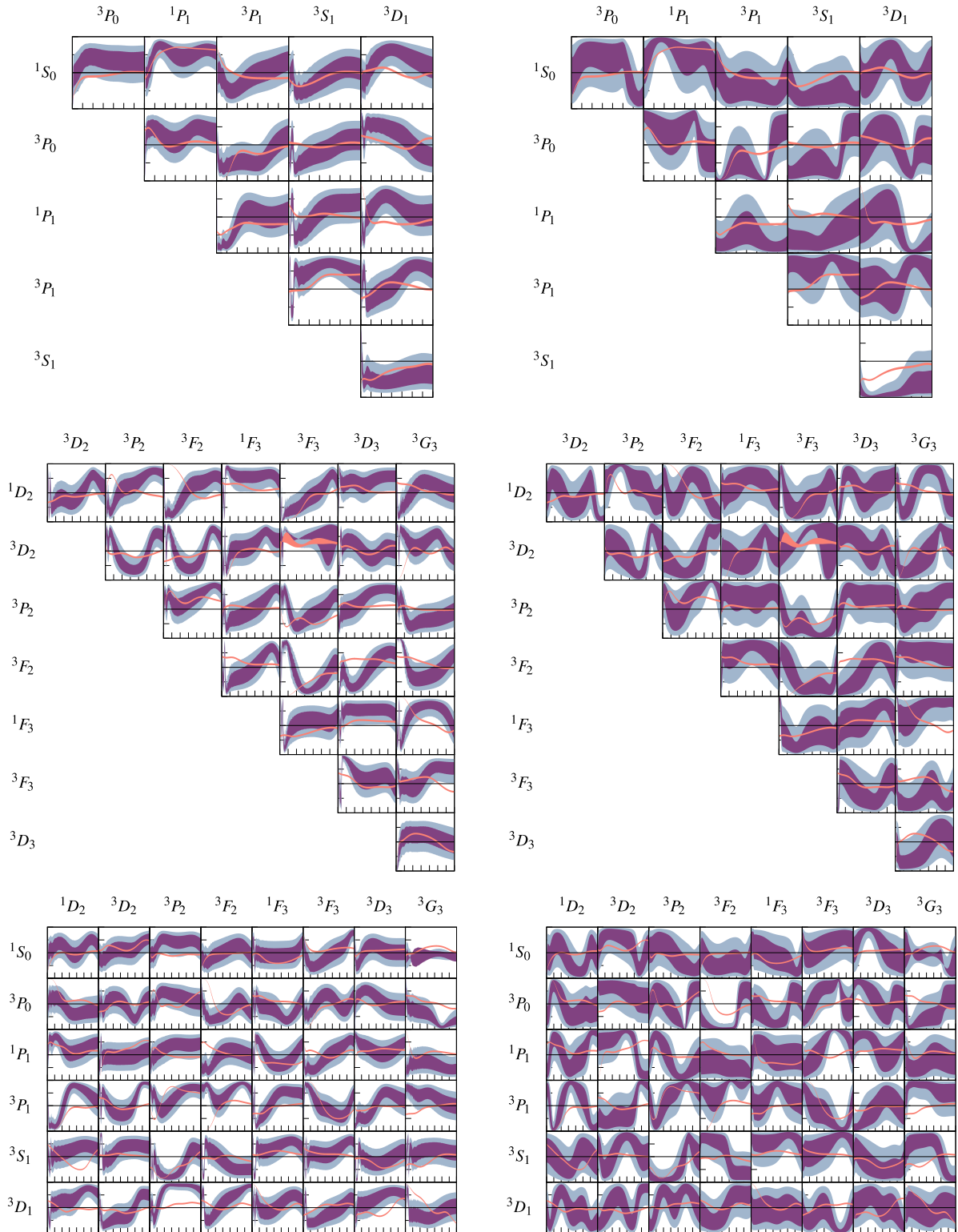


FIG. 3. Partial wave correlation coefficients  $-1 \leq r \leq 1$  with confidence level as a function of the nucleon laboratory energies for  $0 \leq T_{\text{laboratory}} \leq 350$  MeV. The larger (light blue) band corresponds to the systematic uncertainty at the  $2\sigma$  confidence level. The medium band (purple) corresponds to the systematic uncertainty at the  $1\sigma$  confidence level. The smaller (orange) band corresponds to the statistical uncertainty at the  $1\sigma$  confidence level as described in the text. Top: Central phases with total angular momentum  $J \leq 1$ . Middle: Peripheral phases with  $J \geq 2$ . Bottom: Central-peripheral correlations. We show the results for the 13 HQ potentials quoted in the text (left) and the 6 Granada potentials (right).

price to pay, however, is that this implies dealing an order of magnitude larger uncertainties in the phase shifts.

Ignoring correlations in the fits is then justified only at the  $2\sigma$  level, namely, when we *enlarge* their mean standard deviation of the 13 potentials, which roughly corresponds to 20 times larger uncertainties than in the PWA fitting and selecting the  $3\sigma$  self-consistent 2013 Granada database. In practice this adds further uncertainties to the already existing ones, to *ab initio* nuclear structure calculations in terms of potentials obtained by this procedure.

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### APPENDIX: STATISTICS OF CORRELATIONS

We start by considering a univariate and normalized distribution  $P(x)$ . For such a distribution we have the expectation value of a function  $O(x)$  defined as

$$\langle O \rangle = \int_{-\infty}^{\infty} dx O(x) P(x), \quad (\text{A1})$$

where  $\langle 1 \rangle = 1$  is the normalization condition, and  $\mu_x \equiv \langle x \rangle$  is the population mean and  $\sigma_x \equiv \langle (x - \langle x \rangle)^2 \rangle = \langle x^2 \rangle - \langle x \rangle^2$  is the population mean squared distribution. For a sample  $(x_1, \dots, x_N)$  of size  $N$  extracted from this distribution  $P$  we introduce the conventional statistical mean and variance as unbiased estimators:

$$\bar{x} = \frac{1}{N} \sum_{i=1}^N x_i, \quad (\text{A2})$$

$$s_x^2 = \frac{N}{N-1} \overline{(x - \bar{x})^2}, \quad (\text{A3})$$

which fulfill the properties

$$\langle \bar{x} \rangle = \langle x \rangle = \mu_x, \quad (\text{A4})$$

$$\langle s_x^2 \rangle = \langle (x - \langle x \rangle)^2 \rangle = \sigma_x^2. \quad (\text{A5})$$

The sample mean  $\bar{x}$  is itself a random variable since any different extraction of size  $N$  will generally produce a different result. The corresponding distribution function fulfills for large samples,  $N \gg 1$ , the well-known central limit theorem,

$$P_N(z) = \prod_{i=1}^N \int dx_i P(x_i) \delta(z - \bar{x}) \rightarrow \frac{e^{-\frac{1}{2} \frac{(z-\mu)^2}{\sigma^2/N}}}{\sqrt{2\pi\sigma^2/N}}, \quad (\text{A6})$$

where  $\delta(x)$  is the usual Dirac delta function. This result is customarily summarized by stating that  $\bar{x} = \mu \pm \sigma/\sqrt{N}$  with a 68% confidence level. Inverting this relation one finds an estimate of the population mean in terms of the sample mean and sample variance,  $\mu = \bar{x} \pm s_x/\sqrt{N}$ .

The corresponding extension to a normalized joint bivariate probability function  $P(x, y)$  is straightforward and we define accordingly the expectation value as

$$\langle O \rangle = \int dx dy O(x, y) P(x, y). \quad (\text{A7})$$

For our discussion it will be useful to define standardized variables

$$\hat{x} = \frac{x - \mu_x}{\sigma_x}, \quad \hat{y} = \frac{y - \mu_y}{\sigma_y}. \quad (\text{A8})$$

Thus, by construction we have

$$\langle \hat{x} \rangle = \langle \hat{y} \rangle = 0, \quad (\text{A9})$$

$$\langle \hat{x}^2 \rangle = \langle \hat{y}^2 \rangle = 1, \quad (\text{A10})$$

and introduce the linear correlation coefficient  $\rho$  and its variance  $\sigma_\rho^2$ ,

$$\rho = \langle \hat{x} \hat{y} \rangle = \frac{\sigma_{xy}}{\sigma_x \sigma_y}, \quad (\text{A11})$$

$$\sigma_\rho^2 = \langle (\hat{x} \hat{y} - \langle \hat{x} \hat{y} \rangle)^2 \rangle, \quad (\text{A12})$$

where  $\sigma_{xy} = \langle (x - \mu_x)(y - \mu_y) \rangle$  is the covariance of  $x$  and  $y$ .

The correlation  $\rho$  between the  $x$  and  $y$  variables can be estimated by taking a finite sample of size  $N$  and calculating the correlation coefficient defined in Eq. (15) of the main text. Similar to the sample mean  $\bar{x}$ ,  $r$  is also a random variable since a different sample of the same size  $N$  will result, generally, in a different value for  $r$ . Therefore, the distribution function for the linear correlation coefficient of  $N$  pairs is given by the  $\delta$ -constrained integral

$$P_N(r) = \left\{ \prod_{i=1}^N \int d\hat{x}_i d\hat{y}_i P(\hat{x}_i, \hat{y}_i) \right\} \delta(r - \mathcal{C}(\hat{x}, \hat{y})), \quad (\text{A13})$$

which fulfills the proper normalization condition

$$\int_{-1}^1 dr P_N(r) = 1. \quad (\text{A14})$$

For a standardized bivariate Gaussian distribution of the form

$$P(x, y) = \frac{1}{2\pi\sqrt{1-\rho^2}} e^{-\frac{x^2+y^2-2\rho xy}{2(1-\rho^2)}}, \quad (\text{A15})$$

the distribution function  $P_N(r)$  was evaluated analytically long ago [61]:

$$P_{\rho,N}(r) = \frac{(N-1)}{\sqrt{2\pi}} \frac{\Gamma(N)}{\Gamma(N+\frac{1}{2})} (1-r^2)^{\frac{N-3}{2}} (1-\rho^2)^{N/2} \\ \times (1-r\rho)^{\frac{1}{2}-N} F\left(\frac{1}{2}; \frac{1}{2}; N+\frac{1}{2}; \frac{1}{2}(r\rho+1)\right), \quad (\text{A16})$$

where  $\Gamma(x)$  is Euler's gamma function and  $F(a, b, c, x)$  is the hypergeometric function, whose power series around  $x=0$  reads

$$F(a, b, c, x) = \sum_{n=0}^{\infty} \frac{(a)_n (b)_n}{(c)_n} \frac{x^n}{n!} \quad (\text{A17})$$

and  $(a)_n = a(a+1)\dots(a+n-1)$  is the Pochhammer symbol. For example, for uncorrelated Gaussian distributions, corresponding to  $\rho=0$ , the exact result simplifies to

$$P_{0,N}(r) = \frac{(1-r^2)^{\frac{N-3}{2}} \Gamma(\frac{N}{2})}{\sqrt{\pi} \Gamma(\frac{N-1}{2})}. \quad (\text{A18})$$



In the general  $\rho \neq 0$  case one has

$$\langle r \rangle = \rho, \quad \sigma_r^2 = \langle r^2 \rangle - \langle r \rangle^2 = \frac{1 + \rho^2}{N}, \quad (\text{A19})$$

which means that for a finite sample we may observe finite correlations  $r \in (-1, 1)/\sqrt{n}$  even though the original popula-

tion is free of them with  $\approx 68\%$  confidence level. For example, for  $N = 16$  a correlation coefficient of  $|r| \leq 0.25$  is largely compatible with no correlation. Plots of the  $P_{\rho, N=13}(r)$  distribution for different values of  $\rho$  can be seen in Fig. 1 of the main text.

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