Spin-orbit coupling rule in bound fermions systems

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Spin-orbit coupling characterizes quantum systems such as atoms, nuclei, hypernuclei, quarkonia, etc., and is essential for understanding their spectroscopic properties. Depending on the system, the effect of spin-orbit coupling on shell structure is large in nuclei, small in quarkonia, perturbative in cold atomic gases, atomic nuclei far from stability, etc., and is essential for understanding their spectroscopic properties. Depending on the system, the effect of spin-orbit coupling on shell structure is large in nuclei, small in quarkonia, perturbative in cold atomic gases, atomic nuclei far from stability, etc., and is essential for understanding their spectroscopic properties.

I. INTRODUCTION

Spin-orbit coupling, known since the early days of quantum mechanics, is among the most studied effects related to the spin of a particle. After nearly a century, spin-orbit effects continue to provide a basis for a variety of new phenomena in diverse fields of quantum physics, such as spintronics, topological insulators, cold atomic gases, atomic nuclei far from stability, etc., and is essential for understanding their spectroscopic properties. Depending on the system, the effect of spin-orbit coupling on shell structure is large in nuclei, small in quarkonia, perturbative in cold atomic gases, atomic nuclei far from stability, etc., and is essential for understanding their spectroscopic properties.

II. SPIN-ORBIT COUPLING IN ATOMIC NUCLEI

In the nuclear relativistic mean-field framework, a nucleus is considered as a system of independent nucleons moving in local self-consistent scalar and vector potentials. The single-nucleon dynamics is governed by the Dirac equation:

\[ [\vec{\alpha} \cdot \vec{p} + V + \beta(m + S)] \psi_i = E_i \psi_i \]  (1)

where \( \psi_i \) denotes the Dirac spinor:

\[ \begin{pmatrix} \phi_i \\ \chi_i \end{pmatrix} \]  (2)

for the \( i \)-th nucleon. For simplicity we only consider spherical nuclei and assume time-reversal symmetry (pairwise occupied states with Kramers degeneracy), which ensures that the only non-vanishing components of the vector fields are the time-like ones and thus there is no net contribution from nucleon currents. The local vector \( V \) and scalar \( S \) potentials are uniquely determined by the actual nucleon density and scalar density of a given nucleus, respectively. In the ground state A nucleons occupy the lowest single-nucleon orbitals determined self-consistently by the iterative solution of the Dirac equation [1]. If one expresses the single-nucleon energy as \( E_i = m + \varepsilon_i \), where \( m \) is the nucleon mass, and rewrites the Dirac equation as a system of two equations for \( \phi_i \) and \( \chi_i \), then, noticing that for bound states \( \varepsilon_i << m \),

\[ \chi_i \approx \frac{1}{2M(r)}(\vec{\sigma} \cdot \vec{p}) \phi_i \]  (3)

to order \( \varepsilon_i/m \), and

\[ M(r) \equiv m + \frac{1}{2}(S(r) - V(r)) \]  (4)

The equation for the upper component \( \phi_i \) of the Dirac spinor reduces to the Schrödinger-like form [10, 11]

\[ \left[ \vec{p} + U(r) + VLS(r) \right] \phi_i = \varepsilon_i \phi_i \]  (5)
for a nucleon with effective mass $M(r)$ in the potential $U(r) \equiv V(r) + S(r)$, and with the spin-orbit potential:

$$V^{LS} = \frac{1}{2M^2(r)} \frac{1}{r} \frac{d}{dr} (V(r) - S(r)) \vec{l} \cdot \vec{s}. \quad (6)$$

The spin-orbit coupling plays a crucial role in nuclear structure, and its inclusion in the effective single-nucleon potential is essential to reproduce the empirical single-nucleon numbers. The relativistic mean-field framework, in particular, naturally includes the nucleon spin degree of freedom, and the resulting spin-orbit potential emerges automatically with the empirical strength [12]. The nuclear-spin potential originates from the difference between two large fields: the vector potential $V$ (short-range repulsion) with typical strength of $\approx 350$ MeV, and the scalar potential $S$ (medium-range attraction), typically of the order of $-400$ MeV in nucleonic matter and finite nuclei. In the context of in-medium QCD sum rules [13], the strong scalar and vector mean fields experienced by nucleons can be associated with the leading density dependence of the chiral (quark) condensate, $\langle \bar{q}q \rangle$, and the quark density $\langle \bar{q}q \rangle$. In the mean-field phenomenology the sum of these two fields $V + S \approx -50$ MeV provides the confining potential that binds the nucleons in a nucleus, whereas the large difference $V - S \approx 750$ MeV determines the pronounced energy spacings between spin-orbit partner states in finite nuclei, of the order of several MeV [7][8][12][14][15]. A puzzling coincidence that we would like to explore is that the largest spin-orbit splittings for intruder states are comparable in magnitude to the energy gaps between major shells of the nuclear potential.

The aim of this study is to evaluate the typical ratio between the energy spacings of levels characterized by principal single-particle quantum numbers and the energy splitting of spin-orbit partner states (fine structure). Even though the values of this ratio span orders of magnitude for different bound quantum systems, we will show that it is basically governed by two quantities that characterize a given system, irrespective whether the binding and spin-orbit potentials originate from the strong (nuclei) or electromagnetic (atoms) interactions.

In the nuclear case the interaction is of short range and the self-consistent potentials display a spatial distribution that corresponds to the actual single-nucleon density. The expression for the spin-orbit potential Eq. [6] can, therefore, be rewritten in the following form:

$$V^{LS} \approx F(r) \frac{\rho'(r)}{2\rho(r)r} \vec{l} \cdot \vec{s}, \quad (7)$$

where

$$F(r) \equiv \frac{V(r) - S(r)}{[m - \frac{1}{2}(V(r) - S(r))]^2}, \quad (8)$$

and $\rho(r)$ denotes the self-consistent ground-state density of a nucleus with $A$ nucleons. For a typical approximation of the single-nucleon potential, such as the harmonic oscillator, or the more realistic Woods-Saxon potential, one can show [16]:

$$<\rho'(r)> \sim -\frac{1}{R_0^2} \quad (9)$$

where $R_0 = r_0 A^{1/3}$, $r_0 \approx 1.2$ fm and, together with $<\vec{l} \cdot \vec{s}> = l/2$ for $j = l + 1/2$, and $<\vec{l} \cdot \vec{s}> = -1/2(l + 1)$ for $j = l - 1/2$, the energy spacing between spin-orbit partner states can be approximated by:

$$|\Delta <V^{LS}> | \approx \frac{F \hbar^2}{R_0} \quad (10)$$

Let us consider the ratio between the major energy spacings and the spin-orbit splitting. For the harmonic oscillator potential one finds [17]

$$h\omega_0 = \frac{\hbar}{R_0} \sqrt{\frac{-2U_0}{m}}, \quad (11)$$

where, in our case, the depth of the potential is $U_0 \equiv U(r = 0) = V(0) + S(0)$. Therefore,

$$x = \frac{h\omega_0}{|\Delta <V^{LS}> |} = K|\eta - 1 + \frac{1}{4\eta}|, \quad (12)$$

where $K = \sqrt{-2mU_0R_0/\hbar}$, and

$$\eta \equiv \frac{m}{V - S}. \quad (13)$$

K is typically of the order $1 - 5$ for $1 \geq 3$ (corresponding to the magic spin-orbit gaps). Since for the nucleon mass $m \approx 940$ MeV and $V - S \approx 750$ MeV: $\eta = 1.25$, it follows from Eq. [12] that for the nuclear system the ratio $x$ is of the order $1 - 5$, that is, in nuclei the energy splitting between spin-orbit partner states is comparable in magnitude to the spacings between major oscillator shells. This is because of the near equality of the mass $m$ and the potential $V - S$ in nuclei. It should be noted than in the case of the pseudo-spin symmetry [18] $(V = S)$, Eq. [13] yields $\eta = m/2V$. An aspect that can be generalised to different quantum systems is the specific functional dependence of $x$ on the ratio of the particle mass $m$ and the effective potential whose gradient determines the spin-orbit force.

III. OTHER SYSTEMS OF BOUND FERMIONS

In the case of atomic systems the binding of an electron is determined by the Coulomb potential $V(r) = -Ze/r$, where $Z$ is the charge of the nucleus and the fine-structure constant $\alpha = 1/137$. One can again perform the non-relativistic reduction of the Dirac equation for the electron (Eqs. [1] - [3]), and the resulting spin-orbit potential reads:

$$V^{LS} = \frac{1}{2M^2(r)} \frac{1}{r} \frac{dV(r)}{dr} \vec{l} \cdot \vec{s}, \quad (14)$$
with \( 2M(r) \equiv 2m - V(r) \). In this case, of course, \( U(r) \) in Eq. (9) is just the Coulomb potential. The energy spacing between successive levels with different principal quantum number \( n \) is proportional to \( \alpha^2 \), whereas the first-order spin-orbit splitting is \( \sim \alpha^4 \). The ratio between the principal energy spacings and the spin-orbit splittings (fine structure) is much larger than in the nuclear case, that is \( \sim 1/\alpha^2 \approx 10^4 \), known from the early seminal work of Sommerfeld [19]. The interesting fact is that, starting from Eq. (14), this ratio can again be expressed with the same functional dependence on \( \eta \) as in Eq. (12):

\[
\eta = m/V \quad \text{is now negative and, with} \quad m = 0.5 \text{ MeV and} \quad V(r_0) = -2.72 \times 10^{-5} \quad \text{MeV for the hydrogen atom and} \quad \text{the Bohr's radius} \quad r_0, \quad \text{it follows that in the atomic case the characteristic value is} \quad \eta \sim 1/\alpha^2 \approx -2 \times 10^4. \quad \text{For large absolute values of} \quad \eta, \quad \text{the expression Eq. (12) reduces to} \quad x \sim 1/\alpha^2 \approx 10^4, \quad \text{in agreement with the empirical value quoted above. The fine structure of atomic spectra thus becomes a limit of the spin-orbit rule (12). It should be noted the validity of the spin-orbit rule in Coulomb-like systems is due to the 1/r behavior of the potential. The spin-orbit rules also applies to the case of ions having Z protons: in these systems the fine structure is known to be \( Z^2 \alpha^2 \). In the present approach the \( Z^2 \) factor comes from the Z one of Eq. (13) and the Z one from the \( r_0/Z \) typical size of the ion. Figure 1 displays the quantity representing the spin-orbit rule:

\[
x \sim |\eta - 1 + \frac{1}{4\eta}| \quad (15)
\]

as a function of the ratio \( \eta \) between the mass of the particle and the effective potential that determines the spin-orbit force in a given quantum system. As shown above, for nuclei \( \eta \) is slightly larger than one and, depending on the specific orbital, \( x \) lies in the interval 1 - 5. In atoms \( \eta \) is negative and of the order of \( 10^4 \) and, therefore, the characteristic value of \( x \) is \( \sim 1/\alpha^2 \approx 10^4 \).

The main results of the spin-orbit rule quantitatively apply to nuclei and atoms. It may be relevant to test it in a few other quantum systems although a more qualitative agreement is expected, due to additional effects which would not be included in the present approach. For instance, experimental evidence indicates that in \( \Lambda \) hypernuclei the \( \Lambda \)-nuclear spin-orbit interaction is very weak compared to the strong spin-orbit interaction in ordinary nuclei [20][21]. Available data show that the energy spacings between \( \Lambda \) spin-orbit partner states are of the order of \( \approx 100 \) keV, although some microscopic models also predict 2 MeV values in some cases [22]. Even though a quantitative study of the smallness of the \( \Lambda \) spin-orbit interaction necessitates a rather involved analysis based on in-medium chiral SU(3) dynamics [23], one can qualitatively understand the reduction of the spin-orbit splitting in \( \Lambda \) hypernuclei already at the relativistic mean-field level [21][25]. A finite-density QCD sum-rule analysis [15][24] indicates that, when compared the strong scalar and vector mean fields experienced by nucleons in ordinary nuclei, the corresponding self-energies of a \( \Lambda \) hyperon are reduced by a factor \( \approx 0.4 - 0.5 \), and even smaller if corrections from in-medium condensates of higher dimensions are taken into account. With \( m_\Lambda = 1.12 \text{ GeV} \), this means that \( \eta \) in Eq. (13) is of the order \( 3 - 4 \), leading to larger \( x \) value than in nuclei, in qualitative agreement with empirical values of \( x \) in such systems. Since the energy spacing between major oscillator shells in \( \Lambda \) hypernuclei (for instance, \( 13^\circ \text{C}, 16^\circ \text{O}, 40^\circ \text{Ca} \)), is of the order of \( \approx 10 \text{ MeV} \) [20], the empirical ratio \( x \) ranges from a few units to a few dozens. Our mean-field estimate is closer to the small values of \( x \) but, as shown in Ref. [25], a considerable additional reduction of the splitting between \( \Lambda \) spin-orbit partner states arises as the effect of the hypernuclear tensor coupling. As explained above, a quantitative explanation of the small spin-orbit splitting in hypernuclei must include beyond-mean-field effects.

An interesting example of quantum systems that are governed by the strong interaction but exhibit negative values of \( \eta \), are quarkonia such as, for instance, charmonium \( cc \) and bottomonium \( bb \). The center-of-mass is different, compared to the present one-body approach, but this only generates a global scaling factor of 2 on the energy positions, due to the reduced mass. Since we are dealing with order of magnitudes, and most importantly with energies ratios, it is relevant to check if the present approach applies in the case of quarkonia. The use of potential models for these system can be justified by the fact that the bottom and charm masses are large in comparison to the typical hadronic scale of QCD. Most phenomenological approaches to the dynamics of two heavy
quarks interacting through a potential are variants of the Cornell model \[20\], which consists of a superposition of the one-gluon-exchange that leads to a Coulomb-like attractive vector potential at short distances:

\[
V = -\frac{4}{3} \frac{\alpha_s(r)}{r}, \tag{16}
\]

plus a scalar linear confining potential \( S = \sigma r \), with \( \sigma \approx 0.18 \text{ GeV}^2 \). Therefore, \( V - S \) is negative in the quarkonia case. The masses of the \( c \) quark \( b \) quark are \( m_c \approx 1.27 \text{ GeV} \) and \( m_b \approx 4.2 \text{ GeV} \), respectively. At radial distances that correspond to the mean-square radii of the quarkonia states the Coulomb-like attractive vector potential Eq. (16), with a depth of the order of \(-1 \text{ GeV} \), dominates over the scalar potential \[22\]. The mass of the lowest charmonium state is \( \approx 3 \text{ GeV} \), while that of the lowest bottomonium state is \( \approx 9.5 \text{ GeV} \). The energy spacing between 1S and 2S states is of the order of \( 600 \text{ MeV} \) for charmonia, and \( 560 \text{ MeV} \) for bottomonia \[23\, 29\]. The fine splittings between \( 1P \) states are less than \( 100 \text{ MeV} \) for the charmonium (\( \Delta M_{21} = 45.6 \pm 0.2 \text{ MeV} \) and \( \Delta M_{10} = 95.3 \pm 0.4 \text{ MeV} \)), and less than \( 40 \text{ MeV} \) for the bottomonium (\( \Delta M_{21} = 19.4 \pm 0.4 \text{ MeV} \) and \( \Delta M_{10} = 33.3 \pm 0.5 \text{ MeV} \)). This means that, in the case of quarkonia, the empirical ratio between the energy spacings characterized by the principal quantum numbers and the fine spin-orbit splittings is of the order of 5 to 10, in qualitative agreement with Fig. 1.

The particular dependence of this ratio on \( \eta \), shown in Fig. 1 displays interesting features. For positive values of \( \eta \), states for which the orbital angular momentum and spin are aligned are found at lower energy with respect to states for which the orbital angular momentum and spin are anti-aligned (nuclei, hypernuclei), whereas the opposite energy ordering is found for negative \( \eta \) (atoms, quarkonia). The ratio \( x \) (Eq. (15)) diverges at \( \eta = 0 \), that is, in the limit of massless particle.

An interesting situation is found in the vicinity of \( \eta=1/2 \), for which \( x = 0 \). More precisely, \( \eta \) values close to 1/2 are in the validity domain of the approximation performed to derive the present spin-orbit rule. This occurs when the mass of the particle is close to \((V - S)/2\), and the energy spacings between states are characterized by very large spin-orbit coupling (giant LS). Such states could be obtained in particular cases for which one would be able to choose the strength of the effective potential whose gradient determines the spin-orbit force. In a hypothetical case this limit is approached when the effective potential becomes very deep as it would occur, for instance, for bound antibaryon-nuclear systems which, in addition to ordinary nucleons, contain antibaryons (\( \bar{B} = \bar{p}, \bar{\Lambda}, \ldots \)) (cf. Figs. 10 and 21 of Ref. \[30\]). Two cases can be considered. For the antibaryon spectrum the spin-orbit splitting remains small, of about few hundreds keV \[31\]. The corresponding V-S potential is smaller than in the nucleon case because V has the opposite sign in the case of antibaryons \[31\] and, therefore, the value of \( \eta \) becomes larger (Fig. 4). This is both the case for the antiproton and anti-L nuclei \[22\, 32\]. in the last case a good quantitative agreement is found for the relative amplitude of the spin-orbit splitting predicted by the spin-orbit rule (\( x \approx 40 \)).

The case of nucleons in antibaryon-nuclei is closer to the giant LS state: the gradient of the potential obtained from self-consistent calculations increases and the spin-orbit splitting not only gets larger, but displays a pronounced increase with respect to the spacing between major shells (Fig. 1). However, such systems have not been observed and this is just an illustrative example, with antibaryon-nucleus potentials subject to large uncertainties \[30\]. A similar effect, although much weaker, is predicted for single-nucleon spectra in \( \Lambda \)-hypernuclei \[33\]. Even though the presence of a \( \Lambda \) induces only a fractional change in the central mean-field potential, through a purely relativistic effect it increases the spin-orbit term in the surface region, providing additional binding for the outermost neutrons. To emphasize this region of giant spin-orbit splittings, in Fig. 1 we also plot the inverse of \( x \). For negative values of \( \eta \) the ratio \( x \) does not vanish, but again one finds a region of small absolute values of \( \eta \) for which the splitting between spin-orbit partner states is comparable in magnitude to the energy spacing between successive levels with different principal quantum number.

### IV. SUMMARY

In conclusion, we have investigated an interesting effect of spin-orbit coupling in systems of bound fermions (electrons, quarks, nucleons, hyperons). By performing the usual non-relativistic reduction of the Dirac equation, the single-particle mean-field equation takes a Schrödinger-like form which, in addition to the confining potential, exhibits the spin-orbit potential explicitly. Starting from the relativistic mean-field approximation in the nuclear case, we have derived an analytic expression for the ratio between the energy spacings characterized by principal single-particle quantum numbers and the energy splitting of spin-orbit partner states. This quantity explicitly depends on the ratio of the particle mass and the effective potential whose gradient determines the spin-orbit force (cf. Eq. (15)). In nuclei the near equality of the mass of the nucleon and the difference between the large repulsive vector and attractive scalar potentials explains the fact that the spin-orbit splittings are comparable to the energy spacing between major oscillator shells. The same universal functional form also applies to other bound quantum systems, regardless of whether the spin-orbit potential originates from the strong or electromagnetic interaction, and for which the ratio between the principal energy spacings and the spin-orbit splittings is orders of magnitude larger than in the nuclear case. For a given particle mass this ratio could be altered, in principle, by modifying the potential that generates the spin-orbit coupling effect. When this ratio
is $\eta \approx 1/2$, our study predicts the occurrence of giant spin-orbit splittings, that is, a single-particle excitation spectrum dominated by large energy spacings between spin-orbit partner states.

The extension of the derivation of the spin-orbit rule to exotic nuclei, where the densities are more diffuse shall be undertaken in a forthcoming work. This includes halo nuclei involving coupling to the continuum [34–37]. It would also be relevant to derive a pseudo-spin rule, providing the typical magnitude of the related degeneracy raising due to the breaking of the pseudo-spin symmetry [18, 38], with respect to the main shell structure.

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