Partial Wave Analysis of Nucleon-Nucleon Scattering below pion production threshold

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We undertake a simultaneous partial wave analysis to proton-proton and neutron-proton scattering data below pion production threshold up to LAB energies of 350MeV. We represent the interaction as a sum of delta-shells with electromagnetic effects. We obtain $\chi^2/\text{d.o.f.} \lesssim 1$ after discarding about 20% of the 3σ inconsistent data [5] (see however [4] where $\sigma_2$ and $\sigma_1$ are the single nucleon Pauli matrices. $\mathbf{I}$, $\mathbf{m}$, $\mathbf{n}$ are three unitary orthogonal vectors along the directions of $\mathbf{k}_f + \mathbf{k}_i$, $\mathbf{k}_f - \mathbf{k}_i$ and $\mathbf{k}_f$, $\mathbf{k}_i$ are the final and initial relative nucleon momenta respectively. To determine these parameters and their uncertainties we find that a convenient representation to sample the short distance contributions to the NN interaction can be written as a sum of delta-shells

$$V(r) = \sum_{n=1}^{18} O_n \left[ \sum_{l=1}^{N} V_{l,n} \delta(r-r_l) \right] + V_{\text{OPE}}(r) + V_{\text{em}}(r) \theta(r-r_c),$$

where $O_n$ are the set of operators in the AV18 basis [7], $r_i \leq r_c$ are a discrete set of $N$-radii, $\Delta r_i = r_{i+1} - r_i$ and $V_{l,n}$ are unknown coefficients to be determined from data. The $r > r_c$ piece contains a CD OPE and electromagnetic (EM) corrections which is kept fixed throughout. The solution of the corresponding Schrödinger equation in the (coupled) partial waves $^{2S+1}L_J$ for $r \leq r_c$ is straightforward since the potential reads

$$V_{l,J}^{2S}(r) = \frac{1}{2\mu_{\alpha\beta}} \sum_{i=1}^{N} (\lambda_i^{S})^{J/2} \delta(r-r_i) \quad r \leq r_c$$

with $\mu_{\alpha\beta} = M_{\alpha} M_{\beta}/(M_{\alpha} + M_{\beta})$ the reduced mass with $\alpha, \beta = n, p$. Here, $(\lambda_i^{S})^{J/2}$ are related to the $V_{l,n}$ coefficients by linear transformation at each discrete radius $r_i$. Thus, for any $r_i < r < r_{i+1}$ we have free particle solutions and log-derivatives are discontinuous at the $r_i$-radii so that one generates an accumulated S-matrix at any sampling radius providing a discrete and

I. INTRODUCTION

The NN interaction plays a central role in Nuclear Physics (see e.g. [1, 2] and references therein). The standard procedure to constrain the interaction uses a partial wave analysis (PWA) of the proton-proton (pp) and neutron-proton (np) scattering data below pion production threshold [5] although there are accurate descriptions up to 3GeV for pp and 1.3GeV for np [4]. The Nijmegen PWA uses a large body of NN scattering data giving $\chi^2/\text{d.o.f.} \lesssim 1$ after discarding about 20% of 3σ inconsistent data [5] (see however [4] where $\chi^2/\text{d.o.f.} = 1.4$ without the 3σ criterium). This fit incorporates charge dependence (CD) for the One Pion Exchange (OPE) potential as well as electromagnetic, vacuum polarization and relativistic effects, the latter being key ingredients to this accurate success. The analysis was more conveniently carried out using an energy dependent potential for the short range part. Later on energy independent high quality potentials were designed with almost identical $\chi^2/\text{d.o.f.} \sim 1$ for the gradually increasing database [6, 8]. While any of these potentials provides individually satisfactory fits to the available experimental data, an error analysis would add a means of estimating quantitatively the impact of NN-scattering uncertainties in Nuclear Structure calculations. In the present work we provide a new high-quality potential implementing an analysis of its parameter uncertainties using the standard method of inverting the covariance matrix [10].

The work is organized as follows. In Section II we briefly review the main aspects of the formalism. After that, in Section III we present our numerical results and fits as well as our predictions for deuteron properties and scattering amplitudes. Finally, in Section IV we summarize our results and come to the conclusions.
purely algebraic version of Calogero’s variable phase equation \[\text{[17]}\].

This form of potential effectively implements a coarse graining of the interaction, first proposed 40 years ago by Aviles \[\text{[18]}\]. We have found that the representation \[\text{[4]}\] is extremely convenient and computationally cheap for our PWA. The low energy expansion of the discrete variable phase equations was used already in Ref. \[\text{[19]}\] to determine threshold parameters in all partial waves. The relation to the well-known Nyquist theorem of sampling a signal with a given bandwidth has been discussed in Ref. \[\text{[20]}\]. Some of the advantages of directly using this simple potential for Nuclear Structure calculations have also been analyzed \[\text{[21]}\].

The fact that we are coarse graining the interaction enables to encode efficiently all effects operating below the finest resolution \(\Delta r\) which we identify with the shortest de Broglie wavelength corresponding to the pion production threshold, \(\lambda_{\text{min}} \sim 1/\sqrt{m_N}\) or \(0.55\) fm, so that a maximal number of delta-shells \(N = r_c/\Delta r \sim 5\) (for \(r_c = 3\) fm) should be needed. In practice, we expect the number of sampling radii to decrease with angular momentum as the centrifugal barrier make irrelevant those radii \(r_i \lesssim (l + 1/2)/p\) below the relevant impact parameter, so that the total number of delta-shells and hence fitting strengths \(V_{1N}\) will be limited and smaller than \(N = 5\).

The previous discretization of the potential is just a way to numerically solve Schrödinger equation for any given potential where one replaces \(V(r) \to \tilde{V}(r) = \sum V(r_i)\Delta r_i \delta(r - r_i)\), but the number of delta-shells may be quite large for \textit{fixed} strengths \(V_{1N}\). For instance, for the \(1S_0\) wave and for the AV18 \[\text{[7]}\] potential one needs \(N = 600\) delta-shells to reproduce the phase-shift with sufficient accuracy (below \(10^{-4}\) degrees) but just \(N = 5\) if one uses \(V(r_i)\) as fitting parameters to the \textit{same} phase shift \[\text{[21]}\].

The EM part of the NN potential gives a contribution to the scattering amplitude that must be taken into account properly in order to correctly calculate the different observables. Each
Thus we should have exact in strong interactions for $r$ to be equidistant with the purely EM scattering amplitude to high-precision and are known with much higher accuracy and to shorter distances (see e.g. Ref. [7]) so that one might extend the vacuum polarization term of the pp and np channels and the necessary corrections to the nuclear amplitude coming from the electromagnetic phaseshifts.

III. NUMERICAL RESULTS

A. Coarse graining EM interactions

Of course, once we admit that the interaction below $r_c$ is unknown there is no gain in directly extending the well-known charge-dependent OPE tail for $r \leq r_c$. Unlike the purely strong piece of the NN potential the electromagnetic contributions are known with much higher accuracy and to shorter distances (see e.g. Ref. [7]) so that one might extend $V_{em}(r)$ below $r_c$ adding a continuous contribution on top of the delta-shells, so that the advantage of having a few radii in the region $r \leq r_c$ would be lost. To improve on this we coarse-grain the EM interaction up to the pion production threshold. Thus, we look for a discrete representation on the grid of the purely EM contribution $V_{em}(r)$, i.e. we take $V_{em}(r) = \sum_n V_n^{c} \Delta r_n \delta(r-r_n) + \theta(r-r_c)V_{em}(r)$, where the $V_n^{c}$ are determined by reproducing the purely EM scattering amplitude to high-precision and are not changed in the fitting process. The result using the EM potential of Ref. [7] just turns out to involve the Coulomb contribution in the central channel and the corresponding delta-shell parameters $\lambda_n^{c} = V_n^{c} \Delta r_n M_0$ are given in the first line of Table 1. As expected from Nyquist sampling theorem, we need at most $N = 5$ sampling points which for simplicity are taken to be equidistant with $\Delta r_n = 0.6fm$ between the origin and $r_c = 3fm$ to coarse grain the EM interaction below $r \leq r_c$. Thus we should have $V_{l}^{pp} = V_{l}^{np} + V_{l}^{c}$ if charge symmetry was exact in strong interactions for $r < r_c$, although some corrections are expected as documented below.

B. Fitting procedure

In our fitting procedure we coarse grain the unknown short range part of the interaction from the scattering data. We use the $(\lambda_n)^{bf}_{l,f}$ as fitting parameters and minimize the value of the $\chi^2$ using the Levenberg-Marquardt method where the Hessian is computed explicitly [24]. Actually, this is a virtue of our delta-shell method which makes the computation of derivatives with respect to the fitting parameters analytical and straightforward. As a consequence, explicit knowledge of the Hessian allows to a faster search and finding of the minimum.

We start with a complete database compiling proton-proton and neutron-proton scattering data obtained till 2007 [25–27] and add two new data sets till 2013 [28, 29]. We carry out at any rate a simultaneous pp and np fit for LAB kinetic energy below 350MeV to published data only. Unfortunately, some groups of these data have a common but unknown normalization. We thus use the standard floating [30] by including an additional contribution to the $\chi^2$ as explained in detail, e.g., in Ref. [9]. The extra normalization data are labeled by the subscript “norm” below. We also apply the Nijmegen PWA [5] 3σ-criterion to reject possible outliers from the main fit with a 3σ-confidence level, a strategy reducing the minimal $\chi^2$ but also enlarging the uncertainties. Initially we consider $N = 2717|pp,exp + 151|pp,norm + 4734|np,exp + 262|np,norm = 2868|pp + 4996|np$ fitting data and get $\chi^2_{min} = 3310|pp + 8518|np$ yielding $\chi^2$/d.o.f. = 1.51. Applying the 3σ-rejection and re-fitting the remaining $N = 2747|pp + 3691|np$ data we finally obtain $\chi^2_{min} = 2813|pp + 3985|np$ yielding a total $\chi^2$/d.o.f = 1.06.

While the linear relations of the $(\lambda_n)^{bf}_{l,f}$ and $V_{l,n}$ parameters are straightforward, limiting the number of operators $O_n$ reduces the number of independent components of the potential in the different partial waves. The fitting parameters $(\lambda_n)^{bf}_{l,f}$ entering the delta-shell potentials as independent variables,

1 The most recent np fit to these data was carried out in Ref. [6].
FIG. 2. (Color on-line) np and pp phase shifts and their propagated errors (blue band) corresponding to independent operator combinations of the fitted potential. We compare our fit (blue band) with the PWA [5] (dotted, magenta) and the AV18 potential [7] (dashed-dotted, black) which gave $\chi^2$/d.o.f $\lesssim 1$ for data before 1993.
FIG. 3. Color on-line, np (left) and pp (right) Wolfenstein parameters (in fm) as a function of the CM angle (in degrees) and for $E_{\text{LAB}} = 50\text{MeV}$. We compare our fit (blue band) with the PWA [5] (dotted,magenta) and the AV18 potential [7] (dashed-dotted,black) which provided a $\chi^2/\text{d.o.f} \lesssim 1$ for data before 1993.

FIG. 4. Same as in Fig. 3 but for $E_{\text{LAB}} = 100\text{MeV}$. 

$E_{\text{LAB}} = 100\text{MeV}$
\[ T_{\text{LAB}} = 200\, \text{MeV} \]

**FIG. 5.** Same as in Fig. [3] but for \( E_{\text{LAB}} = 200\, \text{MeV} \).

\[ T_{\text{LAB}} = 350\, \text{MeV} \]

**FIG. 6.** Same as in Fig. [3] but for \( E_{\text{LAB}} = 350\, \text{MeV} \).
Eq. (3), are listed in Table I with their deduced uncertainties. All other partial waves are consistently obtained from those using the linear relations between $(\lambda_l)_{1}$ and $V_{ij}$. Our final results allow to fix the same pp and np potential parameters with the exception of the central components of the potential as it is usually the case in all joint pp+np analyses carried out so far [5–8]. We find that introducing more points or equivalently reducing $\Delta r$ generates unnecessary correlations and does not improve the fit. Also, lowering the value of $r_c$ below 3fm, requires overlapping the short-distance potential, Eq. (3), with the OPE plus EM corrections. We find that independent fits to pp and np, while reducing each of the $\chi^2$-values, drive the minimum to incompatible parameters and erroneous np phases in isovector channels. Actually, the pp data constrain these channels most efficiently and in a first step pp-fits where carried out to find suitable starting parameters for the corresponding np-phases. Quite generally, we have checked that the minimum is robust by proposing several starting solutions.

As a numerical check of our construction of the amplitudes we reproduced the Wolfenstein parameters for the Reid93 and NijmII potentials to high accuracy using $N = 12000$ delta-shells grid points, which ensures correctness of the strong contributions. As a further check of our implementation of the long-range EM effects along the lines of Refs. [5, 22, 23] we have also computed the $\chi^2$/d.o.f. for Reid93, NijmII and AV18 potentials (fitted to data prior to 1993) which globally and bin-wise are reasonably well reproduced when our database (coinciding with the one of Ref. [9] for np) includes only data prior to 1993.

C. Comparing with other database

In order to check the robustness of our database against other selections of data we take the current SAID world database [26] where unpublished data are also included and some further data have been deleted from their analysis although the total number exceeds our selected data. If we consider these $N_{\text{SAID}} = 3061[pp,exp + 188][pp,norm + 4147][np,exp + 461]_{pp,norm} + 3249]_{np} + 4558]_{np}$ data (without including their deleted data) we get for our main fit (without re-fitting) the value $\chi^2/N_{\text{SAID}} = 1.65$. Applying the $3\sigma$-rejection to this database we get $\chi^2/N_{\text{SAID}} = 1.04$. If instead we fit our model to this data base we initially get $\chi^2/N_{\text{SAID}} = 1.31$ which after $3\sigma$ selection of data becomes $\chi^2/N_{\text{SAID}} = 1.04$.

D. Error propagation

We determine the deuteron properties by solving the bound state problem in the $^3S_1 - ^3D_1$ channel using the corresponding parameters listed in Table I. The predictions are presented in table II where our quoted errors are obtained from propagating those of Table I by using the full covariance matrix among fitting parameters. The comparison with experimental values or high quality potentials where the deuteron binding energy is used as an input is satisfactory [5–9].

The outcome and tiny theoretical error bands for the Deuteron form factors (see e.g. [31]) are depicted in Fig. I and are almost invisible at the scale of the figure. The rather small discrepancy between our theoretical results and experimental form factor data is statistically significant and might be resolved by the inclusion of Meson Exchange Currents. In Fig. 2 we show the active pp and np phases in the fit with their propagated errors and compare them with the PWA [5] and the AV18 potential [7] which provided a $\chi^2$/d.o.f. $\lesssim 1$. Note that the $J = 1$ phases show some discrepancy at higher energies, particularly in the $e_1$ phase, where it is about the difference between the PWA and the AV18 potential. Likewise, in Figs. 3, 4, 5 and 6 we also show a similar comparison for the pp and np Wolfenstein parameters for several LAB energies.

Finally, as the previous analyses [5–9] and the present paper show the form of the potential is not unique providing a source of systematic errors. A first step along these lines has been undertaken in Ref. [32]. Thus, the uncertainties will generally be larger than those of purely statistical nature estimated here.

IV. CONCLUSIONS

To summarize, we have determined a high-quality proton-proton and neutron-proton interaction from a simultaneous fit to scattering data and the deuteron binding energy with $\chi^2$/d.o.f. $= 1.06$. Our short range potential consists of a few delta-shells for the lowest partial waves. In addition, charge-dependent electromagnetic interactions and one pion exchange are implemented. We provide error estimates on our fitting parameters. Further details will be presented elsewhere.

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We do not include 14 data of total pp cross section as our theoretical model includes all long range EM effects with no screening and, as is well known, the calculation diverges.
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