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Reliability of the pseudospin symmetry in atomic nuclei

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Abstract. The reliability of the pseudospin symmetry (PSS) in atomic nuclei is analyzed in the framework of the relativistic Hartree approach. We find that the nuclear surface strongly increases the effect of the pseudospin-orbit potential (PSOP), spoiling the possibility of the exact realization of the PSS even in the limit of a vanishing PSOP. It is also shown that the PSS cannot be explained by the fact that $\Sigma_S \simeq -\Sigma_0$. New arguments to explain the PSS in finite nuclei are given. The important role the spin-orbit interaction plays in the achievement of the PSS is also discussed.

PACS. 24.10.Jv Relativistic models – 21.60.Cs Shell model – 21.10.Pc Single-particle levels and strength functions – 24.80.+y Nuclear tests of fundamental interactions and symmetries

1 Introduction

In the recent years considerable attention has been paid in nuclear physics to the pseudospin symmetry (PSS) [1–16]. Each two single-particle states of a nucleus labelled by "a" and "b" with the quantum numbers n_a, l_a, $j_a = l_a + 1/2$ and $n_b = n_a - 1$, $l_b = l_a + 2$, $j_b = l_a + 3/2$, where n, l, and j are the radial, orbital and total angular-momentum quantum numbers, respectively, make a pseudospin doublet (PSD). If the PSS were exact, the two states a and b would be degenerate. Thus, in the pseudospin formalism, the same pseudo-orbital angular-momentum quantum number $\tilde{l} = \tilde{l}_a = \tilde{l}_b = l_a + 1 = l_b - 1$ is assigned to these two states. In a more general form $\tilde{l}$ is defined as $\tilde{l} = (2j - l)$.

Though the idea of the PSS appeared many years ago, only recently several authors have established that the PSS has its origin in the relativistic symmetry of the Dirac equation (see refs. [3–12], and references therein). Ginocchio realized that $\tilde{l}$ is identical to the relativistic quantum number l' of the small component $F(r)$ of the nucleon Dirac spinor and he attributed to this fact a key role in the PSS [4].

At present, the understanding of the PSS in the framework of the single-particle relativistic models[1] is based on the following hypotheses: 1) The nucleons inside the nucleus move in a scalar Σ_S and vector Σ_0 potentials which are almost equal in magnitude but have different signs, so that $\Sigma_S + \Sigma_0$ is small enough to consider the PSS slightly broken in nuclei [3–7]. 2) In the limit of small pseudospin-orbit potential (PSOP) the PSS becomes exact [8–11]. 3) The PSOP is small enough to justify the PSS [8–11].

The aim of this work is: A) To show that these three commonly accepted statements fail to describe PSS in finite nuclei because of the nuclear surface. B) To propose a new explanation of the PSS quite different from the one commonly accepted.

In sect. 2, we write the basic Dirac equation in the relativistic Hartree approximation (or relativistic mean-field approximation) [13–18], and discuss the interpretation of the PSS on the grounds of the equivalent Schrödinger-like equation for the small component of the Dirac spinor. In sect. 3, the nature of the PSS in finite nuclei is investigated. Firstly, we consider a mathematical extension of this latter equation and we apply it in sect. 3.1 to non-physical situations in order to study the properties of the bound-state solutions of a quite general hypothetical model satisfying two kinds of exact PSS. The role of the nuclear surface in the PSS is analyzed in detail. In sect. 3.2, new arguments to interpret the PSS are given.

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[1] Until now, the relativistic self-consistent models used to investigate the PSS have been restricted to the mean-field approximation, with the only exception of a work made by our group using the relativistic Hartee-Fock approximation [14]. We shall not refer here to this work, where the Fock terms bring important qualitative features to the PSS.

In sect. 3.3, the role of some terms breaking the PSS is discussed. In sect. 3.4, we analyze the relation between the spin-orbit and pseudospin-orbit schemes. In sect. 3.5, we give a number of arguments suggesting that the PSS cannot be justified by the smallness of $\Sigma_S + \Sigma_0$. Finally, our conclusions are drawn in sect. 4.

2 The Dirac equation and the pseudospin symmetry

The simplest relativistic Lagrangians allowing a qualitative description of the fundamental nuclear properties include the exchange of σ, ω and ρ mesons between nucleons. The corresponding Dirac equation for the single-particle spinors in the relativistic Hartree approximation yields the following equations:

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}r}G(r) &= -T\,G(r) + W\,F(r),\\ \frac{\mathrm{d}}{\mathrm{d}r}F(r) &= V\,G(r) + T\,F(r),\end{aligned} \tag{1}$$

where (G/r) and (F/r) represent the radial part of the upper (big) and lower (small) components of the nucleon Dirac spinor, respectively.

We have introduced the following notations:

$$\begin{aligned}T &\equiv \frac{\kappa}{r} + \Sigma_T, \qquad V \equiv \Sigma_S + \Sigma_0 - \epsilon,\\ W &\equiv 2M + \epsilon + \Sigma_S - \Sigma_0,\end{aligned} \tag{2}$$

where $\kappa \equiv (2j+1)(l-j)$ and $\epsilon = E - M$ is the single-particle energy (SPE) of a nucleon with bare mass M and relativistic energy E. The quantities Σ_S, Σ_0, and Σ_T are the scalar, vector, and tensor components of the nucleon self-energy, respectively. We shall neglect the small component Σ_T hereafter.

From the Dirac equation (1), one can get the following second-order differential equation for the small component $F(r)$ of the nucleon Dirac spinor:

$$\begin{aligned}\mathcal{F}_\kappa[F] \equiv \frac{1}{2M}\Bigg\{ &- F'' + \Bigg[\frac{V'}{V}\left(\frac{F'}{F} - \frac{\kappa}{r}\right) + \frac{\tilde{l}(\tilde{l}+1)}{r^2}\\ &+2M(\Sigma_S+\Sigma_0) + 2\epsilon\Sigma_0 + (\Sigma_S^2-\Sigma_0^2) - \epsilon^2\Bigg]F\Bigg\} - \epsilon F = 0\,.\end{aligned} \tag{3}$$

This equation has the structure of a Schrödinger-like equation with a pseudo-centrifugal term $\left[\hat{V}_{\mathrm{cf}} \equiv \frac{\tilde{l}(\tilde{l}+1)}{r^2}\right]$ and a potential which includes terms strongly energy dependent $(2\epsilon\Sigma_0, \epsilon^2)$ and state dependent $\left[\frac{V'}{V}\left(\frac{F'}{F} - \frac{\kappa}{r}\right)\right]$. Since for the two states a and b of a PSD we have $\kappa_a \neq \kappa_b$, the *κ-term* $[\hat{V}_\kappa \equiv -V'/V \times \kappa/r]$ appearing in eq. (3) breaks the PSS. However, in practice, the PSS can be considered as an approximate symmetry if $|\epsilon_a - \epsilon_b|_{(\tilde{l}_a=\tilde{l}_b)} \ll |\epsilon_c - \epsilon_d|_{(\tilde{l}_c\neq\tilde{l}_d)}$. Thus, it has been frequently argued that the PSS would be expected if the inequality $|\hat{V}_\kappa| \ll \hat{V}_{\mathrm{cf}}$ is satisfied [8–11]. In these references, this condition is considered to be valid because $|V'| = |\Sigma_S' + \Sigma_0'|$ is quite small in nuclei. However, the inequality is not satisfied in the nuclear surface because $V(r_0) = 0$ and $\hat{V}_\kappa$ is singular at $r = r_0$, having opposite signs for $r < r_0$ and $r > r_0$. Actually, for $r \to r_0$, $V'/V \sim (r - r_0)^{-1}$, and although the concrete value of r_0 depends on V, the structure of V'/V around r_0 does not. Thus, for $r \to r_0$ $\hat{V}_\kappa$ has always the functional form $\kappa/(r - r_0)r$, independent of V!. The contribution $\langle F|\hat{V}_\kappa|F\rangle$ to the SPE (we assume $\langle F|F\rangle = 1$), which we shall call the perturbative contribution of $\hat{V}_\kappa$, is a finite quantity, obtained as a result of the quasi-cancellation of two infinite quantities around r_0. However, we have found that, because of the singularity, the self-consistency effects of the κ term are very important though $\langle F|\hat{V}_\kappa|F\rangle$ can be quite small in comparison with the contribution of the pseudo-centrifugal term $\langle F|\hat{V}_{cf}|F\rangle$ [13,14].

3 Nature of the pseudospin symmetry

The Dirac equation (1) and eq. (3) for the small component F of the single-particle spinor have physical meaning only for integer values of κ. However, in order to understand the influence of the κ term on the F function, we shall consider hereafter eq. (3) just as a mathematical differential equation in which the parameter κ appearing in the κ term becomes a *real number* denoted by $\bar{\kappa}$. However, we do not modify the definition of $\tilde{l}$. In other words, we maintain the relation $\tilde{l}(\tilde{l}+1) = \kappa(\kappa-1)$, κ being the integer quantum number appearing in the Dirac equation (1). The generalized equation for F reads

$$\begin{aligned}\mathcal{F}_{\bar{\kappa}}[F] \equiv \frac{1}{2M}\Bigg\{ &- F'' + \Bigg[\frac{V'}{V}\left(\frac{F'}{F} - \frac{\bar{\kappa}}{r}\right) + \frac{\tilde{l}(\tilde{l}+1)}{r^2}\\ &+2M(\Sigma_S+\Sigma_0) + 2\epsilon\Sigma_0 + (\Sigma_S^2-\Sigma_0^2) - \epsilon^2\Bigg]F\Bigg\} - \epsilon F = 0\,.\end{aligned} \tag{4}$$

We can construct a Dirac equation, formally equivalent to eq. (4), by replacing the nucleon mass M entering W in eq. (2) by the quantity $\bar{M}(r)$ defined as

$$\bar{M}(r) \equiv M + \frac{V'}{2V^2}\frac{\kappa - \bar{\kappa}}{r}\,. \tag{5}$$

The generalized Dirac equation reads

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}r}G(r) &= -T\,G(r) + [2\bar{M} + \epsilon + \Sigma_S - \Sigma_0]\,F(r),\\ \frac{\mathrm{d}}{\mathrm{d}r}F(r) &= V\,G(r) + T\,F(r)\,.\end{aligned} \tag{6}$$

Thus, in this equation, the nucleon moves under the influence of an additional effective potential transforming its free-nucleon mass M to the effective mass $\bar{M}(r)$.

The case of exact PSS obtained in the limit $\Sigma_S + \Sigma_0 = 0$ has been checked by Ginocchio in refs. [3]

and [4]. He found, in this case, that not only the two states of a pseudospin doublet (PSD) are degenerate but, furthermore, their F functions are equal up to a phase (hereafter, we shall denote this particular form of symmetry as PSS*, whereas we keep the PSS notation for the case in which only the degeneracy of the two pseudospin partners is required). Ginocchio also claimed that, although the limit $\Sigma_S + \Sigma_0 = 0$ is not realistic for atomic nuclei, $\Sigma_S + \Sigma_0$ is small enough to explain the approximate degeneracy found for the states of some pseudospin doublets and the similarity of their corresponding F_a and F_b components [4].

3.1 Role of the nuclear surface

3.1.1 The nuclear surface prohibits the PSS*

It would be interesting to investigate whether the conclusions obtained by Ginocchio for the states of a pseudospin doublet (PSD) in the extremely simplified model mentioned above with $\Sigma_S + \Sigma_0 = 0$ are, in fact, exclusive among models generating unbound nuclei or they can be also compatible with some more realistic models allowing bound states. Thus, in this section, we shall try to determine whether the PSS* can be also realized in some of these latter models.

In order to find such models, we can consider hypothetical conditions under which the PSS* is supposed to be exact. One possibility is to take the same value of $\bar{\kappa}$ ($\bar{\kappa} = 0$, for instance) for the two states a and b of a PSD, so that F_a and F_b satisfy the same equation (4). Then, we assume that these two states are degenerate ($\epsilon_a = \epsilon_b$) and they can be represented by the same F wave function. The hypothetical nuclear model fulfilling these conditions also should satisfy the Dirac equation (6) with $\bar{\kappa} = 0$. The big component (G) of the Dirac spinor for the two states a and b can be obtained by substituting F in the second line of eq. (6) and taking for the κ parameter the value corresponding to the state we are dealing with (*i.e.*, $\kappa = \kappa_a$ for the a state or $\kappa = \kappa_b$ for the b state). Hereafter, we shall write the G function with the subscript κ to indicate the state a (with $\kappa = \kappa_a$) or b (with $\kappa = \kappa_b$) of the PSD:

$$G_\kappa(r) = \frac{1}{V}\left[\frac{\mathrm{d}}{\mathrm{d}r}F(r) - \frac{\kappa}{r}F(r)\right]. \tag{7}$$

It is worth recalling that V becomes zero at $r = r_0$ (as we are considering $\epsilon_a = \epsilon_b$, r_0 is the same for the two states a and b). Thus, in order to have the G_κ component finite at $r = r_0$, the factor in the brackets in eq. (7) must be zero at r_0. However, $\kappa_a \neq \kappa_b$ (notice that κ_a and κ_b correspond to the physical states and are independent of the parameter $\bar{\kappa}$ entering eq. (4)). Consequently, if the quantity in the brackets in eq. (7) becomes zero at r_0 for the a state it cannot become zero at the same point r_0 for the b state (which, by hypothesis, shares with the state a the same function $F(r)$), except for the *extreme* case in which $F'(r_0) = F(r_0) = 0$. These conditions for $F(r)$ would imply, at least, that $F(r)$ obtained from eq. (4) for $\bar{\kappa} = 0$ would drastically differ from the physical F_a and F_b functions obtained from the same equation with $\bar{\kappa} = \kappa_a$ and $\bar{\kappa} = \kappa_b$, respectively (with exponentially decreasing asymptotic behaviour), showing the strong effect of the $\bar{\kappa}$ term in eq. (4) (or the κ term in eq. (3)) on the $F(r)$ function.

For the exact PSS* we are supposing, the *normal* case ($F(r_0) \neq 0$ and $F'(r_0) \neq 0$) would imply, due to the singularity of the V^{-1} factor in eq. (7), that G_a or G_b were divergent at $r = r_0$ (actually, $G_k(r) \to +\infty(-\infty)$ as $r \to r_0^-$ and $G_k(r) \to -\infty(+\infty)$ as $r \to r_0^+$ for $\kappa = \kappa_a$ or $\kappa = \kappa_b$)[2]. Thus, for the case of exact PSS* and *normal* $F(r)$ function, the singularity of the V^{-1} factor at the nuclear surface does not allow to have two physical solutions for the G_κ functions corresponding to the two states of a PSD. In other words, the nuclear surface prevents, in contrast to the commonly accepted point of view, the possibility of the realization of the exact PSS* in finite nuclei, even in the hypothetical limit $\bar{\kappa} = 0$, except for the *extreme* case considered above (as we shall see later). This crucial result[3] found under the hypothesis that the two degenerate pseudospin partners share the same component F raises the question whether, actually, eq. (4) admits two different solutions for the F function with the same value of $\bar{\kappa}$ and, if they exist, how much do they differ?

3.1.2 The nuclear surface prohibits the PSS for $\bar{\kappa} = 0$

To throw more light on the solutions of eqs. (4) and (6), we have considered, the ^{40}Ca nucleus, which has only one PSD containing the states $a \equiv 2s_{1/2}$ ($\kappa_a = -1$) and $b \equiv 1d_{3/2}$ ($\kappa_b = 2$), and worked out calculations within the relativistic Hartree approximation and the successful NL-SH [17] and NL3 [18] parameter sets.

We have tried to find two solutions of eq. (4) for the same value of $\bar{\kappa}$, by solving eq. (6), considered equivalent to eq. (4), for $\kappa = \kappa_a$ and $\kappa = \kappa_b$[4]. These solutions can include both the physical states when $\bar{\kappa} = \kappa$ and the non-physical ones when $\bar{\kappa} \neq \kappa$. The results for the single-particle energy (SPE) as a function of $\bar{\kappa}$ are shown in fig. 1. We have found two solutions for values of $\bar{\kappa} \leq \kappa_a$ and only one *acceptable* solution for values of $\bar{\kappa}$ in the range $\kappa_a < \bar{\kappa} \leq \kappa_b$. For $\bar{\kappa} > \kappa_b$, no *acceptable* solutions have been found. The figure shows a very stiff variation of

[2] Notice that if $F(r_0) = 0 (\neq 0)$ and $F'(r_0) \neq 0 (= 0)$, both G_a and G_b would be divergent at r_0.

[3] Although we have shown this result in the framework of the relativistic Hartree approximation, this conclusion can be considered quite general and not restricted to this approximation. The necessary condition is that V becomes zero in the nuclear surface. Notice also that the singularity of the factor V'/V in eq. (4) limits the applicability of the usual theorems of uniqueness of solutions to this equation.

[4] We have used a standard fourth-order Runge-Kutta method, imposing only the appropriate asymptotic conditions on the G and F components, corresponding to $\Sigma_S = \Sigma_0 = 0$, and avoiding the denominator V^2 in eq. (5) to become exactly zero.

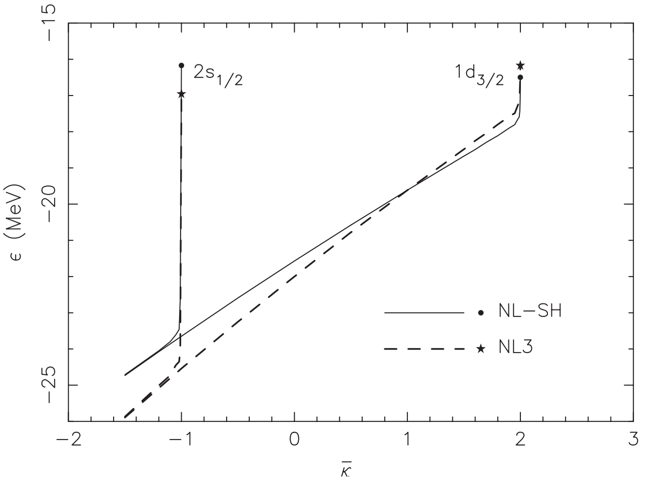

Fig. 1. The neutron single-particle energy ϵ entering eq. (4) as a function of $\bar{\kappa}$ (which is considered as a real number) for the NL-SH (full line) [17] and NL3 (dashed line) [18] parameter sets. For $\bar{\kappa} < -1$ two almost degenerate solutions corresponding to the non-physical single-particle states that exhibit the same features as the $2s_{1/2}$ and $1d_{3/2}$ physical states have been found (they should be degenerate in the exact calculation). The solutions for $\bar{\kappa} = -1$ and $\bar{\kappa} = 2$ corresponding to the $2s_{1/2}$ and $1d_{3/2}$ physical states are indicated by dots (NL-SH) and stars (NL3).

the SPE when the $\bar{\kappa}$ value approaches the physical value κ: κ_a or κ_b (with κ we represent the physical value κ_a or κ_b corresponding to the state under consideration). This result makes evident the extraordinary influence of the $\bar{\kappa}$ term on the solutions of eq. (4) for values of $\bar{\kappa}$ close to the physical ones.

To understand this behavior, we notice that for $\bar{\kappa} < \kappa$, $\bar{M} \to \infty$ as $r \to r_0$, producing a drastic effect in eq. (6) for $r \to r_0$. In fact, from eq. (6), it can be easily seen that the $F(r)$ and $F'(r)$ functions must approach zero as $r \to r_0$ in order the $G(r)$ and $G'(r)$ functions remain finite at r_0. This strong modification of the $F(r)$ function for $\bar{\kappa} \to \kappa^-$ is also reflected in the variation of the SPE ϵ as a function of $\bar{\kappa}$ in fig. 1. For $\bar{\kappa} > \kappa$, $\bar{M} \to -\infty$ as $r \to r_0$. Now, the nucleons move under the influence of a very large negative potential and, although mathematical solutions of the Dirac equation do exist, they are not *acceptable* to describe appropriately the physics of the system[5]. Thus, being these solutions inadequate, from the physical point of view, the possibility of the exact realization of the PSS in the limit of small PSOP (or small κ term) is spoiled.

The results discussed above show that the contribution of the $\bar{\kappa}$ term cannot be estimated by perturbation theory if $\bar{\kappa} \gtrsim \kappa$. Thus, the quasi-degeneracy of the $2s_{1/2}$ and $1d_{3/2}$ states of ^{40}Ca in the NL-SH and NL3 parameter sets cannot be explained by the smallness of the $\bar{\kappa}$ term, as has been considered in refs. [8–11]. In fact, the PSS can be achieved with a $\bar{\kappa}$ term which is not small. This term strongly pushes up the SPE ϵ when $\bar{\kappa}$ approaches the physical values $\kappa_a = -1$ or $\kappa_b = 2$ for the $2s_{1/2}$ or $1d_{3/2}$ states, respectively. Thus, for finite nuclei, the quasi-degeneracy of two pseudospin levels (or PSS) can be achieved, in some cases, the $\bar{\kappa}$ term being big rather than small!

[5] Under these conditions, the single-particle interpretation of the Dirac equation is no longer valid.

3.2 Interpretation of the PSS

In order to better understand how the PSS is achieved, we have to consider in detail the different contributions to the SPE ϵ in eq. (4). Firstly, we notice in fig. 1 that for the b state the $\bar{\kappa}$ term contribution ($\varepsilon(\bar{\kappa})$) to the SPE in the region $\kappa_a \lesssim \bar{\kappa} < \kappa_b$ is an increasing function almost linear in the energy. This behaviour can be explained by the perturbative character of the $\bar{\kappa}$ term in this region (*i.e.*, the F wave function remains almost the same[6]). Actually, into the total perturbative contribution of the $\bar{\kappa}$ term ($\varepsilon(\bar{\kappa}, \epsilon)$) to the SPE ϵ, we have also to include the additional contribution ($\varepsilon(\Sigma, \epsilon)$) coming from the terms $2\epsilon\Sigma_0/2M$ and $\epsilon^2/2M$, which changes necessarily with $\bar{\kappa}$ (through the modification of ϵ brought about by the modification of $\bar{\kappa}$), although F_b remains unchanged. However, as $\epsilon^2/2M$ is very small, the SPE ϵ maintains, approximately, the linearity in $\bar{\kappa}$. Then, considering $\varepsilon(\bar{\kappa}, \epsilon)$, in order for the PSS to be satisfied, it is necessary that the sharp contribution to ϵ in fig. 1 were much larger for the state a than for the state b. In fact, this is what actually happens for all the PSDs of all nuclei, in particular for the pseudospin doublet (PSD) of the ^{40}Ca nucleus. The reason is that the F_a and G_a wave functions of the PSDs with $\kappa_a < 0$ take larger values for $r \gtrsim r_0$ than the F_b and G_b wave functions with $\kappa_b > 0$. Then, as $\bar{\kappa}$ becomes smaller than κ, the effect of $\bar{M}$ in eq. (4), which forces F to approach zero at r_0, becomes larger for the states a with $\kappa_a < 0$ than for the states b with $\kappa_b > 0$. As a result, the sharp contribution to the SPE ϵ in fig. 1 is much larger for the state $2s_{1/2}$ than for the state $1d_{3/2}$, and allows the almost exact PSS for this PSD. This behaviour of the SPE shows that the PSS has a dynamical character. The PSS comes about not as the result of an explicit symmetry of the Dirac Hamiltonian but, rather, as a consequence of the compensation of important contributions to the SPE ϵ coming from different terms in the equation for $F(r)$. This conclusion is compatible with previous investigations [13, 14,16], and will be supported below with extra arguments.

Notice that, as follows from eq. (7), in order for $G_\kappa(r)$ to remain finite at $r = r_0$, the quasi-degenerate states of a PSD must have different F functions[7]. Then, the splitting of the two levels of a PSD does not give us a precise information about how different the corresponding F functions of the two pseudospin partners are.

We have found two solutions of eqs. (4) or (6) for the same value of $\bar{\kappa}$ for $\bar{\kappa} \leq -1$, which correspond to the a and

[6] This happens because, in eqs. (4) and (6), the effect of $\bar{M}$ as a function of $\bar{\kappa}$ is smooth except for $\bar{\kappa} \to \kappa$.

[7] In fact, because of the contribution to the SPE ϵ of the κ and $2\epsilon\Sigma_0$ terms in eq. (3), this is essential to have approximate PSS.

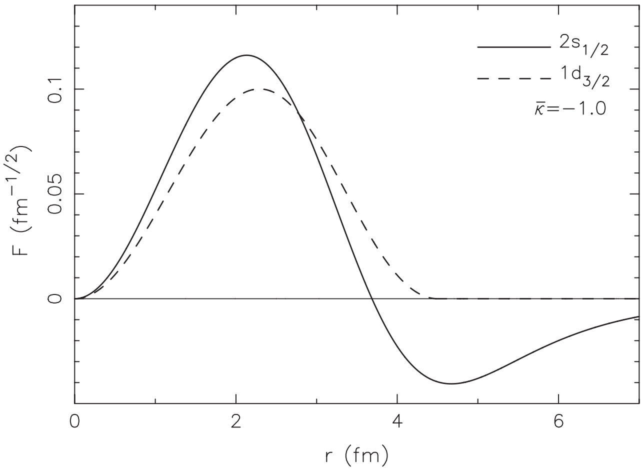

Fig. 2. The small component F of the Dirac spinor for the $2s_{1/2}$ physical neutron state (with $\bar{\kappa} = \kappa_a = -1$, full line) and the $1d_{3/2}$ non-physical neutron state (with the non-physical $\bar{\kappa} = -1$, dashed line), in the ^{40}Ca nucleus.

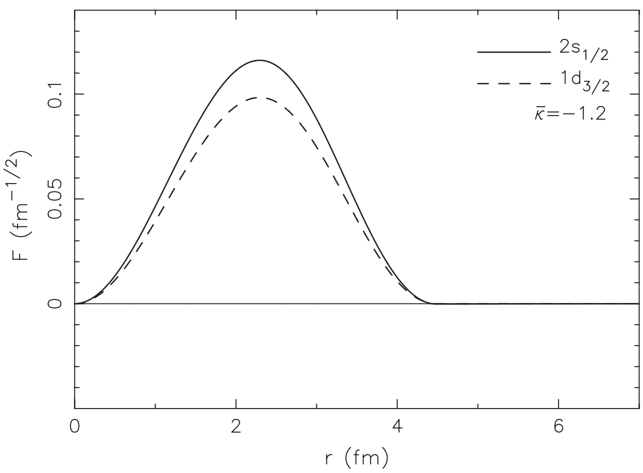

Fig. 3. The same as in fig. 2, but now we take a non-physical $\bar{\kappa} = -1.2$ for both the $2s_{1/2}$ and $1d_{3/2}$ neutron states.

b states. Figures 2 and 3 show the F_a and F_b functions corresponding to $\bar{\kappa} = -1$ and $\bar{\kappa} = -1.2$, respectively, for the NL-SH set [17]. These solutions become almost degenerate for $\bar{\kappa} < -1$. In fact, it can be seen in fig. 3, for the Dirac spinors properly normalized, that these F functions are almost proportional to each other, though their norms are somewhat different. In order to compare properly these two F functions, we have calculated the contributions of the different terms entering eq. (4) to the SPE ϵ. According to this equation, we write the SPE as

$$\varepsilon(F'') + \varepsilon(F') + \varepsilon(\Sigma, \epsilon) + \varepsilon(\tilde{l}) + \varepsilon(\bar{\kappa}) = \epsilon, \qquad (8)$$

where $\varepsilon(F'')$, $\varepsilon(F')$, $\varepsilon(\Sigma, \epsilon)$, $\varepsilon(\tilde{l})$ and $\varepsilon(\bar{\kappa})$ represent the contribution of the terms containing F'', F', Σ and/or ϵ, $\tilde{l}$ and $\bar{\kappa}$ in eq. (4), respectively. These contributions are quoted in table 1 for the NL-SH set. These results show that the proportionality between the two solutions is obtained almost immediately for $\bar{\kappa} < -1$. In fact, for $\bar{\kappa} \to \kappa^-$

Table 1. Contributions of the terms entering eq. (7) to the single-particle energy ϵ in ^{40}Ca for the NL-SH [17] parameter set. All quantities are in MeV.

κ	State	$\varepsilon(F'')$	$\varepsilon(F')$	$\varepsilon(\Sigma, \epsilon)$	$\varepsilon(\tilde{l})$	$\varepsilon(\bar{\kappa})$	ϵ
−1.0	$2s_{1/2}$	18.73	−0.63	−44.83	11.94	−1.38	−16.17
−1.0	$1d_{3/2}$	13.64	3.66	−50.47	11.31	−1.79	−23.65
−1.05	$2s_{1/2}$	13.82	3.59	−50.47	11.36	−1.86	−23.56
−1.05	$1d_{3/2}$	13.66	3.68	−50.51	11.31	−1.89	−23.75
−1.1	$2s_{1/2}$	13.72	3.67	−50.54	11.32	−1.97	−23.80
−1.1	$1d_{3/2}$	13.70	3.68	−50.54	11.31	−1.98	−23.83
−1.2	$2s_{1/2}$	13.72	3.71	−50.62	11.31	−2.17	−24.05
−1.2	$1d_{3/2}$	13.73	3.71	−50.62	11.31	−2.17	−24.05

(but $\bar{\kappa} \neq \kappa$) we expect that small numerical uncertainties increase the differences of the contributions of the terms given in table 1. Thus, our results for $\bar{\kappa} < -1$ are compatible with two functions F_a and F_b exactly degenerate and proportional to each other, corresponding to the *extreme* case $F'(r_0) = F(r_0) = 0$ considered in the sect. 3.1.1. Then, in an exact calculation, fig. 1 should be slightly modified so that the oblique part of the line corresponding to F_a lies exactly over the oblique part of the line corresponding to F_b, whereas the sharp part of F_a and F_b should be exactly vertical. In fact, the sharply increasing part represents the transition from the physical states with $\bar{\kappa} = \kappa$, exhibiting normal asymptotic behaviour, to the non-physical ones with $\bar{\kappa} \neq \kappa$, satisfying the condition $F'(r_0) = F(r_0) = 0$. Thus, the sharp part could be also suppressed, representing only the oblique lines and the points corresponding to the SPE ϵ of the two physical states for each parameter set. In any case, the important result is that, when $\bar{\kappa}$ is slightly decreased from its corresponding physical value, the wave function F and its eigenvalue ϵ are strongly modified, showing the essential role the $\bar{\kappa}$ term plays in eq. (4). In particular, this term is responsible for the normal behaviour of the $F(r)$ and $G(r)$ components of the physical states for $r \gtrsim r_0$. Thus, it determines the nucleon density distribution in the nuclear surface.

The proportionality between F_a and F_b found for $\bar{\kappa} < \kappa_a$ gives us a starting point to explain the similarity of the F wave functions found in some PSDs of many nuclei. The main reason is that, as we have noticed above, F_b remains almost unchanged in the region $\kappa_a \lesssim \bar{\kappa} < \kappa_b$. Then, as $\bar{\kappa} \to \kappa$, $\bar{M} \to M$ in a similar way for the two states a and b. Thus, the strong modification of $\bar{M}$ for $\bar{\kappa}$ near κ produces *important but similar modifications* of the F_a and F_b wave functions except near the point r_0, where the singularity strongly influences the behaviour of F_a and F_b. Thus, F_a and F_b remain proportional in the inner region of the nucleus. Of course, the region of proportionality increases as r_0 increases. This fact favors the similarity of F_a and F_b in heavy nuclei.

In this kind of nuclei, it can be observed that the similarity between F_a and F_b increases rapidly with the number of nodes ($\tilde{n}_r$) of these two components. This result is mainly associated to the increasing of the contribution of the term proportional to F'' in eq. (3) with $\tilde{n}_r$. Thus, the effects of the other terms, including that of the κ term, are, relatively, less important as F'' takes larger values. The κ term always produces significant changes in F and its effect is always essential; however, as $\tilde{n}_r$ increases, the effect on F_a and F_b becomes less asymmetric (*i.e.*, more similar). This seems to be an important point, although not the only one, to understand the similarity between F_a and F_b for $\tilde{n}_r \geq 3$ in finite nuclei, rather than the fact that $\Sigma_S \simeq -\Sigma_0$, which is common for all PSDs and fails if $\tilde{n}_r = 2$ although $|\epsilon_a|$ or $|\epsilon_b|$ were small.

Although in some cases the differences between F_a and F_b near r_0 seem to be not very important, they are always essential because the quantity V^{-1} in eq. (7) acts as a multiplicative factor that produces near r_0 very large effects on the big component G_κ of the Dirac spinors. This fact prohibits, for example, to obtain approximate G_a and G_b big components near r_0 from approximate F_a and F_b components. Even when the big component of a state is obtained from the corresponding big component of the partner using the appropriate pseudospin algebra, there appear important problems [7].

3.3 Role of the term proportional to V′ in the equation for F

We have shown that the κ term cannot be considered small. This fact can be mainly attributed to its divergence at r_0. Since this divergence is cancelled by the term containing F' in eq. (3), it seems interesting to examine the influence of the $h(V') \equiv \frac{V'}{V}\left(\frac{F'}{F} - \frac{\kappa}{r}\right)$ term on the solutions of eq. (3). Several authors have attributed the approximate PSS observed in nuclei to the smallness of $|V'|$ [3–11]. If they were right, the breaking of the PSS brought about by the $h(V')$ term would be small. However, we have observed that the direct contribution of this term to the SPE ϵ is generally larger than the direct contribution of the κ term. One can see in ref. [14] that, in fact, the two addends appearing in $h(V')$ contribute coherently (*i.e.* $\varepsilon(F')$ and $\varepsilon(\kappa)$ have the same sign). This result suggests that the explanation of the PSS based on the smallness of $|V'|$ is not adequate. Furthermore, although, in some cases, eq. (3) without the term $h(V')$ can admit normalizable $F(r)$ solutions, they cannot be considered as the approximate functions of the F_a and F_b components, because they would produce from eq. (7), obviously, divergent $G_\kappa(r)$ functions at the singularity point. Thus, the $h(V')$ term is essential to get physical solutions from eq. (3). Its self-consistent effects are very large, reinforcing the idea that the PSS cannot be justified by the smallness of $|V'|$.

3.4 Relation between spin-orbit and pseudospin-orbit schemes

The Dirac equation (1) can be reduced to an equivalent Schrödinger-like equation for the big component G. It reads

$$-G'' + \left[\frac{W'}{W}\left(\frac{G'}{G} + \frac{\kappa}{r}\right) + \frac{l(l+1)}{r^2} + WV\right]G = 0\,, \quad (9)$$

where κ, V and W are defined in sect. 2 (see eq. (2)).

Equation (3) for F can be written in a similar form as eq. (9) for G, but changing the sign of the κ term and replacing W by V and l by $\tilde{l}$ everywhere.

Equations (3) and (9) formally establish a strong similarity between the spin-orbit (LS) coupling scheme and the pseudospin formalism. This similarity calls for studying the relationship between them. The large energy splitting produced by the LS interaction in relation with the splitting of many PSDs suggests that the κ term plays a less important role in eq. (3) than in eq. (9). However, what actually happens is just the opposite.

The gradual quenching of the κ term in eq. (9) produces a gradual reduction of the energy splittings of the two spin-orbit partners. However, as we have mentioned above, small variations of $\bar{\kappa}$ in eq. (4) can produce very strong modifications of the single-particle energy (SPE) ϵ and the G and F wave functions. Furthermore, for $\bar{\kappa} > \kappa$ the Dirac equation cannot properly describe the state corresponding to κ. This very different behavior of the solutions of eq. (4) (or eq. (3)) and eq. (9), as $\bar{\kappa}$ or κ are modified from their physical values, respectively, is due to the fact that the κ term in eq. (9), can be switched off by adding to V the quantity $-W'/W^2 \times \kappa/r$, which does not bring a strong modification of V. However, as we have explained above, to quench the $\bar{\kappa}$ term in eq. (4) (or the κ term in eq. (3)) it is necessary to introduce in the Dirac equation a divergent term at r_0, which crucially modifies the behavior of the b state for $r \gtrsim r_0$, while this equation, from the physical point of view, is no longer appropriate to describe the a state. This strong difference in the LS and pseudo-LS schemes is mainly due to the fact that $V(r)$ becomes zero at a certain value of r in the nuclear surface for all single-particle bound states, whereas $W(r)$, which determines the LS interaction, is a positive and large quantity everywhere in the nucleus. Thus, one can find solutions of eq. (9) for real values of κ allowing a continuous and smooth (*i.e.*, perturbative) transition between the two states of a spin doublet (and even beyond). This can be achieved, by allowing κ to vary between the two values of κ corresponding to the two states of a spin doublet (or even beyond). On the contrary, we have seen that the solutions of eq. (4) for non-physical values of $\bar{\kappa}$ do not exhibit a good asymptotic behaviour and, consequently, they cannot allow a continuous transition between the two states of a pseudospin doublet (PSD).

Another aspect that is worth noting is that the two states a and b of a PSD have values of j such that $j_a = l_a + 1/2$ and $j_b = l_b - 1/2$. Thus, in a simple shell model approximation, in which the nucleons move in a central potential and a LS potential, the LS term shifts the SPEs ϵ_a and ϵ_b of the PSD in opposite directions. It means that the splitting of the PSDs crucially depends on the strength of the LS interaction. In this not self-consistent picture, two states of a PSD can be forced to be degenerate if the

LS interaction is adequately chosen [1,15]. However, in general, this is not possible by choosing the magnitude of $\Sigma_S + \Sigma_0$ compatible with bound nuclei.

For self-consistent models, the relationship between the LS and pseudo-LS schemes is qualitatively similar, although, in this case, the situation is more complicated because there are additional contributions to the LS splittings of terms in the equation for G different from the LS term, as a result of the self-consistent procedure. It is also worth mentioning that a large LS force increases the relative size of the F function in comparison to the G component, favoring the similarity between F_a and F_b. In fact, this similarity is appreciably spoiled, if the quantity $\Sigma_S - \Sigma_0$ is arbitrarily reduced although the $\Sigma_S + \Sigma_0$ remains unchanged. These facts confirm that the potential $\Sigma_S - \Sigma_0$ plays a more essential role than the $\Sigma_S + \Sigma_0$ one in the PSS, in contrast with some conclusions of the previous investigations [3–11]. All that shows that the PSS and LS schemes are strongly related and the PSS cannot be understood independently of the LS interaction. In fact, in the case with no LS interaction, the two energy levels of a PSD would not be closer to each other than the remaining states of the two spin-orbit doublets involved in the PSD.

3.5 The PSS in finite nuclei cannot be justified by the smallness of $|\mathbf{\Sigma_S + \Sigma_0}|$

As is considered in refs. [3–7], the exact PSS* can be obtained if $\Sigma_S + \Sigma_0$ is neglected in V, *i.e.* if $V = -\epsilon$ in eq. (2) (hereafter we shall designate this case as Model I). Unfortunately, these conditions are incompatible with real nuclei since they do not admit bound states. *The single-particle Dirac spinors corresponding to bound and unbound states are completely different.* Thus, we believe that the PSS properties of Model I cannot be extrapolated to real nuclei[8]. In any case, if the PSS could be based on the fact that $|\Sigma_S + \Sigma_0|$ is small, it would mean, in particular, that the κ term and the $h(V')$ term would be small and, consequently, could be neglected in eq. (3). However, we have shown in sect. 3.3 that this approximation brings about unacceptable solutions of this equation.

It happens also that the main differences between F_a and F_b occur for $r \simeq r_0$ due to the singularity of V'/V. However, near r_0, $V'/V \simeq (r-r_0)^{-1}$, showing only a small dependence on $\Sigma_S + \Sigma_0$ through the value of r_0. All this means that the PSS cannot be justified by the condition that $|\Sigma_S + \Sigma_0|$ is small.

[8] Although this model predicts that $E_a = E_b$ and $F_a = F_b$, if the reason of the similarities $\epsilon_a \simeq \epsilon_b$ and $F_a \simeq F_b$ observed in some cases were the small value of $|\Sigma_S + \Sigma_0|$, then, this property should be exhibited, in a similar way, by all PSDs, and should be regularly improved as $|\Sigma_S + \Sigma_0|$ decreases (remaining $\Sigma_S - \Sigma_0 \simeq$ unchanged). However, this behaviour seems to be not very well respected, suggesting, at least, that other factors should be considered in the explanation of this similarity. Notice that the situation for the Coulomb potential is different [3] because in this case the single-particle level density becomes infinite as ϵ approaches the continuum.

New arguments to support this conclusion can be found by taking into account the effect of the spin-orbit interaction on the PSS discussed in sect. 3.4. The results predicted in refs. [3–6] for the case $\Sigma_S + \Sigma_0 = 0$ are also obtained when, furthermore, $\Sigma_S - \Sigma_0 = 0$ (Model II), which means that there is no spin-orbit interaction. However, as we have discussed above, an adequate spin-orbit interaction is essential to get approximate PSS. Thus, we have Model II that also predicts exact PSS for the states lying in the continuum but, if this model were modified so that $\Sigma_S + \Sigma_0$ took realistic values, the PSS would be considerably spoiled in finite nuclei. Then, the approximate PSS observed in certain pseudospin doublets of these systems cannot be explained by the fact that $|\Sigma_S + \Sigma_0|$ is small, because $\Sigma_S + \Sigma_0 = 0$ in Models I and II but, however, if model II were modified as we have explained above to get bound nuclei, the PSS would be appreciably spoiled. Thus, the magnitude of $\Sigma_S - \Sigma_0$, which determines the spin-orbit interaction in finite nuclei, seems to be more important in explaining the PSS than that of $\Sigma_S + \Sigma_0$.

4 Conclusions

To study the effect of the PSS breaking κ term in eq. (3) for the small component $F(r)$ of the nucleon Dirac spinor, we have considered κ as a real parameter, which is denoted by $\bar{\kappa}$ in eq. (4), and we have constructed an equivalent Dirac equation with the nucleon mass M replaced by an effective mass $\bar{M}$ containing $\bar{\kappa}$.

With this equation, we have investigated the properties of the bound-state solutions of a quite general hypothetical model satisfying the exact PSS* (*i.e.*, $\epsilon_a = \epsilon_b$ and $F_a = F_b$ for the two states of a PSD). We have found that, because of the singularity of V^{-1} at $r = r_0$ in the nuclear surface, the exact PSS* necessarily implies $F'_{a,b}(r_0) = F_{a,b}(r_0) = 0$. This result is important because it means, in particular, that the physical solutions of a realistic model corresponding to the states of a pseudospin doublet are, necessarily, quite different from those of any "approximate" model satisfying exact PSS*.

Our results also show that, because of the singularity of the factor V^{-1}, the κ term is indeed very strong. This term determines, in particular, the behaviour of the nucleon wave functions for $r \gtrsim r_0$ and, consequently, also the density distribution around the nuclear surface. In fact, for $\bar{\kappa} \neq \kappa$, $F(r) = 0$ for $r \geq r_0$. This strong modification of $F(r)$, as $\bar{\kappa}$ differs from its physical value, means that the two states of a pseudospin doublet cannot be continuously connected by a continuous variation of $\bar{\kappa}$, in contrast to what happens with two states of a spin-orbit doublet. For $\bar{\kappa} > \kappa$ the nucleons move in a very negative effective potential and the Dirac equation appears to be unable to describe appropriately the physics of the system. This fact would spoil the exact PSS even for the hypothetical case corresponding to $\bar{\kappa} = 0$, in which the PSS is supposed to be exact. We conclude that in finite nuclei, because of the divergence of the quantity V'/V due to the surface effects, the PSS cannot be explained by the smallness of the κ term.

Our results also indicate that the PSS cannot be justified by the smallness of the $|V'|$ in eq. (3) either. Although solutions of this equation without the $h(V')$ term can be found in some cases with $\epsilon < 0$, they considerably differ from the physical ones and, in any case, the G component obtained from eq. (7) diverge at r_0. Thus, in finite nuclei, the explicit PSS exhibited by eq. (3) without the term $h(V')$ is mathematical rather than physical.

For these finite systems, there exist quasi-degenerate PSDs, but their corresponding states have, necessarily, different F wave functions. Consequently, they can satisfy the PSS with arbitrary precision but not the PSS*. Thus, the single-particle spectrum of a nucleus does not give a precise idea of the degree of similarity between F_a and F_b wave functions, *i.e.* of the degree of accomplishment of the PSS*. Our results for the ^{40}Ca nucleus indicate that the PSS can be exactly realized and it is compatible with the PSS* strongly broken.

Using simple arguments, we have also shown that the PSS in finite nuclei cannot be explained by the fact that $|\Sigma_S + \Sigma_0|$ is small, in contrast to the commonly accepted point of view.

We have found that in the ^{40}Ca nucleus, for $\bar{\kappa} < \kappa_a$, the states $a = 2s_{1/2}$ and $b = 1d_{3/2}$, both solutions of eqs. (4) and (6), are degenerate and their corresponding F functions are proportional to each other. Then, the PSS becomes exact (actually, it is a particular type of the PSS, more general than the PSS*). The PSS found for $\bar{\kappa} < \kappa_a$ in the ^{40}Ca nucleus is a general result valid for all nuclei.

This important result allows us to propose a new interpretation of the PSS, which is based not on the smallness of the potential $|\Sigma_S + \Sigma_0|$ or of the κ term, but, rather, on the strong compensation of different contributions to the SPE. The spin-orbit interaction, through the quantity $\Sigma_S - \Sigma_0$, plays an essential role in this compensation. The two states of a PSD cannot be connected in a perturbative way through a continuous variation of $\bar{\kappa}$, showing the dynamical character of the PSS. Furthermore, the PSS found for $\bar{\kappa} < \kappa_a$ supplies also the "key" to explain the similarity between F_a and F_b in the inner region of the nuclei. This similarity is favored by a large value of the number of nodes $\tilde{n}_r$ of F, which increases the relative importance of the term proportional to F'' in eq. (3), and by a strong spin-orbit interaction.

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