Reply to K. Amos et al  
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Abstract

An expression for the spin–orbit interaction coupling between different levels, which was shown to be aberrant more than thirty years ago persists in the literature without clear indication of what is used. It leads to expressions quite simpler than they should be. After an attempt to warn the community of the nuclear physicists on this strange situation (nucl-th/0312038), the authors of the publication in which the “aberrant” interaction is described and used, try to justify their work (nucl-th/0401055), by a very strange “symmetrization” of something already symmetric. They claim also that their method allows to solve some problem related to the Pauli principle and give some references, among which a book which reports the solution of such problem almost forty years ago, with a very small effect. An examination of their own results shows that their optimism is not completely justified. Nevertheless, any user of ECIS, sensitive to their arguments, is requested to ask their opinion to these five coauthors before publishing.

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After the publication of some article [1] in Nuclear Physic A, I wanted to publish a comment [2] warning the nuclear physicist community that two different deformed spin–orbit are used in the literature for nucleon–nucleus inelastic scattering without notifying which one is employed. Because everybody uses the same expression in nuclear structure studies (for this reason, I qualified it as “normal”), for inelastic scattering, I called “normal” the one which has the same behavior between partial waves and “aberrant” the other one. As I am not of native of English language, I was thinking to be allowed to use this word, because I found on page 3 of [3] :

\textbf{ab–er–rant} (…), \textit{adj.} […] deviating from what is true, correct, normal, or typical.

and on page 3 of the first volume of [4] :

\textbf{ab–er–rant} \ldots \textit{adj} […] 1: straying from the right or normal way : deviating from truth, rectitude, propriety 2: deviating from the usual or natural type : EXCEPTIONAL, ABNORMAL.
(. . . denoting pronunciation and etymology). My problem to publish such an advertisement is that I have only [1] to cite.

On the 14th of June, I was visiting the office of the Nuclear Energy Agency, at Issy–les–Moulineaux, which send nuclear codes to who wants them all over the world (except in USA). We found on the web the answer [5] of which the title is quite terrifying for some body who sent almost 300 ECIS to more than 50 countries. I find this answer largely out of the subject. I have to answer to the spin–orbit question, but also on the antisymmetrization with occupied states, another subject on which I have comments to do but which I did not want to publish.

In [2], Eq. (1) is not the spin–orbit interaction but its coefficient; the spin–orbit interaction involves the two following lines. The six–parameter spin–orbit interaction of ECIS can be used to compare results with the two different deformed spin–orbit interactions and many other expressions by who wants it; anyway, the parameters are read only if a special logical is set true. This is like that since ECIS67. Instead of laughing at, why the authors of [1] do not do the same?

As the authors of [1] say that the “normal” is derived in some extremely hard–to–find publications”, let us resume it. First of all, the two-body spin–orbit interaction as described in [6, 7, 8, 9] 1 is “normal”; therefore, the intermediate step of its use as a one-body interaction, described by the sums of two terms of Eq. (84) of [6], the Eqs. (21-22) of [7], the Eqs. (51-52) of [8], and Eqs. (4,49-50) of [9] are also “normal”. With a finite range, these expressions are a kind of folding potential for the direct term, to which must be added similar expressions for the exchange term. At the zero–range limit (not δ(r – r’), but δ’’(r – r’)), direct and exchange terms for the two–body interaction are identical : they are given by Eq. (30) of [7] and Eq. (55) of [8]. Assuming zero for the eigenvalues of (l . σ) of one particle (which means complete shells for l = j+1/2 and j = l−1/2 with same radial function), one get the same expression as with the “full Thomas term”. The result must be made hermitian, but not in the sense used by the authors of [1, 5] by dropping the derivative term acting on the right side but by replacing it by a derivation on the left side with opposite sign (that is : acting also on the form–factor).

As the “normal” coupled–channel spin–orbit potential is derived in some extremely hard–to–find publications [5] but cannot been published anywhere because it is not new, let us give it here in details. First of all, the spin–orbit obtained when the Dirac equation is changed into its Schrödinger equivalent (“full Thomas form”) can be written as :

\[ V^{LS} = \sum_{\lambda, \mu} \left( \nabla V_\lambda(r) Y_\lambda^\mu(\hat{r}) \right) \times \frac{\nabla}{i} . \sigma \]  

1In [6] there was an error for \( a^J(1, 2) \) as said in [7] : the coefficients of \( V_{J-1} \) and \( V_{J+1} \) are \( J(J-1) \) and \( (J+1)(J+2) \) instead of \( J(J+3) \) and \( (J+1)(J-2) \) respectively. There is also a factor 4 in the three first publications, coming from an error in writing the derivative with respect to \( r_1 - r_2 \) and assimilation of \( \sigma \) to \( s \). In [9], \(-n_{J\sigma\tau}^2\) and a factor 1/4 are missing in the expression of \( d^J(1, 2) \).
which avoids to deal with more equations than necessary: the zeroth order term of [1] is in \( V_0(r) \), the first order term for some \( \beta_2 \) is in \( V_2(r) \), the second order is \( V_4(r) \) and also in \( V_0(r) \) and in \( V_2(r) \) (for the \( n^{th} \) order, it is in all even \( V \), from \( V_0(r) \) to \( V_2n(r) \)). Using the following identities:

\[
\nabla = \frac{r}{r} \frac{d}{dr} - i \frac{r \times \ell}{r^2}, \quad i \sigma \cdot (A \times B) = (\sigma \cdot A)(\sigma \cdot B) - (A \cdot B),
\]

\[
(\sigma \cdot \nabla) = \frac{(\sigma \cdot r)}{r} \left( \frac{d}{dr} - \frac{(\ell \cdot r)}{r} \right), \quad (\sigma \cdot \ell)(\sigma \cdot r) = -(\sigma \cdot r)(\sigma \cdot \ell), \quad (\sigma \cdot r)^2 = r^2;
\]

\( V^{LS}(r) \) can be written as:

\[
V^{LS} = \sum_{\lambda, \mu} - \left( \left[ \frac{d}{dr} + \frac{(\ell \cdot \sigma)}{r} \right] V_\lambda(r) Y^\mu_\lambda(\hat{r}) \right) \left[ \frac{d}{dr} - \frac{(\ell \cdot \sigma)}{r} \right] \]

\[+ \left( \frac{d}{dr} V_\lambda(r) Y^\mu_\lambda(\hat{r}) \right) \frac{d}{dr} - \left( \frac{r \times \ell}{r^2} V_\lambda(r) Y^\mu_\lambda(\hat{r}) \right) \frac{r \times \ell}{r^2} \quad (3)
\]

The terms with two derivatives cancel one another. Noting by \( \ell_i \) and \( \gamma_i \) the angular momentum and the eigenvalue of \((\ell \cdot \sigma)\) of the right side, \( \ell_f \) and \( \gamma_f \) for the left side, \((\ell \cdot \sigma)\) acting on \( Y^\mu_\lambda(\hat{r}) \) can be replaced by \((\gamma_f - \gamma_i)\) because \( \ell_f = \ell_i + \lambda \). The last term can be simplified, using the relation:

\[
(A \times B). (C \times D) = (A \cdot C)(B \cdot D) - (B \cdot C)(A \cdot D)
\]

which replaces the two cross products by \( r^2(\lambda \cdot \ell_i) \). But, as \( \ell_f = \ell_i + \lambda \) and \((\ell \cdot \ell) = (\ell \cdot \sigma)^2 + (\ell \cdot \sigma) \):

\[
-2(\lambda \cdot \ell_i) = \lambda(\lambda + 1) + (\gamma_i - \gamma_f)(\gamma_i + \gamma_f + 1)
\]

With these quite simple manipulations, the result is obtained as:

\[
V^{LS} = \sum_{\lambda, \mu} Y^\mu_\lambda(\hat{r}) \left( \frac{dV_\lambda(r)}{dr} \right) \gamma_i + \frac{V_\lambda(r)}{r} \left[ (\gamma_i - \gamma_f) \frac{d}{dr} \right]
\]

\[+ \frac{V_\lambda(r)}{2r^2} \left\{ \lambda(\lambda + 1) - (\gamma_f - \gamma_i)(\gamma_f - \gamma_i \pm 1) \right\} \]

where \( \pm 1 \) is +1 in this tri–dimensional derivation and is −1 if the wave functions are multiplied by \( r \) as usual. This derivation should not be a problem to people used to angular momenta, \( \sigma \)-matrices, scalar and vector products.

To say that the first term of Eq. (6) is fully consistent with the whole is quite strange. The fact that the two last terms can be replaced \([1, 5, 10]\) by a \((\ell \cdot \ell)\) and a \((s \cdot s)\) interactions as yet to be proven. Note that the first publications which used the “full Thomas term” \([11, 12]\) did not notice the behavior \((\gamma_i - \gamma_f)\) of this term because they ignored the (quite simple) derivation presented above. This interaction is expected to play a role primarily for the asymmetry of the inelastic scattering, but less than the deformed central interaction: it should be so in the relation of the amplitude of this asymmetry with the sign of the deformation in the rotational model \([13]\). Anyway, If the deformed spin–orbit interaction plays no role in their problem \([1]\), why they use it.
The symmetrization of an operator including $d/dr$ acting on the right side is its replacement by $-d/dr$ acting on the left side, that is on the form–factor as well as the function. The use of the deformed spin–orbit [1] is equivalent to the use of:

$$V_{ijkl}^{LS}(r) = V_{ijkl}(r)\{[\ell.s]_i + [\ell.s]_j + [\ell.s]_k + [\ell.s]_l\}$$

(7)

for the two–body spin–orbit interaction, as can be seen after one integration.

In [5], there are many comments and references related to the Pauli principle of which it was not question in [2]. I was allowed by the Service de Physique Theorique to photocopy all the reference [2] of [5] in its library (including the second one in Saclay’s central library) and also the 3 references of the article in Nuclear Physics related to Pauli principle (130 pages for all that) and to borrow [14]. It seems that they never opened this book; I did not remember of its content. There is a very good table of references by which I found myself cited 8 times as RA 67b, once as RA 68 and also twice as GI 67 and once as ME 66. The first [15] of their references [2], of G. Pisent, one of the coauthors, is also cited twice as PI 67c in this book: a footnote on page 103 (In the papers concerned with $^{13}C$ as a compound nucleus the exclusion principle could not be exactly satisfied | ... , ... , PI 67c, ... |), and the last paragraph of page 113 (... and Pisent and Saruis | PI 67c). This various works suffer from the drawback that the Pauli exclusion principle is violated at some stage of the calculation.)

In Spring 1965, I was theoretically at USC, practically at UCLA, in Los Angeles. With M. A. Melkanoff and T. Sawada, we decided to do some calculations on the giant resonance of $^{16}O$ using the shell model with a continuum theory of C. Bloch and V. Gillet [16]. This work has been published in Nuclear Physics A [17] and as a seminar at a Summer School in Varenna [18]; in the same book, there is another seminar from me on the ”Stretch scheme” and a seminar entitled Results of Hartree–Fock calculations with non–local and hard–core potentials, by J. P. Svenne, Canadian of Copenhagen University, who I think to be one of the coauthors of Ken Amos. This work is partly reported in [14]. The space used is described in the book on page 23 in the text together with figure 3.2 and its legend. C. Bloch and V. Gillet could obtain values only at points which they choose for the grid, but we managed to obtain continuous results (footnote on page 77 :Care must be taken because the integrands involve $a'(E'';c)$ which is singular at $E'' = E$ |RA 67b|.) with a minimum number of points and did computation from 16 to 30 MeV (this is scattering on $^{15}O$ for which 16 MeV is the threshold with respect to $^{16}O$). Then, we decided to do the same calculation in the $r$–space instead of the $E$–space. We got different results; looking why, we orthogonalized with the 1$s_{1/2}$ occupied bound-state, thinking that a small mixture of this state give very important effects for $^{16}O(\gamma, n)$, more than for the elastic scattering because this result is the integral of the solution multiplied by $r$ and the hole function. We obtained the same result as in $E$–representation. That was the proof that these two approaches, mathematically equivalent are numerically equivalent (discarding error or imprecision on one of them). This is presented pages 106-110 with
the results in figure 6.1. On page 103, 6.3a. *Coupled channels approach* the first paragraph includes two citations prior to [17] as not taking into account antisymmetrization and quote RA 67b as showing this effect. The second paragraph is: *The most complete coupled channels calculation of the reactions* $^{16}\text{O}(\gamma, n)$ and $^{16}\text{O}(\gamma, n)$ (*for E1 transitions*) *was carried through by Raynal, Melkanoff and Sawada* [RA 67b]. *These authors treat antisymmetrization correctly.* In fact, I never saw the *Pauli principle* expressed more clearly than by Eqs. (19-20) of [18] or Eqs. (55-58) of [17] (Eqs. (59-61) for a zero–range interaction). The reference [19] given in [1] uses only a $1s(\alpha)$ state with no generalization.

More details can be found in [17, 18]: figures 12 and 13 in the first reproduced by figures 4 and 3 in the second show the results obtained respectively for $^{16}\text{O}(\gamma, n)$ and $^{16}\text{O}(\gamma, p)$ with five channels and coupling the ten channels. In neutron figures, there are:

- the five channels result,
- the ten channels one,
- the experimental results known at that time,
- and also results obtained with five channels without taking into account the occupation of the $1s_{1/2}$ state.

Unhappily, this last curve is not given in figure 6.1 of [14] which shows only five channels results and experimental data for neutrons and not this fourth curve which is essential to clarify the point in discussion: there is no noticeable effect up to 20 MeV (4.5 MeV above threshold) but a shift of the maximum around 22 MeV, about the same as between five and ten channels calculations. In the same two publications, we showed that the difficulty to deal with a resonance $d_{3/2}$ in the continuum in E–representation can be overcome by using a bound–state and taking into account the difference of the Saxon–Woods wells in r–representation or E–representation. In [17, 20], we studied the effect of a $2p–2h$ state as quoted GI 67 by [14] on pages 108 and 225.

I foresee Ken Amos’ answer: it is not the same problem, you deal with $^{15}\text{O}$ and $^{15}\text{N}$ and not $^{12}\text{C}$, you use some two–body interaction instead of a pure one–body, and so on, and so on ... But look to their own results, table I, page 86 of [1] the three lines where there are experimental data and results with and without OPP: for the first, the energy is shifted by 33% of what is needed, in the good direction but the width is increased of 20% only instead of 148%; in the second one the energy is shifted of only 4% of what is needed and the width unchanged; in the third one, the energy is shifted of 82% of what is needed, in the good direction (great success) but the width is increased 15% instead of being divided by 4.33; in a fourth case, there is no effect. With these values, they claim that this antisymmetrization is absolutely necessary; with the same values, I feel that it disturbs the results.

On the 25th of June 1975, I participated to the jury for the thesis of J.–M. Normand [21] at Orsay with V. Gillet, P. Benoist–Gueutal, M. Goldman and R. Arvieu as president. He showed the effect of the Pauli principle at threshold...
energies [22]. He studied scattering lengths and effective ranges of neutrons, which I think quite sensitive to these effects, on $^{12}C$, $^{13}C$, $^{16}O$, $^{17}O$, $^{19}F$ and $^{40}Ca$. Only the scattering lengths were known at that time. In table 5, using 4 different interactions with different strengths (in all 14 calculations), he found for $^{12}C$ a decrease of 8% to 21% for the scattering length, of 4% to 7% for the effective range (but, among these 14 calculations, the smallest value is 54% of the largest one for the scattering length and 30% for the effective range, 30% and 20% discarding the largest value). In table 6, for $^{16}O$, also with 4 interactions and 13 calculations, these figures reduce to 5% to 7% for the scattering length, 2% to 4% for the effective range and values spread by 12% for both. In Table 7 for $^{40}Ca$, with 2 interactions and 6 calculations, there is no effect of the $1s_{1/2}$ state (less than 0.3%) but a large effect of the $2s_{1/2}$, 21% to 42% for the scattering length, 15% to 31% for effective range, leading to almost identical results; the variation of this last results are 0.6% and 1.1% for a variation of 4.2% and 3.3% of the strength of the interaction (very special case for which the Pauli principle is more important than the model, id est, than the strength of the interaction). In table 8 are given 6 results for $^{13}C$ and 2 for $^{17}O$ ; in this table, there are results for two values of $J$. In all these cases, one can see that the corrected results are quite near the uncorrected ones obtained with an increase of the interaction by about 3%. Results for $^{19}F$ show the importance of the choice of the space of configuration.

Even if the effects are more important for $^{12}C$ than $^{16}O$, I do not see in this very sensitive calculation a justification of the assertion of Ken Amos that the Pauli principle affects strongly results at low energy and it is not their publication which can convince looking their table 1. Anyway, such phenomena are weaker with a complex potential (because the wave function is damped inside the nucleus) and ECIS was not written for such problems. As said in the title, any user of these codes who has the smallest doubt about this subject should ask their opinion to K. Amos et al. Anyway, it is a lot easier to add that to ECIS than to introduce a quadratic spin-orbit which was never seriously used in DWBA90.

In [5], these is a reference to page 426 of Hodgson’s book [23]; in the following pages, there is a presentation of [10] and of some publications of G. Pisent, before or after [15] with no allusion to the “Pauli exclusion principle”. In the subject index, seven pages are indicated for this topic:

- page 90 on semiclassical optical model,
- page 113 for application in nuclear medium,
- pages 130, 131, 132 for the calculation of the imaginary part of the optical potential,
- page 162 related to consequences for nuclear medium,
- page 581 consider the effect of the excess of neutrons on the difference between the number of reactions $(p,n)$ and $(n,p)$. 
The “Pauli exclusion principle” applied to the scattering wave is completely ignored in this book where this effect is only applied to nucleon–nucleon scattering in nuclear medium as needed in [24] : the critics of [5] on the conception of ECIS are also valid for it. There is no question of spin–orbit deformation : [11, 12] are not cited. My own thesis is cited for different points (an error on page 148, not reproduced on pages 231, 235 and 244) including figure 10.6 on elastic deuteron scattering.

The third book [25] cited in [5] is not available at Saclay. I cannot afford to buy it and analyze it as I did above for the two first ones.

I hope that every user of ECIS will make his own opinion on [5] and my answer, even those who use it for heavy–ion scattering because the title does not exclude this subject. If they have any doubt, they should communicate their results to the five coauthors of which they can find the e–mail address in [1].

Conclusions

• When they say : the spin–orbit expression we use is fully consistent with the S.L term that comes from the full–fledged Thomas term, they forget to add that they pluck.

• If they open the books which they give as reference, they can see that the effects which they claim to be at low energy are seen only at higher energy. Even if they are some effects [21, 22], they can disappear if there is a search on parameters as in [1].

• If they look at the table which they publish, they have to agree that the Pauli principle is inefficient to give good results : readers can conclude that their method is bad or that the Pauli principle has no notable effects but cannot agree with their optimistic comments.

Anyway, the Pauli principle was not the subject of [2] but the fact to see in the literature an expression which I believed forgotten since a long time and was certainly used many times without being quoted. The “normal” expression is easy to derive as shown by equations (2) to (6) there in. The allusion to a mosquito and an elephant at the end of [5] reminds a tale of La Fontaine about a frog and an ox. Errare humanum est (see footnote); perseverare diabolicum.

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