NARROWING THE CONFIDENCE INTERVALS IN NUCLEAR STRUCTURE PREDICTIONS THROUGH ELIMINATION OF PARAMETRIC CORRELATIONS*

I. Dedes[a], J. Dudek[a,b]

[a]Université de Strasbourg, CNRS, IPHC UMR 7178, 67 000 Strasbourg, France
[b]Institute of Physics, Maria Curie Skłodowska University
Radziszewskiego 10, 20-031 Lublin, Poland

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As it is well-known, the existence of correlations among the parameters of mathematical models such as typical physics theories implies that any attempt of optimisation of the parameters becomes impossible or highly unstable. When this happens, one says that the parameter determination (usually referred to as inverse problem) becomes an ill-posed mathematical problem. In this article, we suggest a regularisation method of ill-posed or nearly ill-posed inverse problems in the context of the nuclear mean-field applications with the help of the Monte Carlo methods. We present the approach and illustrate its numerical results on the example of the parameter adjustments of the phenomenological Woods–Saxon Hamiltonian in the ^{208}Pb nucleus treated as a test case.

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1. Introduction: statistical significance of model predictions

Any modelling of the realistic nuclear structure phenomena, and for that matter of the great majority of physical effects of interest in various other domains of research, requires adjustments of parameters. Their so-called 'optimal values' are then used to perform the calculations, usually in order to interpret the results of measurements, to predict the new effects as well as to optimise the conditions for the future experiments. Whereas an interpretation of the already known experimental results can be considered a category apart, the *meaningful* theoretical predictions of various effects, mechanisms and phenomena outside of the fit area require some special care. Indeed,

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it has been shown in numerous publications related, *e.g.*, to the Skyrme–Hartree–Fock nuclear structure calculations, *cf.* for instance Ref. [1] and references therein, that of the order of hundreds of various parameterisations of the Skyrme-type interactions have been used to successfully reproduce some already known data, whereas the predictions for (extrapolations into) the new nuclear ranges in the (Z, N)-plane gave diverging results. This latter, usually undesired effect, often has to do with the instabilities of the parameterisations deemed optimal. (The reader interested particularly in the problem of optimisation of the Skyrme-type interactions in the nuclear structure applications is referred *e.g.* to the recent Refs. [2,3] and references therein.)

1.1. Instabilities of the model predictions caused by ill-posedeness

The problems of this type are well-known in *applied mathematics* within the so-called Inverse Problem Theory[1] and usually signify the presence of what is called an ill-posed inverse problem (see below). These problems often have to do with the fact that when performing the parameter adjustments to the selected samples of experimental data, the 'optimal' solutions manifest parametric correlations[2], which happen to be present quite frequently within most of the realistic models of complex physical phenomena. Such parametric correlations depend on both the model itself (through the interaction Hamiltonian) *and* the sampling, *i.e.*, the choice of the number of data points and the type of the experimental data, *cf. e.g.* Ref. [10] and references therein. Thus, when increasing or decreasing the number of data points selected for the fit, certain parametric correlations may disappear and possibly contribute to a stabilisation of the final parametrisation. However, one can demonstrate, *cf.* discussion in Sect. 2.1, that the presence of parametric correlations implies ill-posedness of the inverse problem. Since there exist powerful methods of testing for the presence of parametric correlations — thus ill-posedeness and instabilities of the obtained parametrisation of the model — it becomes clear that each meaningful parameter determination must include such tests; the reader is referred to Ref. [11] for a pedagogical discussion of the related issues. All parameter determination procedures

[1] The literature within the extremely fast developing field of Inverse Problem is impressive, including dozens of books and recently published lecture notes and it would be out of place to attempt here any overview of this subject. We will limit ourselves to mention merely a few examples such as Refs. [4–8] or [9].

[2] Parametric correlations manifest themselves by the fact that one or more parameters can be expressed as function(s) of the others without influencing the r.m.s. deviations in any significant manner. These correlations may result from the fact that the experimental data used do not constrain the model satisfactorily (for some illustrations, see below).

which manifest parametric correlations are mathematically guaranteed unstable when attempting predictions outside of the fit area, and their use is not advised for meaningful theoretical predictions under such circumstances.

1.2. Modelling results and the associated probability distributions

The problem of a meaningful determination of the 'optimal parameters' of the model is further complicated by the fact that the experimental data used as the input for fitting procedures are known only within the uncertainty intervals related to the error bars. Thus, strictly speaking, the experimental results represent probability distributions (often Gaussians) rather than numbers. This implies that the *results of the fitting* are associated with certain probability-distributions — possibly centred around the optimal parameter values — the probability-distributions which themselves characterise the parametric uncertainties. The latter observation provides the conceptual basis for the Monte Carlo simulations as a very powerful tool for studying the underling uncertainties and their probability distributions (*cf. e.g.* Ref. [10]) and by the same token, the related uncertainty distributions of the final theoretical predictions. This observation has been used in some previous publications, *cf. e.g.* Ref. [12], and an extension of these techniques will be presented and illustrated briefly in this article.

1.3. Probability distributions: the impact of incompleteness of the model

As it turns out, in the nuclear structure applications, the experimental error-bars are very often relatively small leading to only very insignificant widths of the mentioned parametric uncertainty distributions[3]. This is much less so, as far as theory uncertainties are concerned, the latter related to the incompleteness of the modelling. It will be instructive at this point to remind the reader about the mechanism in question by using an example. Suppose, the nuclear structure Hamiltonian contains the central and the spin-orbit interactions whereas, say, tensor interactions are not taken into account. By fitting the parameters to the experimental data, necessarily the parameters of the interactions *present* in the model will be 'contaminated' by the fact that a part of the interactions is *absent*, neglected or unknown. Thus the parameters — in the discussed case of the central and spin-orbit interactions, which are deemed optimal — are 'guaranteed falsified'. Even though the fit of the parameters to the actually used experimental input data

[3] An important exception from this rule is provided by the so-called *experimental single-particle levels and their energies*, which, as it is well-known, are not directly observable and depend on various model-dependent hypotheses *e.g.* about the stripping and pick-up reaction cross sections, coupling with the surface vibrations *etc.*, *cf. e.g.* Ref. [10] and references therein.

may lead to satisfactory-looking r.m.s. deviations, the predictions related to the extrapolated nuclear regions can only accidentally be meaningful[4]. In other words, the probability-uncertainty distributions of the 'optimal' parameters impacted by the experimental errors mentioned just above will be *de facto* much broader when taking the theory uncertainties into account. The consequences of not including certain interactions in the Hamiltonian (leading to model incompleteness) for the parameter adjustment procedure are generally difficult to evaluate, *cf.* also the discussion in Ref. [11]. This is not only because of the difficulties in the estimating of the impact of the terms *absent* in the actual Hamiltonian, but also because it is difficult to estimate the impact of falsified parameter values of the interactions present in an incomplete Hamiltonian and caused by the absence of certain terms. These difficulties increase in all the cases in which a part of the interactions is yet simply unknown.

1.4. Stochastic interpretation and stochastic significance of predictions

Observations in the preceding section bring us to the problem of stochastic significance of the theoretical modelling of various physical phenomena. In other words: Since the optimal parameters of the models are known only up to their uncertainty probability distributions, both because of the experimental errors and incompleteness of the modelling, so are the final results of the modelling and it becomes of primordial importance to be able to estimate such uncertainties basing on the 'best information available'. The model predictions with narrower uncertainty distributions can be considered of higher statistical significance for a given physics case (*cf.* Figs. 4 to 7). The widths of such distributions determine what is referred to as *confidence intervals*.

As it turns out, the issue of model's capacity to predict the results before experiment is gaining in importance in many domains of quantum physics and, in particular, in the nuclear structure. There are not only the international conferences devoted entirely to this subject, *cf.* Ref. [14], but also some scientific journals begin imposing the conditions according to which the articles which involve the theoretical modelling must discuss the issue of the 'uncertainty of the model', *cf. e.g.* Ref. [15].

[4] The authors of the book *Numerical Recipes*, Ref. [13], p. 651, in their introduction to the chapter *Modelling of Data* observe with sarcasm:

"Unfortunately, many practitioners of parameter estimation never proceed beyond determining the numerical values of the parameter fit. They deem a fit acceptable if a graph of data and model look good. This approach is known as chi-by-the-eye. Luckily, its practitioners get what they deserve."

[These are the present authors who have chosen to underly certain words in the above quotation.] In other words: very likely "they" do not get any meaningful result.

The mathematical methods needed for this type of the analysis have been developed intensively in the past, and are actually in an intensive progress in the domain of Inverse Problem Theory, *cf.* Refs. [6–8] as an example, but literally thousands of articles on the subjects appear every year, in particular in the devoted journals, and dozens of books appeared in the recent years.

In this article, we wish to present and discuss certain concepts of the regularisation of the ill-posed inverse problem focussing our illustrations on a particular subject of the nuclear theory predictions *viz.* those of the single nucleonic levels in spherical nuclei. We will employ for this purpose the nuclear mean-field theory using the phenomenological Woods–Saxon model. The latter turns out to be particularly well-suited for illustrations of certain mathematical methods of evaluating the parametric uncertainties which, even though standard in various fields of applications, are still rather seldom applied systematically in the nuclear structure physics.

The present article follows the main lines of the 'Stochastic Approach to the Modelling Uncertainties', as proposed in Ref. [10]. The latter can be formulated as follows:

> *Given quantum phenomenon $\mathcal{P}$ described using the model $\mathcal{M}$ with the help of observables $\{\mathcal{F}\}$*
>
> $$\mathcal{M}: \quad \hat{\mathcal{F}}_1, \hat{\mathcal{F}}_2, \ldots \hat{\mathcal{F}}_p \,.$$
>
> *These observables will be characterised not only by the related eigenvalues, whose ensembles are denoted $\{f_j\}$ and thus:*
>
> $$\left[\hat{\mathcal{F}}_1 \to \{f_1\}, \quad \hat{\mathcal{F}}_2 \to \{f_2\}, \ldots \; \hat{\mathcal{F}}_p \to \{f_p\}\right]$$
>
> *but also by distributions of probability of their validity*
>
> $$\mathcal{P}_1 = \mathcal{P}_1(f_1)\,, \qquad \mathcal{P}_2 = \mathcal{P}_2(f_2), \; \ldots \; \mathcal{P}_p = \mathcal{P}_1(f_p)\,.$$
>
> *These distributions need to be derived with the help of stochastic methods on the basis of all the uncertainties both known, or possible to estimate for the model considered at a given time of its evolution.*

The above formulation can be seen as an evolutive-research approach, a way to follow when trying to obtain the more and more stochastically and physically[5] significant parameter estimates while going beyond 'just simple

[5] It may be considered disturbing if in a number of publications, the non-equivalent parametrisations of the same Hamiltonian are obtained (by non-equivalent we mean not only that the values of parameters differ considerably but even the signs of certain coupling constant differ from one article to another implying that the attractive character of the same term goes into a repulsive one, depending on the author) whereas the r.m.s. deviations of the considered physical observables are comparable and comparably 'acceptable' in terms of the 'chi-by-the-eye' criterion of footnote 4.

χ^2-minimisation'. In the following, we will present certain illustrations of what is meant.

2. Inverse problem and Monte Carlo simulations

In any non-relativistic quantum-mechanical problem, one of the principal goals consists in finding the solutions of the Schrödinger equation. In such an equation, the Hamiltonian of a physical system contains the interaction potential $\hat{V} = \hat{V}(p, \ldots)$, with the ensemble of all parameters, $p \equiv \{p_i\}$, for $i = 1, 2, \ldots f$. In applied mathematics, the solution of the problem

$$\hat{H}(p, \ldots)\psi_m(p; \vec{r}) = e_n(p)\psi_n(p; \vec{r})\,, \tag{1}$$

in which all the parameters, usually referred to as optimal, are considered known, is called *solving the direct problem*. At the same time, the algorithm employing the parameters to generate the solutions, the latter called in the jargon 'data' and denoted d, is usually abbreviated using an equivalent shorthand notation

$$\hat{\mathcal{O}}\, p = d\,. \tag{2}$$

One says: An operator $\hat{\mathcal{O}}$ acting on the known parameters p provides the data d. In the case of interest for this article, the 'data' are identified with the eigen-energies of the underlying Hamiltonian and the corresponding wave functions whereas, more generally, in the quantum many-body theories, the operator $\hat{\mathcal{O}}$ should be identified with the many-body Hamiltonian.

However, in order to be able to solve the direct problem, in one way or another, the optimal parameters must be found first. Formally, the corresponding solution can be written down in the form of

$$\hat{\mathcal{O}}^{-1}\, d^{\,\mathrm{exp}} = p^{\,\mathrm{opt}}\,. \tag{3}$$

One says: Equation (3) represents the so-called *inverse problem* in which the inverse of the original operator $\hat{\mathcal{O}}$, here denoted $\hat{\mathcal{O}}^{-1}$, when acting on the selected experimental data set $d^{\,\mathrm{exp}}$ (called 'sample'), provides the optimal parameter set.

2.1. Parametric correlations and singularities of the inverse problem

This compact mathematical representation of the issue of the direct and inverse problem remains strictly formal in the cases of interest in this article and, more generally, in the nuclear structure theory constructed around the many-body nuclear interaction Hamiltonian — simply because the inverse of the many-body Hamiltonian remains unknown. As a consequence of this fact, we will limit ourselves to a few observations, which in place of the formal inverse problem considerations address a much more 'practical' issue: a linearised approach to the χ^2-minimisation in the vicinity of the solutions.

Recall that parameter estimates involve the minimisation of the measure of the distance between the model (in the present case: nucleon) energies and the corresponding experimental data, the latter, up to a normalisation factor usually taken in the form of

$$\chi^2(p) = \sum_{j=1}^{N^{\rm exp}} w_j \left[e_j^{\rm exp} - e_j^{\rm th}(p) \right]^2 \to \frac{\partial \chi^2}{\partial p_k} = 0\,, \qquad k = 1 \ldots f\,, \tag{4}$$

where $N^{\rm exp}$ represents the number of data points and f the number of model parameters, whereas $\{w_j\}$ are the physicist-defined weight factors, which remain a subjective element of the full approach (here, however, to present the arguments we are interested in, it will not be necessary to consider them explicitly).

Let us express the energies using an approximate Taylor linearisation which in the vicinity of the 'optimal' solution, $p^{\rm opt}$, can be written down as

$$e_j^{\rm th}(p) \approx e_j^{\rm th}\left(p^{\rm opt}\right) + \sum_{k=1}^{f} \left(\frac{\partial e_j^{\rm th}}{\partial p_k} \right) \Bigg|_{p=p^{\rm opt}} \left(p_k - p_k^{\rm opt} \right)\,. \tag{5}$$

Such an expression approaches the exact result when the parameters approach the optimal solution. Introducing a short-hand notation for the Jacobian matrix taken at the optimal parameter set, $J_{jk}^{[\rm opt]} \leftrightarrow J_{jk}$:

$$J_{jk} \stackrel{df}{=} \left(\frac{\partial e_j^{\rm th}}{\partial p_k} \right) \Bigg|_{p=p^{\rm opt}} \qquad \text{and} \qquad b_j = \left[e_j^{\rm exp} - e_j^{\rm th}\left(p^{\rm opt}\right) \right] \tag{6}$$

allows to express, within the Taylor approximation, the $\chi^2(p)$ using the Jacobian matrix as

$$\chi^2(p) = \sum_{j=1}^{N^{\rm exp}} \left[\sum_{k=1}^{f} J_{jk} \left(p_k - p_k^{\rm opt} \right) - b_j \right]^2\,. \tag{7}$$

The minimum condition, after shortening the notation $J_{jk} \to J$, takes now an algebraic form of

$$\frac{\partial \chi^2}{\partial p_i} = 0 \to \left(J^T J \right) \left(p - p^{\rm opt} \right) = J^T\, b\,. \tag{8}$$

The above expression represents a system of linear equations for the unknown parameters p. Let us introduce a square matrix $\mathcal{A} \equiv J^T J$; we have

$$p = \mathcal{A}^{-1} \left(J^T\, b \right) + p^{\rm opt}\,, \tag{9}$$

and it becomes clear that the existence of the solutions depends on the existence of the inverse matrix $\mathcal{A}^{-1}$. However, one may show that when the ensemble of parameters of the problem contains correlations (some parameters are functions of some others) some lines (columns) of the Hessian matrix become linearly dependent and it follows that $\mathcal{A}$ has no inverse.

The above result has devastating consequences for the parameter evaluation procedures. This is not so much because of the *strict* non-existence of the inverse matrix in question, but rather because of the fact that the 'practical' *i.e.* numerical calculation of the matrix $\mathcal{A}$ in Eq. (9) takes place *close to the singularity point*. Under such conditions, the numerical procedures seem to be working rather satisfactorily, some inverse matrices can be calculated numerically without computer's signalling algorithm errors, the equations of the structure of the ones in (9) — or equivalent — are numerically solved and, moreover, the resulting r.m.s. deviations may seem acceptable (according to the *chi-by-the-eye* criterion of footnote 4). However, the closeness to the singularity point implies the instability of the final results: A minimal modification of the input conditions such as *e.g.* slight change of the experimental input implies divergence of the final result for the 'optimal parameters' — paradoxically, without a big impact on the r.m.s. estimates, which often remain fairly insensitive to the singularities discussed.

It, therefore, becomes clear that the detection of the presence of parametric correlations in any given parameter evaluation problem and the research of physically motivated methods of their possible removal are of primary importance for the stability of the optimal parametrisation and the implied predictive power of the modelling. In the following sections, we describe the results of the Monte Carlo based procedure of the elimination of parametric correlations in the case of the spherically symmetric Woods–Saxon Hamiltonian; we refer to this process as 'regularisation'.

2.2. Parameters and uncertainty probability distributions

The starting point in the posing of the problem in this section will be the observation that the energy-positions of each of the so-called experimental single-nucleon levels are uncertain. The uncertainties are usually represented by the error bars which, in turn, are directly related to the width at half maximum of the corresponding Gaussian uncertainty distribution. This width, as discussed in the preceding section, will be non-negligible in the considered case since it has to account for not only the purely experimental/instrumental uncertainties but, most of all, of the incompleteness of the model. Thus, each single-nucleon energy $e_i^{\exp}$, which will be used as the element of sampling (the full set of the input data used for the parameter optimisation procedures), together with its uncertainty, will be represented by the Gaussian probability distribution

$$P_i\left(e;\sigma_i,\, e_i^{\exp}\right) = \frac{1}{\sqrt{2\pi}\sigma_i} \exp\left[-\left(e - e_i^{\exp}\right)^2 / 2\sigma_i^2\right] . \tag{10}$$

It then follows that the optimal solutions should be represented not only by the set of numbers $\{p^{\rm opt}\}$ but rather by the corresponding probability distributions

$$\mathcal{P}_k = \mathcal{P}_k\left(p_k, p_k^{\rm opt}\right) . \tag{11}$$

To illustrate the results of the present pilot project, which can be seen as an element of a more complete analysis[6], we will use the spherical Woods–Saxon phenomenological mean-field model known to represent the experimental single-nucleon energies in a realistic manner.

2.3. The Woods–Saxon mean-field model: parameters and motation

For the sake of the presentation of the issue of the parametric correlations, it will be necessary to introduce the corresponding Hamiltonian and its parameters. The Hamiltonian has the form of

$$\hat{H}_{\rm WS} = \hat{t} + \hat{V}_{\rm cent} + \hat{V}_{\rm so}\left[+\hat{V}_{\rm Coulomb} \text{ for protons}\right] , \tag{12}$$

where the subscript "so" stands for spin-orbit and $\hat{t}$ represents the nucleon kinetic-energy operator, whereas

$$\hat{V}_{\rm cent} \equiv \frac{V_{n,p}^{\rm cent}}{1 + \exp\left[-\left(r - R_{n,p}^{\rm cent}\right)/a_{n,p}^{\rm cent}\right]} \quad \text{with} \quad R_{n,p}^{\rm cent} = r_{n,p}^{\rm cent}\, A^{1/3} \tag{13}$$

and

$$\hat{V}_{\rm so} \equiv \frac{1}{r}\frac{{\rm d}V_{\rm so}}{{\rm d}r}\, \hat{\ell}\cdot\hat{s}\,, \tag{14}$$

with

$$V_{\rm so} \to V_{\rm so}(r) \equiv \frac{V_{n,p}^{\rm so}}{1 + \exp\left[-\left(r - R_{n,p}^{\rm so}\right)/a_{n,p}^{\rm so}\right]} \quad \text{with} \quad R_{n,p}^{\rm so} = r_{n,p}^{\rm so}\, A^{1/3}\,. \tag{15}$$

Above we have two sets of parameters, every set containing 6 parameters for the protons and neutrons each. These parameters are denoted

$$p^{n,p} \equiv \left\{V_{n,p}^{\rm cent}\,,\; V_{n,p}^{\rm so}\,,\; r_{n,p}^{\rm cent}\,,\; r_{n,p}^{\rm so}\,,\; a_{n,p}^{\rm cent}\,,\; a_{n,p}^{\rm so}\right\} , \tag{16}$$

where the subscripts n and p refer to the neutrons and protons, respectively. In what follows, the neutron and proton parameter sets are treated as strictly independent so that the minimisation of the χ^2-tests will be performed separately for the neutrons and for the protons.

[6] Such a more advanced analysis involves several nuclei at the same time and includes dependence of the Gaussian widths on the individual nucleonic quantum numbers (n, ℓ, j); the corresponding results will be published elsewhere.

3. Monte Carlo simulations and parametric correlations

To illustrate certain selected mathematical properties of the results of the parameter determination procedures, we will focus on an example of the spherical doubly magic ^{208}Pb nucleus. We will introduce the numbers of experimental levels, $N_{n,p}^{\rm exp}$, for the neutrons and protons. The latter are: $N_n^{\rm exp} = 11$ for the neutrons and $N_p^{\rm exp} = 7$ for the protons. The experimental data used will be the same as those used in Ref. [10].

The energy uncertainty of each single-nucleonic level is defined by specifying σ_i, *cf.* relations of type of Eq. (4), and, in principle, each level has its own uncertainty characteristics. However, the problem of the individual characteristics of the uncertainty distributions depending on the individual sets of quantum numbers $\{n, \ell, j\}_i$, *i.e.*, $\sigma_i \leftrightarrow \sigma_{(n,\ell,j)_i}$ for each considered quantum state is a relatively complex one and the corresponding detailed discussion will be published elsewhere.

The purpose of the following series of illustrations will be two-fold: Firstly, to detect the presence/absence of parametric correlations and secondly, to examine the possibilities of the elimination of parameter correlations and its impact on the predictive power of the modelling. To simplify the analysis from the start, we would like to begin with the search of the possible absence of certain parametric correlations in the phenomenological Woods–Saxon Hamiltonian. Next, we would focus on the presence and the precise form of the existing correlations by expressing, if possible, the dependence of some parameters as function(s) of some others. This problem does not have any general solution and needs to be examined case-by-case. The parametric correlations of this type have been studied in the past *cf. e.g.* Ref. [12], but in the present case, after having determined the form of the correlations, we wish to eliminate the dependent parameters and examine the impact of the implied regularisation of the originally ill-posed problem. We chose for this purpose, as the testing ground, the Monte Carlo generated uncertainty distributions of the predicted (calculated) single-nucleon levels.

To follow this strategy, we will introduce a single uncertainty width $\sigma = \text{const.}$, in Eq. (10), *i.e.* independent of i, and considered as an average characteristic which represents at the same time the theoretical and the experimental uncertainties of the single-nucleon energies. Such an approach has certain advantages since it allows to look for the presence (or identify the absence) of possibly systematic tendencies as *e.g.* an evolution of the final prediction uncertainties with increasing main shell-number N, or with the orbital angular momentum ℓ quantum number, *etc.*

We will consider fitting the parameters of the Hamiltonian according to the principles of the Monte Carlo methods: We will generate with the help of the random number generator a big number, $\mathcal{N}_{n,p}^{\rm trial}$, of the trial, so-called

pseudo-experimental level-sets, each set composed of $N_{n,p}^{\mathrm{exp}}$ levels. These sets will be generated according to the Gaussian distributions of Eq. (10). By minimising the χ^2 function for the neutrons and protons separately, we will obtain $\mathcal{N}_{n,p}^{\mathrm{trial}}$ sextuplets of parameters listed in Eq. (16), *i.e.*:

$$\text{Neutrons}: \quad \left\{V_n^{\mathrm{cent}},\ r_n^{\mathrm{cent}},\ a_n^{\mathrm{cent}},\ V_n^{\mathrm{so}},\ r_n^{\mathrm{so}},\ a_n^{\mathrm{so}}\right\}, \tag{17}$$

for the neutrons and

$$\text{Protons}: \quad \left\{V_p^{\mathrm{cent}},\ r_p^{\mathrm{cent}},\ a_p^{\mathrm{cent}},\ V_p^{\mathrm{so}},\ r_p^{\mathrm{so}},\ a_p^{\mathrm{so}}\right\}, \tag{18}$$

for the protons. As it is well-known, *cf. e.g.* Refs. [10, 12] and references therein, several hypotheses related to the possible absence of the parametric correlations can be verified by the projection techniques. Briefly: Consider a model depending on parameters $\{p_k\}$ for $k = 1, 2, \ldots f$. With the help of the Monte Carlo generated f-plets of the parameter sets $\{p_k\}_n$ for $n = 1, 2, \ldots \mathcal{N}^{\mathrm{trial}}$, we will be able to construct the planar projections of the type $\{p_{k_\kappa}, p_{k_\rho}\}$. If the corresponding distribution represents approximately a radial symmetry (*cf.* figures 1–2), we conclude that parameters p_{k_κ} and p_{k_ρ} are independent. Conversely, any pattern which can be interpreted as lines or systems of lines gives rise to the detection of parametric correlations.

As it can be seen from figures 1–2, the shapes of the distributions of the six-dimensional points projected onto the two-dimensional planes of the appropriately chosen axes manifest nearly radial symmetry suggesting that the parameters V^{cent} and a^{cent} as well as r^{cent} and a^{cent} can be considered uncorrelated.

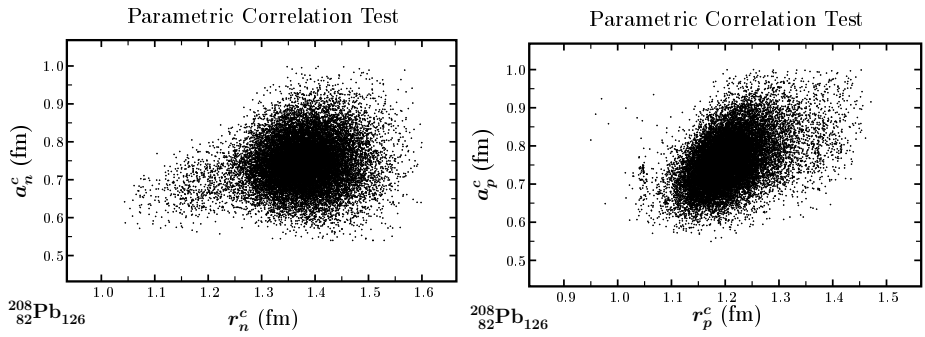

Fig. 1. Results of the Monte Carlo simulations corresponding to the condition $\sigma_i = \sigma = 500\,\mathrm{keV}$ and $\mathcal{N}^{\mathrm{trial}} = 50\,000$. The near radial symmetry of the distributions of points in these diagrams indicates that the radius parameter and diffuseness parameter of the Woods–Saxon central potential can be considered uncorrelated. This conclusion applies to the neutron parameters, left-, and to the proton parameters, right-hand side [see the text for further comments].

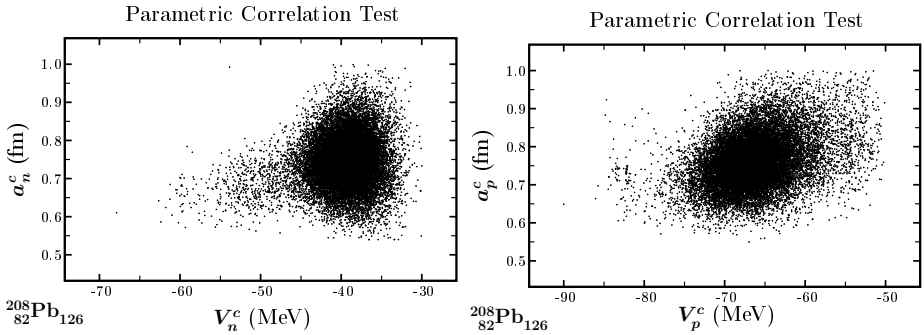

Fig. 2. Illustration similar to that in Fig. 1, but for the test of the possible parametric correlations between the diffusivity and the potential depth parameters of the central Woods–Saxon potentials for the neutrons (left) and protons (right). Similar conclusion applies: These two parameters may be considered uncorrelated.

Analogous illustration for the combination of the radius and the potential depth parameters is given in Fig. 3 showing parabolic correlations.

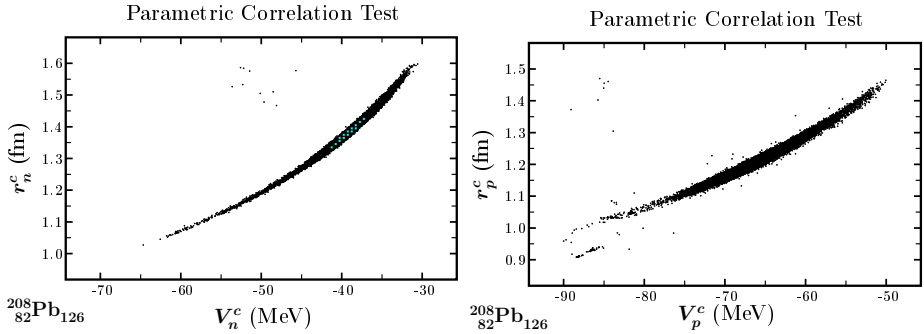

Fig. 3. Illustration analogous to the preceding ones here, however, showing a well-defined correlations demonstrated to be parabolic as discussed in the text, with the parabolic fit demonstrating very small r.m.s. values. Here, we have selected the representation in the form of r^{cent} *vs.* V^{cent} dependence. Left-hand side shows the results for the neutrons, right-hand side the ones for the protons.

The parabolic correlations have been demonstrated by a direct fit using the expressions

$$r^{\mathrm{cent}} = \alpha * \left(V^{\mathrm{cent}}\right)^2 + \beta * V^{\mathrm{cent}} + \gamma \tag{19}$$

with the results

$$\alpha = 0.0001323\ \mathrm{fm\,MeV^{-2}}\,, \quad \beta = 0.0302132\ \mathrm{fm\,MeV^{-1}}\,, \quad \gamma = 2.6264104\ \mathrm{fm} \tag{20}$$

for the protons and

$$\alpha = 0.0003616\ \mathrm{fm\,MeV^{-2}}\,, \quad \beta = 0.0499522\ \mathrm{fm\,MeV^{-1}}\,, \quad \gamma = 2.7840453\ \mathrm{fm} \tag{21}$$

for the neutrons. Results of the calculations for the spin-orbit potential parameters (not shown) confirm the independence between the spin-orbit strength and diffuseness, and the spin-orbit radius and the diffuseness parameters, and at the same time show the correlations between the strength and the radius parameters. This latter correlation is a more complex one as compared to that for the central potential. Since it will not be needed for the following discussion, those results will not be presented here.

4. Level uncertainty distributions and elimination of parametric correlations

Whereas determination of the presence and/or of the absence of the parametric correlations is an essential element of the *ex post* analysis of any procedure of the parameter adjustment — such an element can merely be considered as the first step. In this section, we will present the results of our Monte Carlo study focussing on the uncertainties of the final predictions of the single-nucleon levels.

4.1. Prediction uncertainties caused by the input uncertainties

In what follows, we report on the results of eliminating the parametric correlations in order to examine the possible consequences in terms of the final prediction uncertainties. The needed information is obtained, in fact, simultaneously with the Monte Carlo test of the parametric correlations discussed in the preceding section.

Indeed, when fitting the sixtuplets of parameters in Eqs. (17)–(18), we also each time obtain the single-particle spectra and this information can be used to construct the occurrence histograms as the ones shown in the figures 4 to 7. To construct these histograms, we divide the energy axis into small intervals and count the number of times each given eigenvalue falls into any given interval. In this way, we obtain distributions, which after the normalisation become the uncertainty probability-distribution for each nucleonic level.

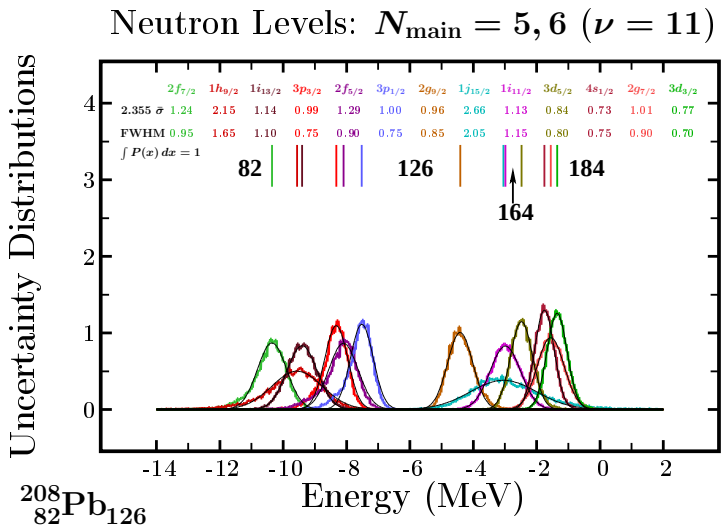

Fig. 4. The normalised histograms representing the probability distributions of uncertainties of each individual level in the neutron main shells $N = 5$ (the group below the 126-gap) and $N = 6$ (the group above the 126-gap) in ^{208}Pb. The two rows of numbers in the upper part of the figure represent two measures of the half-maximum widths as discussed in the text. These results illustrate the uncertainties obtained *before* the removal of the parametric correlations assuming that the combined theory and experimental input uncertainties are given by $\sigma = \sigma_i = 500\,\mathrm{keV}$.

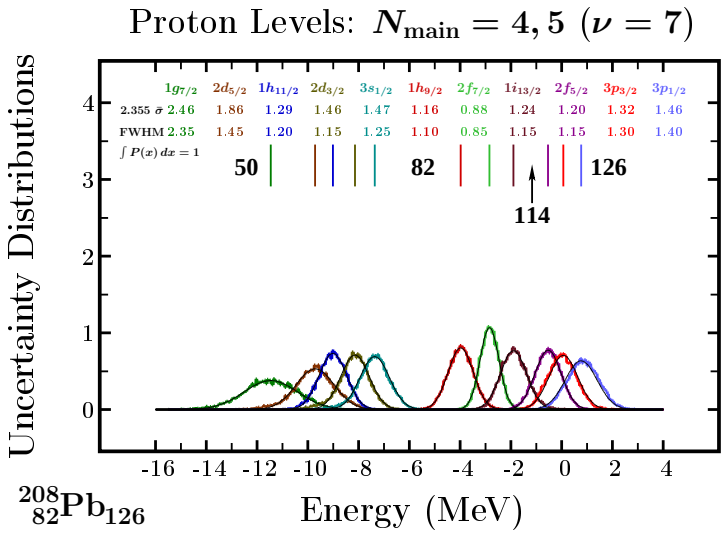

Fig. 5. Similar to the preceding one but for the protons in ^{208}Pb.

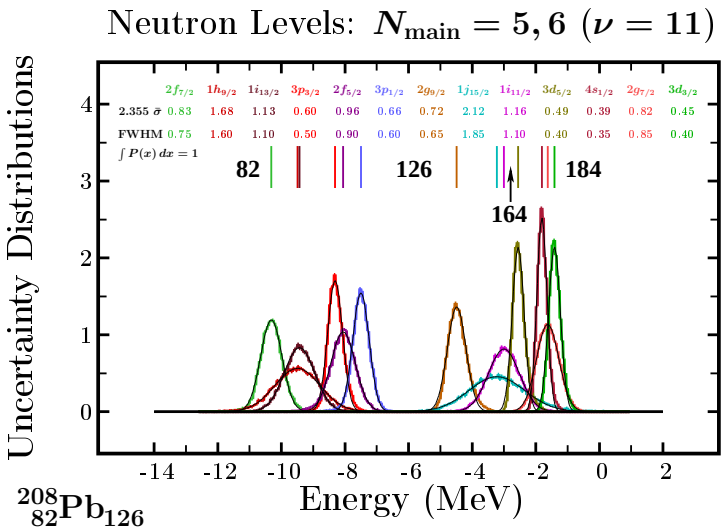

Fig. 6. Illustration similar to that in Fig. 4, but for the results obtained after parametric correlation removal. Observe that the histograms are systematically narrower as compared to the previous case, what indicates a systematic *decrease* in terms of the uncertainties associated with the probability distributions. Moreover, the two rows of numbers in the upper part of the figure give very similar estimates what signifies that the structure of the histograms has been markedly 'purified' in the sense that they represent to a good approximation the Gaussian structures, in the present case.

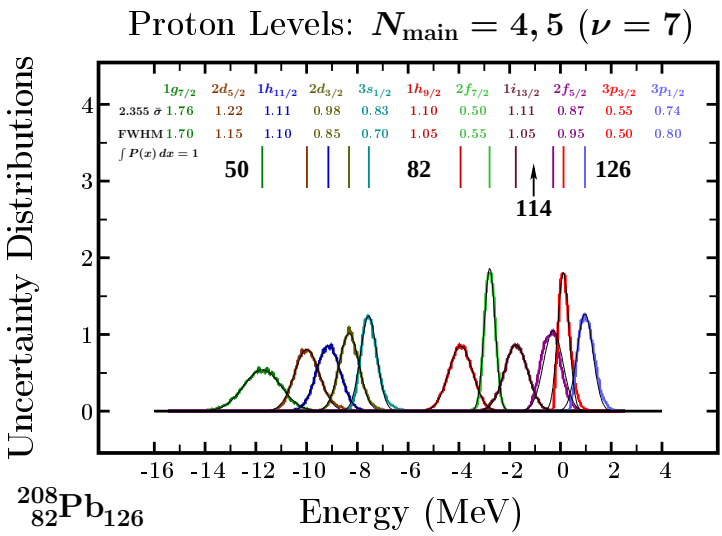

Fig. 7. Illustration similar to the one in Fig. 6 but for the protons.

The histograms have been compared and analysed using two approaches presupposing the *a priori* Gaussian nature of the discussed distributions. In the first case, we directly fit the Monte Carlo generated histograms using the two-parameter Gaussian form in order to obtain the expected energy positions $\bar{e}_{n\ell j}$ and the corresponding $\bar{\sigma}_{n\ell j}$-values. In the second case, we define the expected value of the energy position of the given level $\bar{e}_{n\ell j}$ with the help of the expressions of the form of

$$\bar{e}_{n\ell j} = \frac{1}{\mathcal{N}^{\rm trial}} \sum_{i=1}^{\mathcal{N}^{\rm trial}} [e_{n\ell j}]_i \,, \tag{22}$$

whereas the corresponding estimate of the $\bar{\sigma}_{n\ell j}$ is defined by

$$\bar{\sigma}_{n\ell j} = \left\{ \frac{1}{\mathcal{N}^{\rm trial}} \sum_{i=1}^{\mathcal{N}^{\rm trial}} \left[(e_{n\ell j})_i - \bar{e}_{n\ell j} \right]^2 \right\}^{1/2} . \tag{23}$$

For the ideal Gaussian distributions and the very large numbers of trials, the two ways of evaluation should give the same results. However, in the case of perturbed-Gaussian form of the histograms, differences are to be expected. The first rows in the figures marked with '$2.335\,\bar{\sigma}$' give the results obtained using Eq. (23), whereas the second ones give the results of the direct fitting.

The results in figures 4 and 5 were obtained before the parametric correlation removal. They indicate that the widths of the distributions estimated using the two approaches may differ considerably. This can be qualified as representing certain 'contamination' of the Gaussian structure of the corresponding histograms.

Comparison of the results in figures 4 and 6, *i.e.*, before and after the parametric correlation removal (here: for the neutrons) indicates the presence of a couple of characteristic tendencies. Firstly, the corresponding widths are systematically narrower after the parameter correlation removal. Secondly, the width estimates for the single-particle level uncertainties obtained with the help of two algorithms introduced above lie systematically closer to each other after the parameter removal signifying a 'cleaner' Gaussian form of the considered distributions.

The results for the protons are similar to the ones for the neutrons as can be seen from comparison of figures 5 and 7.

5. Summary and conclusions

We have presented examples of an analysis of the adjustment of the phenomenological mean-field Hamiltonian parameters focussing on the determination of the parametric correlations by using the Monte Carlo approach

and examining their consequences for the predictive power of the modelling. The main purpose of this article is to present and illustrate our realisation of the *mathematical and numerical applications of the Monte Carlo methods* in the regularisation of the ill-posed inverse problems which, to our knowledge, is the first attempt of this kind in the nuclear mean-field context. For the purpose of this illustration, we have used a simple but realistic Woods–Saxon Hamiltonian applied to the analysis of single-nucleon levels in the doubly magic ^{208}Pb nucleus.

We have focussed on the *a priori* known parametric correlations of the Woods–Saxon type between the central-potential radius and central-potential depth parameters, r^{cent} and V^{cent}, respectively, and profited from the fact that the third, the diffusivity parameter a^{cent} is not correlated with the others. This offers a 'scholarly' test ground for this type of considerations. We have eliminated the resulting parabolic dependence $r^{\mathrm{cent}} = r^{\mathrm{cent}}(V^{\mathrm{cent}})$ by reducing the number of fitting parameters from 6 [*cf.* Eqs. (17)–(18)] to 5. Next, we have used as the testing-tool the histograms characterising the uncertainties of the predicted positions of the single particle levels and compared their widths obtained using the Monte Carlo simulations before and after the removal of the parametric correlations. Our preliminary tests indicate that the removal of the parametric correlations leads to narrowing the uncertainty probability distributions thus suggesting an improvement in terms of predictive power.

The generalisation to the more realistic situations involving simultaneously more parameters and other forms of the Hamiltonian is in progress and will be published elsewhere.

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