NUCLEAR MEAN-FIELD TECHNIQUES: ADEQUACY OF INTERACTIONS AND IMPLIED PREDICTIONS*

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In this article, we present strategic lines necessary in order to construct general nuclear mean-field Hamiltonians as allowed by symmetry principles, keeping in mind a possible increase of their predictive power.

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1. Posing the problem

One of the, so far, most successful approaches to the nuclear structure many-body problem has certainly been the nuclear mean-field theory. Often used realisations involved self-consistent methods like the Skyrme–Hartree–Fock theory. However, despite an impressive number of publications using these methods, very little is known about the predictive power of such theories, especially when it comes to performing calculations extended into regimes that lie outside of the areas used for the parameter fit (extraneous predictions). In fact, it can be shown that the mutual inter-dependence of certain parameters of the model, *cf.* Ref. [1] for illustrations, destabilises the implied theory predictions: Small changes in the input imply significant changes in the theory results — effectively destroying the predictive power. In the case of the mentioned Skyrme–Hartree–Fock Hamiltonian, this problem can be considered serious: There exist over 250 different parametrizations of the corresponding Hamiltonian, non-equivalent and occasionally, mutually contradicting *e.g.* terms attractive within one parameterization are repulsive within another, *cf.* Ref. [2]. The corresponding Hamiltonians generally lead to extraneous predictions which can hardly be considered compatible.

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Constructing quantum theories of the nuclear many-body problem and at the same time imposing the condition that the theory's extraneous predictions are stable, is generally a complex issue. It has to do with the notion of the inverse problem of *applied mathematics* which we recall briefly. Given theory $\mathcal{T}$ represented by an operator $\hat{\mathcal{O}}$ which allows to obtain the theory results[1] referred to as *data*, d^{th}, through action on parameter set p. When operating on parameters to obtain theory predictions, $\hat{\mathcal{O}}(p) = d^{\mathrm{th}}$ — we say that we solve the direct problem. However, to be able to perform such calculations, to start with we need to know the parameters what implies that at least once at the beginning we must solve the

$$\text{Inverse Problem}: \quad \hat{\mathcal{O}}^{-1}(d^{\mathrm{exp}}) = p\,, \tag{1}$$

where d^{exp} represents the set of all the experimental data. When theory parameters are correlated (as it is the case of the Skyrme–Hartree–Fock Hamiltonian), one can demonstrate rigorously that the inverse in the above relation does not exist — in which case the formalism does not provide any relation between the experimental data and parameters: The formalism simply cannot be parametrized.

However, the parameter finding algorithms in all cases of practical importance involve the χ^2 parameter-fitting rather than the formal analysis of the inverse problem with the misleading consequences: The χ^2 algorithm most of the time provides a very good fit to the experiment so that the *graph* of comparison between the theory and data "looks good". Since, however, in this case the inverse problem is ill-posed the so-obtained parameters may lie in the unphysical ranges and, moreover, the implied parameterization is unstable.

There exists no satisfactory remedy known today for the nuclear physics inverse problem discussed — however, perhaps surprisingly — the underlying mathematical formalism is rather well known. It involves the techniques of elimination of parametric inter-dependencies as well as the so-called regularisation techniques among which the method of Tikhonov and the so-called Singular Value Decomposition are about the best known. From what has been said it follows that the choice of the underlying Hamiltonian plays a crucial role: If one or more terms of physical significance are missing, the remaining terms will be parametrized incorrectly since the absence of certain components of the interaction (an ignorance) will be numerically compensated by over- (under-) evaluated parameter values. If that happens the predictive power is lost.

As a consequence, Hamiltonians underlying the constructed theory should contain all possible terms permitted by the fundamental symmetries which

[1] In some cases $\hat{\mathcal{O}}$ can be identified with the Hamiltonian of the system; sometimes it may involve other formalisms such as the theory of the electromagnetic transitions.

the considered interaction must obey. In other words: All the mean-field interaction components which are permitted by the fundamental symmetries must appear in the formalism at the very beginning. Their relative importance is to be determined *only* as the next step.

In order to construct the most general form of the nucleon–nucleon interaction as allowed by symmetry considerations, one may employ the so-called spin-tensor decomposition [3, 4]. Within this formalism, one constructs the following six tensors of rank $k = 0, 1, 2$ in spin-space

$$S_1^{(0)} = 1\,, \qquad S_2^{(0)} = \{\vec{\sigma}_1 \otimes \vec{\sigma}_2\}^{(0)}\,, \qquad S_3^{(1)} = \vec{\sigma}_1 + \vec{\sigma}_2\,, \quad (2)$$

$$S_4^{(2)} = \{\vec{\sigma}_1 \otimes \vec{\sigma}_2\}^{(2)}\,, \qquad S_5^{(1)} = \{\vec{\sigma}_1 \otimes \vec{\sigma}_2\}^{(1)}\,, \qquad S_6^{(1)} = \vec{\sigma}_1 - \vec{\sigma}_2\,, \quad (3)$$

where $\vec{\sigma}_1$ and $\vec{\sigma}_2$ represent the spins of the two nucleons, labelled "1" and "2", respectively. These spin tensors can, in turn, be coupled to tensors in the configuration space $X_\mu^{(k)}$ and $Y_\mu^{(k)}$ with the same rank k to form scalar interactions

$$V(1,2) = \sum_{\mu=1}^{6} \left(\left\{ X_\mu^{(k)} \otimes S_\mu^{(k)} \right\}^{(0)} P_{T=0} + \left\{ Y_\mu^{(k)} \otimes S_\mu^{(k)} \right\}^{(0)} P_{T=1} \right)\,, \quad (4)$$

$P_{T=0}$ and $P_{T=1}$ denoting isospin projectors. Expression (4) is the required form of the nucleon–nucleon interaction which will enter the mean-field description. Coupling of tensors with $k = 0$, $k = 1$ and $k = 2$ leads to the scalar, vector and tensor forces, respectively.

Of course, the form-factors of such an interaction cannot be derived from symmetry considerations, and have to be deduced by adjustment of some parameters to the appropriately chosen experimental data whose instrumental and systematic uncertainties are well under control. At this point, a number of important questions immediately arise. For example, is there any hierarchy in the importance of various contributions? How can one adequately determine their relative importance knowing that the adjusted parameters generally depend on the sampling (experimental data input)? Another fundamental issue is related to possible interrelations between parameters controlling different terms of the interaction. Are some parameters related to other ones? If yes, how can one overcome, totally or at least partially, this difficulty, since this would lead to instabilities of the theoretical calculations and eventually to the impossibility of extraneous predictions?

Surprisingly, such issues belong to the everyday research program in many domains of science, but have been seldom posed in subatomic physics. As an example of typical parametric correlations, imagine a phenomenological mean-field Hamiltonian including a central and a spin-orbit field. If a contribution due to a nucleon–nucleon tensor-force is added (symmetry

principles allow its presence) but if such a term is omitted for so-called simplicity, the form-factors of the central and spin-orbit terms with parameters fitted to experiment will partially 'compensate' for this absence. The consequence of such a procedure would be (at least partially) a loss of physical adequacy of such interactions. [Note in passing that it is well known that both the nucleon–nucleon tensor and spin-orbit interactions give raise to contributions of the spin-orbit splitting in nuclei.]

Among many advantages of the mean-field approach, one can notice that, even if some terms in the spin-tensor decomposition are *sensu stricto* forbidden by symmetry considerations for the nucleon–nucleon interactions, they may be incorporated, however, in effective one-body formalisms. This is the case for instance for the so-called anti-symmetric spin-orbit interaction that may be constructed out of the terms $S_5^{(1)} = \{\vec{\sigma}_1 \otimes \vec{\sigma}_2\}^{(1)}$ and $S_6^{(1)} = \vec{\sigma}_1 - \vec{\sigma}_2$, in contrast to $S_3^{(1)} = \vec{\sigma}_1 + \vec{\sigma}_2$ which is at the origin of the standard spin-orbit potential.

2. Summary

In this article, we emphasise the fundamental problem of the predictive power of theories in the domain of nuclear structure calculations. The accent has been put on the concept of the nuclear mean-field, whose components should, as a matter of principle, stem from the more fundamental nucleon–nucleon interaction. The structural form of the latter interaction is governed by symmetry principles, and this can be achieved in a systematic way by using the spin-tensor decomposition technique. However, the form factors entering the various terms have to be parametrized in some phenomenological way, rendering unavoidable the introduction of some parameter sets. New questions arise at this stage, as possible hierarchization of different contributions as well as possible interrelations between the parameters. This, in turn, leads to the necessity of controlling the predictive power of the theory by analysing the parametric correlations and possibly finding some ways to remedy this difficulty via regularisation techniques.

The loss of predictive power in any mathematical modelling is related to the fact that the associated inverse problem (*cf. e.g.* Ref. [5]) is ill-posed. The ill-posedeness is a very common phenomenon in many scientific domains in which the inverse problem theory is applied, *cf.* Sect. 6 in Ref. [1], however very importantly, in particular also in the case of Skyrme–Hartree–Fock calculations in nuclear structure physics, *cf. e.g.* Fig. 7 in the same reference. This ill-posedeness is a direct result of the fact that the parameters of the Hamiltonian used turn out to be correlated. [There exist certain well known regularization procedures which can be applied to diminish the implications of the parametric correlations, those former ones, however, have generally

not been applied so far, at least in most of the sub-atomic physics studies.] It turns out that the actual nuclear mean-field Hamiltonians suffer from parametric correlations — thus from ill-posedeness — and consequently the instability of the extraneous predictions (for the distinction between intraneous and extraneous predictions *cf.* Ref. [1]).

In the case of the nuclear mean field applications, the situation, already grave because of the ill-posedeness due to the parametric correlations, can even be made worse(!) by adjusting the parameters to the observables which these Hamiltonians are not constructed to reproduce. For instance: by adjusting the parameters of the mean-field Hamiltonians, the latter representing merely the mean-field degrees of freedom such as single particle energies, to the nuclear masses, the latter sensitive to the nucleon–nucleon interactions, which are absent in the mean-field approximation, we deliberately falsify the fit (sometimes referred to as 'wrong fitting') by forcing the parameters of the mean field to describe partly the effects of the 2-body correlations — absent in these Hamiltonians.

In the situation of ill-posedeness, and thus with the issue of theory's predictive power resting on the 'shaky' grounds, there are some observables on which the damaging impact may be less important than on the others. For instance, it seems quite reasonable to expect that predictions based on single-particle properties used for the parametric fits as well as for the observables directly related to those of the single particle properties should suffer less severely from the lack of predictive power than other quantities. As an example, giant resonances essentially imply particle-hole excitations related to the single-particle degrees of freedom, and may, therefore, benefit from better extrapolations properties in such a case.

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