Raynal’s use of the word ‘‘aberrant’’ appears more appropriate for his ECIS formulation

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Abstract

Recently, we published a paper (Nucl. Phys. A 728 (2003) 65) presenting a new calculational method for nucleon-nucleus elastic scattering at low energies. That method is particularly appropriate for analyses in the region of narrow resonances. The method is based upon the sturmian representation of the S-matrix, and allows inclusion of nonlocality effects due to Pauli principle. It also provides a systematic identification of narrow-resonance spectra and subthreshold bound states. A phenomenological test calculation for low-energy (below 4 MeV) neutrons on $^{12}\text{C}$ (including the first two excitations of the target) was presented to illustrate the validity of the approach. The model calculation received a violent criticism (see nucl-th/0312038) by the developer of a method (ECIS) which to date cannot handle nonlocality effects and cannot be used easily to identify all narrow resonances. We demonstrate that Raynal’s opposition to our development is not well founded by the arguments he presents. Indeed the work we published shows, on rewording the title of nucl-th/0312038, that it is “aberrant” phenomenologically to analyze resonant low-energy nucleon-nucleus processes with coupled-channel methods without taking into account the nonlocalities due to the Pauli principle; problems typically encountered in the ECIS formulation.

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In the comment of Ref. [1], it is implied that we generate our coupled-channel spin-orbit potential by taking the standard elastic spin-orbit potential in channel c, $(1 \cdot s)_c$ and make it “coupled-channel” with the phenomenological
prescription:
\[ W_{ls}[\ell, s] c \delta_{c'c} \rightarrow \frac{W_{ls}}{2} \{ [\ell_s] c' + [\ell_s] c \} . \]  

(1)

This is not the case, but one could be misled so by Eq. (1) of Ref. [1], where one small piece of a complex formula is taken out of context.

Then Raynal makes an illegitimate comparison of this piece alone, set apart from the context, with the six-parameter model coupled-channel spin-orbit potential used in his code ECIS and derived in some extremely hard-to-find publications. In his article, Ref. [1], he persists in the erroneous claim that we do such limited kind of coupled-channel generalisation of the elastic spin-orbit term [see Eqs. (5-6)].

Given that the false criticism could be disguised by his presentation we restate here how we generate the coupled-channel \( L \cdot S \) term in our phenomenological test calculation and what are the considerations involved.

The use of a deformed optical potential to reproduce a low energy spectrum of resonances is quite a peculiar problem. The literature on the argument can be traced back (to our knowledge) to few references [2]. The problem has been also summarised by P.E. Hodgson in his book [3]. With respect to usual (central or deformed) optical model analyses, this specific problem is characterised by the low energies involved and the discrete structure of the resonance spectrum. Since the potential parameters collectively influence the resonance spectrum, the inverse-problem solution (derivation of the potential parameters from fitting the background and resonances) therefore is particularly cumbersome.

Ref. [4] discusses a particular technique of algebraization of the multichannel scattering problem through finite–rank expansion of the interaction. The technique is particularly suitable for the problem because it allows one: (a) systematically to find the narrow and super-narrow (compound) resonances through the study of sturmian trajectories, by-passing the major computing problem of using an extremely fine energy grid, and (b) to eliminate the Pauli–forbidden states from the channel couplings.

The last point is particularly important. In table I of Ref. [4] we compare the spectra obtained with and without elimination of the Pauli–forbidden states. Pauli blocking matters significantly, and points to a known but unfortunately frequently forgotten issue: when nucleon–nucleus processes are described by collective degrees of freedom, the associated calculations typically disregard the antisymmetrization effects. Note that these effects are also relevant for DWBA calculations of scattering [5].

The particular choice made for the input-potential form in no way detracts from these major points of our paper. However, Raynal has misrepresented what we have used and so we review the model potential we have employed in our test calculation. The choice of the phenomenological potential is an old form [2], namely a central part plus a spin–orbit term (with surface–type radial dependencies) plus spin–spin and orbit–orbit terms (with volume–type radial dependence). All coefficients are considered as adjustable parameters, to be determined through the fitting procedure. Raynal objects to the spin-orbit aspect arguing for a form derived from reduction of the Thomas term. But all
are merely phenomenological representations.

Using the notation given in our paper [4], we write the Thomas term as follows:

\[ V_{th} = -iV_{ls} \mathbf{S} \cdot (\nabla f \times \nabla), \] (2)

where \( \mathbf{S} \) is the nucleon spin operator and \( f \) is defined by Eq. (37) of Ref. [4] in the case of central interaction.

One can write the Laplacian in the form

\[ \nabla = \frac{\mathbf{r}}{r} \nabla_r + \frac{1}{r} \nabla_\Omega ; \quad \mathbf{L} = -i \mathbf{r} \times \nabla. \] (3)

Then, for central potentials [\( f = f(r) \)], the usual expression is easily found, namely:

\[ V_{th} = V_{ls} \frac{1}{r} \frac{df}{dr} \mathbf{S} \cdot \mathbf{L}. \] (4)

We now introduce distortion as in the Tamura model [6]. The new distorted potential is described by equations (38) and (39) of Ref. [4]. If we consider for the moment first-order expansion in the deformation parameter \( \beta \) of the factor \( f \) as given in Eq. (12) of Ref. [4], we obtain

\[ V = V_{ls} \left\{ \frac{1}{r} \frac{df}{dr} + \epsilon \frac{d}{dr} \frac{df}{dc} \right\} \mathbf{S} \cdot \mathbf{L} - i \frac{df}{dc} \left[ (\nabla_\Omega \epsilon) \times \nabla \right]. \] (5)

Here and in the following all derivatives of \( f \) are meant to be calculated in the limit \( \epsilon = 0. \)

In this potential the first two terms correspond (apart from some different notation) to Eqs. (3) and (5.1) of Ref. [7], and are usual spin–orbit potentials. The third term refers to Eq. (5.2) of Ref. [7].

If one substitutes Eq. (39) of Ref. [4] (up to first order) into Eq. (4), one obtains exactly the first two terms of Eq. (5), namely:

\[ V = V_{ls} \frac{1}{r} \frac{df}{dr} + \epsilon \frac{d}{dr} \frac{df}{dc} \] (6)

However, in our approach we introduce also distortions to second order. For simplicity, we introduce distortions directly in the spin-orbit Eq. (4) [instead of using Eq. (2)]. In addition, we consider a phenomenological spin–spin and also an orbit–orbit potential. Note, in particular, that a spin–spin potential in our model was necessary to have the correct separation between \( J^\pi = \frac{3}{2}^+ \) and \( J^\pi = \frac{5}{2}^+ \) resonances in the spectrum; an aspect extensively discussed by Tanifugi et al. in Ref. [2].

Going to second order, namely assuming complete expansion as in Eq. (39) of Ref. [4], similar results are obtained. Eq. (5) then becomes:

\[ V_{th} = V_{ls} \left\{ \frac{1}{r} \frac{df}{dr} + \epsilon \frac{d}{dr} \frac{df}{dc} + \epsilon^2 \frac{d^2 f}{dr d\epsilon} \right\} \mathbf{S} \cdot \mathbf{L} - i \frac{df}{dc} \left\{ \left[ \frac{d}{d\epsilon} (\nabla_\Omega \epsilon) + \frac{d^2 f}{d\epsilon^2} (\nabla_\Omega \epsilon^2) \right] \nabla \right\}, \] (7)

and Eq. (6) assumes now the following form:

\[ V = V_{ls} \frac{1}{r} \frac{df}{dr} + \epsilon \frac{d}{dr} \frac{df}{dc} + \epsilon^2 \frac{d^2 f}{dr d\epsilon^2} \] (8)
This corresponds exactly to the first part of Eq. (7), and is the spin–orbit part of our interaction, which includes channel-coupling and deformations.

The second part of Eq. (7) is generally disregarded in calculations because it leads to a very complicated form and certainly it does not represent a conventional spin-orbit \((\mathbf{S} \cdot \mathbf{L})\)-type term. It can be shown that it contains some type of spin-spin structure and note that an effective spin-spin interaction is already included in our model potential.

Clearly, the form we use [see Eq. (8)] is fully consistent with the \(\mathbf{S} \cdot \mathbf{L}\) that comes from the Thomas term. That it can be considered inconsistent or aberrant, as stated by Raynal, is simply false. Note that we never claimed that the term in Eq. (8) represents the fully complete spin structure of the deformed optical potential. The model we use has indeed additional spin and orbital terms contributing to the spin-structure of the deformed optical potential.

Now we come to the problem of the symmetrization of the potential. Symmetrization is needed because our low-energy potential (which is purely a real operator) is not symmetric when all the spin operators (spin-spin, orbit-orbit and spin-orbit) are coupled with the deformation operator. Thus symmetrization is needed to recover unitarity in the S-matrix.

In absence of deformation the global interaction is given by Eq. (36) of Ref. [4], with \(f\) and \(g\) given by Eqs. (37) therein. When deformation is switched on, we may write in operatorial and schematic form:

\[
V = f\left[V_0 + V_{0L}\mathbf{L} \cdot \mathbf{L} + V_{ss}\mathbf{S} \cdot \mathbf{I}\right] + g V_{ls}\mathbf{L} \cdot \mathbf{S},
\]

where now \(f\) and \(g\) are operators derived by introducing deformation into the expressions \(f(r, R)\) and \(g(r, R)\) of Eq. (37) of Ref. [4].

The expression of \(\epsilon\) in Eq. (38) of Ref. [4] implies\(^1\) that the operators \(f\) and \(g\) contain tensor terms of the type \(Y_2(\hat{r}) \cdot Y_2(\hat{s})\) and \(Y_4(\hat{r}) \cdot Y_4(\hat{s})\) (\(\hat{s}\) standing for the internal target coordinates) and Eq. (41) of Ref. [4] gives the detailed expression of \(f\). In our representation, these terms originate the channel couplings.

Since, in general, these tensor operators do not commute with the spin– and orbit–dependent operators, it is necessary to symmetrize Eq. (9), as follows:

\[
V = V_0 f + V_{0L}[\mathbf{L} \cdot \mathbf{L} f + f \mathbf{L} \cdot \mathbf{L}] + V_{ss}[\mathbf{S} \cdot \mathbf{I} f + f \mathbf{S} \cdot \mathbf{I}] + V_{ls}[\mathbf{L} \cdot \mathbf{S} g + g \mathbf{L} \cdot \mathbf{S}].
\]

Finally, projection on states defined by Eq. (35) of Ref. [4], and use of completeness properties, give rise to Eq. (42) therein. This expression is similar but more general than the expression reported in Eq. (7) of Ref. [7].

It is important to note that we used this phenomenological model interaction to test the sturmian algebraic method for narrow-resonance identification and to exhibit the relevance of the Pauli principle in the bound and resonance spectra. For neutron-\(^{12}\)C scattering that interaction was sufficiently structured (but not exceedingly complicated) to determine S-matrices from which

\(^1\)Note that in our case \(L = 2\)
the elastic scattering data at very low energy was well reproduced. Never did we claim use of a unique starting model interaction. Nonetheless, the terms involved (central, spin-orbit, spin-spin, and orbit-orbit) are ones that typically appear in semi-relativistic reductions, *e.g.* using, the Foldy-Wouthuysen transformation in atomic and molecular processes. We, and many others, have used them in the nucleon-nucleus context in a purely phenomenological sense. These terms, however, do not saturate all the possible type of operators that can be constructed to describe semi-relativistic and many-body effects that can be possibly contained in this extremely complicated nucleon-nucleus optical potential. There is no claim in our work that the terms in our model calculation represents “the most general and complete form of optical potential that can be constructed at a given order in the deformation parameter”. That is, in our opinion, beyond present-day knowledge.

One should consider also that involved spin-spin and even tensor structures naturally appear in the multinucleon interaction operators, and precisely in this particular symmetrized form, if one combines pion-exchange dynamics with two-nucleon correlations in a rigorous three-nucleon calculation. These specific forms are known to have important effects for the vector analyzing powers of nucleon-deuteron scattering at low energy[8].

As a matter of fact, the interaction so defined is sufficiently structured and flexible with respect to parameter variation that a sound phenomenological analysis was possible, *provided that* the Pauli principle is taken into account and a powerful technique of resonance identification is used. According to Raynal, the merit of our work is only to show that some physicists are still using certain expressions for the deformed spin-orbit interaction, which in Ref. [7] is shown to give slightly different results with respect to use of the “complete” Thomas term in DWBA calculations. But these effects are at higher energies and specifically for the analysing powers of the inelastic transitions.

Raynal fails to realize that we use a model interaction which is much more rich in structure (spin-spin, orbit-orbit, with addition of linear and quadratic deformation operators) with respect to what has been used in the references he cites. Most importantly, our analysis is of the low-energy regime where only the elastic channel is accessible and the main issue concerns the structure of the resonant spectrum as seen in the elastic process. Here our analysis show that inconsistent results can be produced if nonlocalities due to the Pauli principle are not taken into account, a problem that points directly to a serious flaw in the use of the ECIS formulation for such kind of problems. This means simply that the relevance of the detailed structure of the deformed spin-orbit potential, in this low-energy domain and for the kind of observable that we consider, is still an open question. Instead of producing sterile polemics Raynal should try to overcome these methodological difficulties embedded in his ECIS calculational scheme.

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2However, the results by Blair and Sherif suggest that it is a question needing answer if one deals with inelastic spin observables and not with cross section
Conclusions

We have replied to the criticism by Raynal in nucl-th/0312038. Because the issue was poorly explained in that reference, we had first to make it intelligible. To summarise, the criticism is centered on the fact that we tested our calculation method within a model scheme which contains a spin-orbit term Raynal termed “aberrant”. We showed in this reply that this is not the case, since the spin-orbit expression that we use is fully consistent with the $S \cdot L$ term that comes from the full-fledged Thomas term.

In case of deformed nuclei, it is known that the $S \cdot L$ term does not exhaust all the possible spin structures of the (coupled-channel) potential. In fact, to reproduce the data we phenomenologically included additional deformed (coupled-channel) spin-spin and orbital-orbital terms, and carried over deformations to second order. Moreover, our coupled-channel potential is suited for very low-energy, and has to be hermitian. Because spin and/or orbital operators do not commute in general with the deformation operators, it has to be made hermitian by a symmetrization prescription. This puts a further constraint in the spin structure, which has been duly taken into account.

To support the criticism, Raynal refers to old calculations. Of those quoted calculations, only that by Sherif and Blair in Ref. [7] can be found with ease in the literature. These DWBA-type calculations refer to much higher energies (above 20 MeV), and specifically to the analysing powers for the inelastic process. Some differences were found at forward angles for this specific observable, between results obtained with the full Thomas term compared with those found using the symmetrized $L \cdot S$ part of the Thomas term. However, Raynal seems to have missed that the very same reference warns that already at 18.6 MeV incident protons, this claim is not anymore fully consistent.

In conclusion, the criticism moved by Raynal against our analysis is not based on firm grounds because:

(i) our analysis is for the nucleon-carbon process at significantly lower energies where the main problem is specified by the structure of the resonance spectrum. Our computational method is particularly designed for this kind of problem.

(ii) our analysis refers to elastic processes and observables, since these are the only possible observables in nucleon scattering at such low energies. Instead, the effect of the full Thomas term has been seen mainly at higher energies and for an inelastic scattering spin observable.

(iii) our model interaction is richer in its coupled-channel spin structure with respect to that analysed so far by the references quoted in nucl-th/0312038. It contains additional deformed spin-spin and orbit-orbit terms and all terms are carried to second order in the deformation parameter. For the specific physical problem considered that structure has been proved to be sufficiently rich to obtain a good reproduction of the resonant spectra, of the background cross section, and of the elastic analysing power below 4 MeV.

(iv) most importantly, our work has clearly shown that phenomenological analyses such as those based on the ECIS formulation are seriously flawed because they ignore in the coupled-channel optical potential the effects due to the Pauli principle and, more specifically, of spurious states and resonances.
The coupling of the single-particle dynamics with collective-type degrees of freedom of the target has been long known to lead to an explicit violation of the exclusion principle. This fact is clearly stated in old books [9] as well as in widely used modern nuclear physics textbooks [10]. The combined use of the sturmian representation (aka Weinberg states) with the technique of orthogonalizing pseudo-potentials allows one to incorporate in the optical potential, formed by a collective model of the target structure, the strongly nonlocal effects of the projectile-bound nucleon indistinguishability, thus finally overcoming this notorious violation of the Pauli exclusion principle. Bound and super-narrow resonance spectra are strongly affected by this additional nonlocal term. Without this additional nonlocal piece the corresponding spectra are largely inconsistent, and this points to a serious limitation in the use of the ECIS method in phenomenological analyses for low-energy nucleon-nucleus scattering processes. Given this problem, Raynal’s polemics about the precise structure of the deformed spin-orbit potential in our low-energy neutron-$^{12}$C test analysis suggests the curious situation of a person trying to call everybody’s attention to a tiny mosquito outside a closed window, while an elephant is sitting right in the middle of his dining room.

References

[1] J. Raynal, “An aberrant ...” nucl-th/0312038

[2] G.Pisent, A.M.Saruis, Nucl. Phys. 91 (1967) 561; A.Pascolini, G.Pisent, F.Zardi, Lett. Nuovo Cimento 1 (1969) 643; J.T.Reynolds, C.J.Slavik, C.R.Lubitz, N.C.Francis, Pys. Rev. 176 (1968) 1213; A.C.L.Barnard, Phys. Rev. 155 (1967) 1135; 1213; O.Mikoshiba, T.Teresawa, M.Tanifugi, Nucl. Phys. A168 (1971) 417.

[3] P.E.Hodgson, Nuclear Reactions and Nuclear Structure, Clarendon Press (1971), 426

[4] K.Amos, L.Canton, G.Pisent, J.P.Svenne, D. van der Knijff, Nucl. Phys. A728 (2003) 65.

[5] K. Amos, P.J. Dortmans, H. V. von Geramb, S. Karataglidis, and J. Raynal, Adv. in Nucl. Phys. 25, 275 (2000).

[6] T. Tamura, Rev. Mod. Phys. 37, 679 (1965).

[7] H. Sherif, J. S. Blair,., Phys. Lett. 26B, 489 (1968).

[8] L. Canton, W. Schadow, Phys. Rev. C 64:031001 (2001)

[9] C. Mahaux H. A. Weidenmuller, Shell model approach to nuclear reactions, North-Holland, Amsterdam, 1969.

[10] W. Greiner J. A. Marhun, Nuclear Models, Springer-Verlag, Berlin, 1996.