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Improving the Predictive Power of Nuclear Mean Fields from Two-Body Interactions

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Abstract. The number of parameters entering the nuclear mean field description, and possible correlations among those parameters, has become a very important issue in the treatment of the nuclear many-body problem. We would like to illustrate on the example of the spin-orbit interaction how a mean field can be constructed out of the two-body interaction, and give some illustrations leading to a better understanding of how such a construction can be handled.

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1 Introduction

The mean-field approach, both in its self-consistent and non self-consistent versions, has proven to be one of the most powerful tools to study the nuclear many-body problem. Starting from the fundamental nucleon-nucleon interaction, one should in principle be able to construct nuclear mean-fields, taking into account basic symmetry considerations to restrict the form of the allowed terms. A natural framework to achieve such a program is provided by the spin-tensor decomposition [1, 2]. However, such methods cannot provide the full contents of the mean-field, and one still has to parametrize in some way the form factors governing the various terms. One is then usually confronted with the questions of which terms are possibly more important, how many parameters should appear, and how these parameters may be correlated [3].

Spin-orbit and tensor forces are examples of interactions that have received much attention in the past, and several approaches have been proposed, as for example the Hartree-Fock self-consistent technique [4, 5].

In this article we would like to focus on the parametrization of the spin-orbit interaction within the framework of the nuclear self-consistent mean-field, for spherical systems preserving time-reversal symmetry. At this limit, many possible terms appearing a priori vanish as the result of symmetry considerations, thus simplifying considerably the underlying mechanisms. After giving the structure of the general terms with the help of various densities, we analyze further their properties with respect to more standard approaches like the historical parametrisations used in the past, as the one proposed very early by Blin-Stoyle [6], or more recent realizations [7], in the case the system preserves time-reversal and spherical symmetry.

2 Hartree-Fock Formulation for the Spin-Orbit Interaction

In the following, we will consider a two-body nucleon-nucleon spin-orbit interaction given by

$$\hat{V}^{SO} = V(\|\vec{r} - \vec{r}\,'\|)\,(\vec{r} - \vec{r}\,') \wedge (\vec{p} - \vec{p}\,') \cdot (\vec{\sigma} + \vec{\sigma}\,')\;, \tag{1}$$

where $V(\|\vec{r} - \vec{r}\,'\|)$ denotes a distance-dependent form factor of the interaction between two nucleons located at positions $\vec{r}$ and $\vec{r}\,'$, possessing momenta $\vec{p}$ and $\vec{p}\,'$, and spins $\vec{\sigma}$ and $\vec{\sigma}\,'$ (here expressed in terms of Pauli operators).

Expanding expression (1), we obtain a sum of eight terms :

$$\begin{aligned}
\hat{V}^{SO} = &\;\; V(\|\vec{r} - \vec{r}'\|)\,(\vec{r} \wedge \vec{p}\,) \cdot \vec{\sigma} && \to T_1 \\
- &\;\; V(\|\vec{r} - \vec{r}'\|)\,(\vec{r}' \wedge \vec{p}\,) \cdot \vec{\sigma} && \to T_2 \\
- &\;\; V(\|\vec{r} - \vec{r}'\|)\,(\vec{r} \wedge \vec{p}') \cdot \vec{\sigma} && \to T_3 \\
+ &\;\; V(\|\vec{r} - \vec{r}'\|)\,(\vec{r}' \wedge \vec{p}') \cdot \vec{\sigma} && \to T_4 \\
+ &\;\; V(\|\vec{r} - \vec{r}'\|)\,(\vec{r} \wedge \vec{p}\,) \cdot \vec{\sigma}\,' && \to T_5 \\
- &\;\; V(\|\vec{r} - \vec{r}'\|)\,(\vec{r}' \wedge \vec{p}\,) \cdot \vec{\sigma}\,' && \to T_6 \\
- &\;\; V(\|\vec{r} - \vec{r}'\|)\,(\vec{r} \wedge \vec{p}') \cdot \vec{\sigma}\,' && \to T_7 \\
+ &\;\; V(\|\vec{r} - \vec{r}'\|)\,(\vec{r}' \wedge \vec{p}') \cdot \vec{\sigma}\,'. && \to T_8
\end{aligned} \tag{2}$$

The contributions of these eight terms, further one denoted $T_1, \ldots, T_8$, to the Hartree-Fock potential can be evaluated separately.

Let us recall here that the Hartree-Fock equations for a system of nucleons described by the single-particle wave functions $\phi_i(q)$, q denoting the coordinates of the particles, read

$$-\frac{\hbar^2}{2m}\Delta\phi_i(q) + U_H\;\phi_i(q) - \int U_F\;\phi_i(q')\,dq' = \varepsilon_i\phi_i(q), \tag{3}$$

where U_H represents the Hartree potential, and U_F the non-local exchange (Fock) term. In the following considerations we will essentially focus on the expression of the Hartree contributions $\hat{U}^{SO}_{H,T_1}, \ldots, \hat{U}^{SO}_{H,T_8}$ of the terms $T_1, \ldots, T_8$, leaving the effect of the exchange terms for further communications.

Following Engel et al. [8], we will denote the particle density by $\rho(\vec{r})$, the current density by $\vec{\jmath}(\vec{r})$, the spin density by $\vec{s}(\vec{r})$ and the vector spin current density by $\vec{J}(\vec{r})$.

Denoting by $\vec{\ell}$ the orbital angular momentum, defined as $\vec{\ell}=\vec{r}\wedge\vec{p}$, one obtains

$$\hat{U}^{SO}_{H,T_1} = \Big[\int d^3\vec{r}\,'V(\|\vec{r}-\vec{r}\,'\|)\rho(\vec{r}\,')\Big]\,\vec{\ell}\cdot\vec{\sigma}, \tag{4}$$

$$U^{SO}_{H,T_2} = \left[-\int d^3\vec{r}\,'V(\|\vec{r}-\vec{r}\,'\|)\,\rho(\vec{r}\,')\,\vec{r}\,'\right]\wedge\vec{p}\cdot\vec{\sigma}, \tag{5}$$

$$\hat{U}^{SO}_{H,T_3} = \left\{\frac{\hbar}{i}\int d^3\vec{r}\,'V(\|\vec{r}-\vec{r}\,'\|)\left[\tfrac{1}{2}\vec{\nabla}'\rho(\vec{r}\,')+i\vec{\jmath}(\vec{r}\,')\right]\right\}\cdot(\vec{r}\wedge\vec{\sigma}), \tag{6}$$

$$U^{SO}_{H,T_4} = \frac{\hbar}{i}\left\{\int d^3\vec{r}\,'V(\|\vec{r}-\vec{r}\,'\|)\,\vec{r}\,'\wedge\left[\frac{1}{2}\vec{\nabla}\,'\rho(\vec{r}\,')+i\vec{\jmath}(\vec{r}\,')\right]\right\}\cdot\vec{\sigma}, \tag{7}$$

$$\hat{U}^{SO}_{H,T_5} = \Big[\int d^3\vec{r}\,'V(\|\vec{r}-\vec{r}\,'\|)\,\vec{s}(\vec{r}\,')\Big]\cdot\vec{\ell}, \tag{8}$$

$$\hat{U}^{SO}_{H,T_6} = \left[\int d^3\vec{r}\,'V(\|\vec{r}-\vec{r}\,'\|)\,\vec{r}\,'\wedge\vec{s}(\vec{r}\,')\right]\cdot\vec{p}, \tag{9}$$

$$\hat{U}^{SO}_{H,T_7} = -\left\{\int d^3\vec{r}\,'V(\|\vec{r}-\vec{r}\,'\|)\left[\hbar\vec{J}(\vec{r}\,')+\frac{1}{2}\vec{p}\,'\wedge\vec{s}(\vec{r}\,')\right]\right\}\cdot\vec{r}, \tag{10}$$

$$\hat{U}^{SO}_{H,T_8} = \int d^3\vec{r}\,'V(\|\vec{r}-\vec{r}\,'\|)\,\vec{r}\,'\cdot\left\{\hbar\,\vec{J}(\vec{r}\,')+\frac{1}{2}\big[\vec{p}\,'\wedge\vec{s}(\vec{r}\,')\big]\right\}. \tag{11}$$

In the following, we will suppose that the system under investigation preserves spherical symmetry as well as time-reversal invariance. It is easily shown that in this case the only non-vanishing contributions to the Hartree potential will originate from the terms T_1, T_2, T_7 and T_8. Grouping terms T_1 and T_2 leads to the following expression [6]

$$\hat{U}^{SO}_{H,T_1}+\hat{U}^{SO}_{H,T_2} = \left[\int d^3\vec{r}\,'V(\|\vec{r}-\vec{r}\,'\|)\rho(r')\Big(1-\frac{\vec{r}\,'\cdot\vec{r}}{r^2}\Big)\right]\vec{\ell}\cdot\vec{\sigma} \tag{12}$$

thus generating a single particle spin-orbit potential for the Hartree mean-field. We will denote by $F(r)$ the corresponding form factor that will be further on discussed

$$F(r) = \int d^3\vec{r}\,'V(\|\vec{r}-\vec{r}\,'\|)\rho(r')\Big(1-\frac{\vec{r}\,'\cdot\vec{r}}{r^2}\Big). \tag{13}$$

In the same way, terms T_7 and T_8 can be grouped into

$$\hat{U}^{SO}_{H,T7}+\hat{U}^{SO}_{H,T8} = \hbar\int d^3\vec{r}\,'V(\|\vec{r}-\vec{r}\,'\|)\vec{J}(\vec{r}\,')\cdot(\vec{r}\,'-\vec{r}). \tag{14}$$

The terms T_7 and T_8 lead to a different structure than the mean-field spin-orbit contributions of T_1 and T_2, and they will not be analyzed further in this communication.

3 Discussion of the One-Body Hartree Spin-Orbit Potential

A very popular approach to handle the form factor given in expression (13) has been suggested long time ago by Blin-Stoyle [6]. In this reference the form factor $F(r)$ is expressed as

$$F(r) = -\int d^3\vec{r}\,'V(\|\vec{r}-\vec{r}\,'\|)\rho(\vec{r},\vec{r}\,'). \tag{15}$$

Writing $\rho(\vec{r},\vec{r}\,') = \rho'(\vec{s},\vec{r})$ with $\vec{s}=\vec{r}\,'-\vec{r}$, and performing a Taylor expansion of $\rho'(\vec{s},\vec{r})$ about $\vec{s}=0$ one obtains, with the help of the mean particle density in closed shell orbitals $\rho_{nl}(r)$:

$$F_{\rm BS}(r) = K\frac{1}{r}\frac{d\rho(r)}{dr}, \tag{16}$$

where

$$K = -\frac{4\pi}{3}\int_0^{+\infty} V(s)s^4 ds. \tag{17}$$

In the above expression of $F_{\rm BS}(r)$ the subscripts “BS" have been introduced to make reference to the Blin-Stoyle calculations.

In order to investigate the validity of the approximation used in the Blin-Stoyle approach, one can perform a comparison between the $F_{\rm BS}(r)$ form factor and the form factor calculated directly with the help of equation (13). To simplify the discussion, let us assume a Fermi shape for the nuclear density distribution, given by the following expression

$$\rho(r) = \rho_\circ\frac{1}{1+\exp[(r-R_\circ)/a]}. \tag{18}$$

We consider R$_\circ = r_\circ A^{1/3}$ with $r_\circ = 1.3$ fm, $\rho_\circ = A/[\frac{4}{3}\pi R_\circ^3]$ (A denoting the mass number of the considered nucleus), and $a = 0.7$ fm.

In our discussion, we will use an interaction given by

$$V(s) = C_{SO}\Big(e^{-\mu s}/\mu s\Big)^2. \tag{19}$$

This interaction, depending on the parameters $C_{SO} < 0$ and $\mu > 0$, has been chosen in order to reproduce two-pion exchange between the nucleons, as it is for example the case for phenomenological nucleon-nucleon forces such as the Hamada-Johnston potential. In this case the calculation of the factor K used in the Blin-Stoyle calculations can be given in analytical form, namely

$$K = -\frac{\pi}{3}\frac{C_{SO}}{\mu^5}, \tag{20}$$

and therefore one obtains, for the Blin-Stoyle form factor, in combination with the Fermi-shape density distribution,

$$F_{\rm BS}(r) = -\frac{\pi}{3}\frac{C_{SO}}{\mu^5}\Big[-\frac{1}{a\rho_\circ}\rho^2(r)\exp[(r-R_\circ)/a]\Big]. \qquad (21)$$

It is interesting to notice that, as it is done for instance in ref. [7], one sometimes uses for K, given in expression (17), a simple constant. The introduction of a realistic Fermi shape for the density, as it is used here, gives a strong support to such a simple estimate for K, as well as an elegant physical interpretation in terms of the two-body spin-orbit coupling constant C_{SO} and parameter μ.

In order to get simple estimates of the parameters of the spin-orbit interaction, and for further possible comparisons between various approaches, it will be of advantage to recall the structure of the spin-orbit mean field used in Woods-Saxon calculations [9]:

$$V_{\rm SO,WS} = F_{\rm WS}(r)\; \vec{\ell}\cdot\vec{\sigma}, \qquad (22)$$

where

$$F_{\rm WS}(r) = \lambda_{SO}\Big[\frac{\hbar}{2mc}\Big]^2\frac{1}{r}\frac{d}{dr}\Big[\frac{-V_\circ}{1+\exp[(r-R_{\rm SO})/a_{\rm SO}]}\Big], \qquad (23)$$

with

$$V_\circ = V\Big[1 \pm \kappa\Big(\frac{N-Z}{N+Z}\Big)\Big] \qquad (24)$$

the sign “$+$" being used for protons, and “$-$" for neutrons. The nucleon mass is denoted by m.

4 Determination of the Parameters of the Spin-Orbit Interaction

As a first approximation we take $\mu = (m_\pi c^2)/(\hbar c)$, the inverse of the Compton wavelength of the pion, as given by the numerical value $\mu = 1/1.4$ fm^{-1}. Once the value of μ is fixed, a simple estimate of the spin-orbit interaction strength parameter C_{SO} can be obtained in the following way: one calculates the Woods-Saxon form factor of eq.(23) at $r = R_{\rm SO}$, which is identified with the form factor $F(r)$ of eq.(13), providing a value for C_{SO}.

In Figure 1 we have plotted, for protons in the nucleus ^{208}Pb, the Woods-Saxon spin-orbit form factor $F_{\rm WS}(r)$ of eq.(23) using the so-called “universal" parametrization, the Blin-Stoyle form factor $F_{\rm BS}(r)$ of eq.(21), and the form factor $F(r)$ of eq.(13). For the latter two cases, the parameters μ and C_{SO} are taken to be identical. They have been obtained by imposing $\mu = 1/1.4$ fm^{-1} and adjusting C_{SO} for $F(r)$ to reproduce the Woods-Saxon potential at $r = R_{\rm SO}$ as explained above. The so obtained value is $C_{SO} = -53.4$ MeV. As seen in the

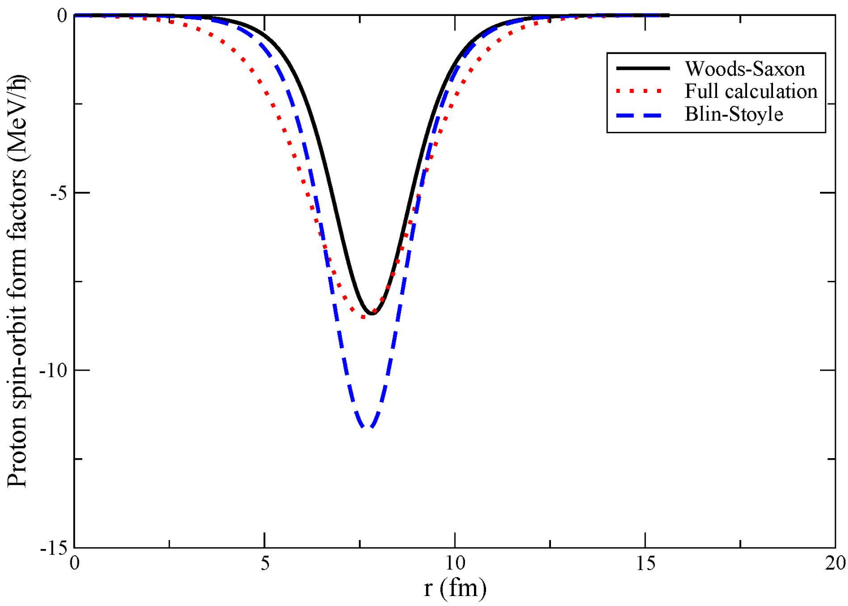

Figure 1. (Color online) Proton spin-orbit form factors plotted in function of r. Full line "Woods-Saxon" refers to (23), dotted line "Full calculations" to (13) and dashed line "Blin-Stoyle" to (21). Spin-orbit interaction parameters are $\mu = 1/1.4$ fm^{-1} and $C_{SO} = -53.4$ MeV.

figure, the Blin-Stoyle approximation to $F(r)$ leads to a deeper potential well, which is, however, narrower.

So far, we have considered a certain value for the coefficient μ, equal to the inverse of the pion Compton wavelength, thus limiting the degrees of freedom to the constant C_{SO}. The question may be raised concerning the variation of the spin-orbit potential with respect to small variations in the parameter μ around this reference value. In order to investigate this point, we have kept fixed C_{SO} to the previously obtained value -53.4 MeV and varied somewhat the value of $\mu = \alpha\mu_\circ$ with $\mu_\circ = 1/1.4$ fm^{-1}. The results are shown in Figure 2 where $\alpha = 0.95$ and $\alpha = 1.05$. The figure indicates a rather strong dependence on the small variation of μ, giving some indication that in the present context this parameter, which has a clear physical meaning, should be considered with special attention.

In order to investigate the influence of small variations of the coefficient C_{SO} when μ is fixed, we have also calculated form factor $F(r)$ of eq.(13) with $C_{SO} = \alpha C_{SO,0}$, taking as a reference the value $C_{SO,0} = -53.4$ MeV. Results are shown in Figure 3. According to the obtained results, it seems that fluctuations of C_{SO} by the same relative amount as for μ have less impact on the shape

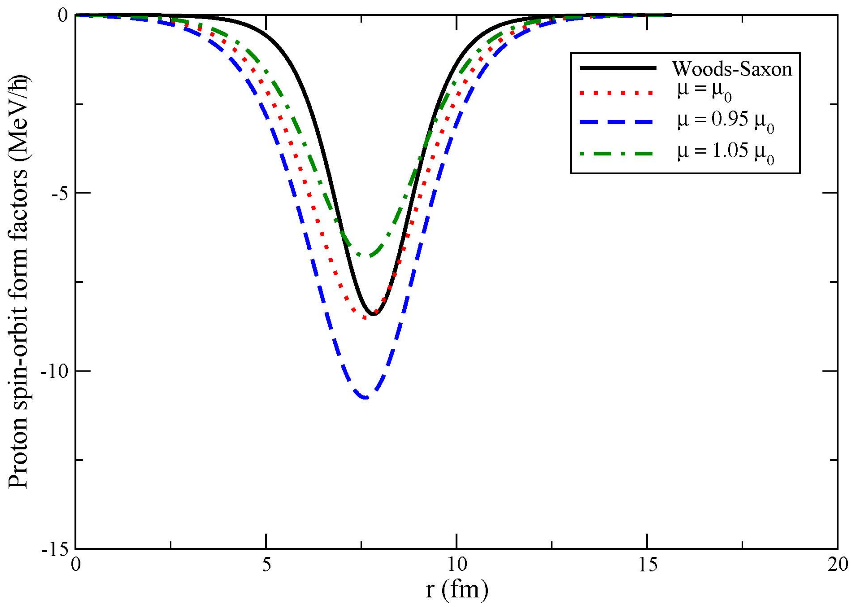

Figure 2. (Color online) Proton spin-orbit form factors plotted in function of r. Full line "Woods-Saxon" refers to (23), the other curves refer to $F(r)$ calculated for fixed $C_{SO} = -53.4$ MeV but different values of $\mu = \alpha\mu_\circ$, with $\mu_\circ = 1/1.4$ fm^{-1} and $\alpha = 0.95$ and 1.05.

and the depth of the single-particle spin-orbit potential, comforting us again with the choice of μ as probably the parameter that should be fixed with higher priority. This is also justified by a more clear physical significance of μ as it directly relates to pion properties.

5 Conclusions and Perspective

In this article we have made a brief comparison between different kinds of approaches used to evaluate the single-particle Hartree part of the spin-orbit interaction: the standard Woods-Saxon approach, the Blin-Stoyle approximation, and the "full calculation" evaluating $F(r)$ of eq.(13). Although results are similar in some aspects, the "full calculation" gives deeper insight into the origin of the mean field stemming directly from nucleon-nucleon interactions, thus being less phenomenological than the Woods-Saxon calculations. Also, the traditional Blin-Stoyle approach based on Taylor expansion does not seem to be justified anymore, since modern computer codes easily handle the full calculations numerically.

But the most important conclusion is that the number of free parameters can be

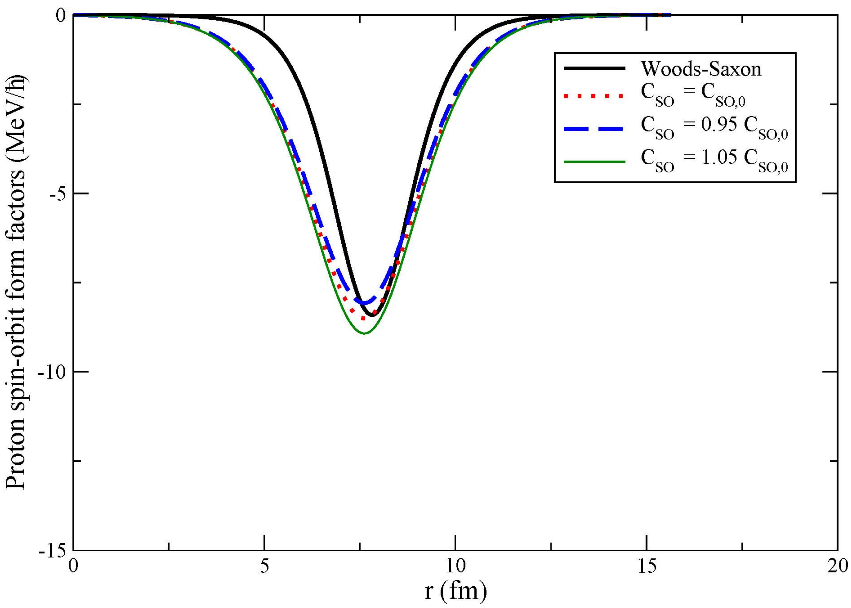

Figure 3. (Color online) Proton spin-orbit form factors plotted in function of r. Full line "Woods-Saxon" refers to (23), the other curves refer to $F(r)$ calculated for fixed $\mu_\circ = 1/1.4\ \text{fm}^{-1}$, but different values of C_{SO} with $C_{SO} = \alpha C_{SO,0}$, and $C_{SO,0} = -53.4$ MeV.

reduced, since for one species of particles, say protons or neutrons, the nucleon-nucleon potential, in our example, can be modeled with only two parameters, or even only one, if the inverse Compton wavelength of the exchanged pions is fixed to start with.

This conclusion is very important when it comes to the question of how to get better parametrizations of the nuclear mean field, by trying to find a way to reduce the number of free parameters of the theory.

Further investigations will take into account the exchange terms, and the inclusion of the isospin dependent spin-orbit interaction. The question of the reduction of the number of free parameters of the theory will get even more importance, especially with respect to the predictive power of the so obtained mean-field.

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