Reply to "Calculation of the Lorentz-weighted average S matrix from high-resolution low-energy neutron scattering data"

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We substantiate our previous results on the danger of identifying the energy-average scattering function with the Lorentz-weighted average of a scattering function fitted to the experimental data in a finite energy interval.

This is a rebuttal to the Comment by MacDonald and Birse[1] against our work[2] and in defense of theirs.[3,4] These papers deal with the following three topics: (i) the definition and the calculation of the energy average of the scattering function from high-resolution low-energy neutron scattering data, (ii) the specific example of the scattering of $p_{3/2}$ neutrons by ^{32}S and (iii) the definition of the optical-model potential.

Definition and calculation of the energy-averaged scattering function

The elastic scattering cross section for pure neutron elastic scattering reads

$$\sigma(E)=\pi k^{-2} g|1-S(E)|^2 \ , \tag{1}$$

where g is the spin statistical factor. The energy average $\langle\sigma(E)\rangle$ of $\sigma(E)$ can be expressed in terms of the average $\langle S(E)\rangle$ of the scattering function $S(E)$ if one makes the usual assumption that the factor k^{-2} need not be averaged over. An energy average can be written in the general form

$$\langle S(E;I)\rangle=\int_{-\infty}^{\infty} dE' F(E,E';I) S(E') \ , \tag{2}$$

where the normalized weight function F should represent the energy profile of the beam.[3] Brown[5] has pointed out that the Lorentzian weight

$$F_L(E,E';I)=\frac{\pi^{-1} I}{(E-E')^2+I^2} \tag{3}$$

is quite convenient. Indeed, one has then

$$\langle S(E;I)\rangle_{L\infty}=S(E+iI) \ , \tag{4}$$

where the indices L and ∞ respectively refer to the Lorentzian and to the integration limits in Eq. (2). The conditions of validity of "Brown's theorem" (4) are that $S(E)$ be analytic in the upper half of the complex E plane and that $|S(E)|$ remain finite for $|E|\to\infty$ in that half-plane.

We have no queries about the validity of this theorem for the actual scattering function and about the identification of $S(E+iI)$ with the average of $S(E)$ in most theoretical works. However, we showed in Ref. 3 that it can be quite inaccurate to approximate the average of $S(E)$ by $S_p(E+iI)$, where $S_p(E)$ is a *parametric approximation* derived from the analysis of high-resolution low-energy neutron scattering experiments. By necessity, the experimental data are affected by uncertainties and only cover a finite energy range $[E_l,E_u]$ that we call the "experimental domain." Most analyses use the convenient R-matrix parametrization[6]

$$S_p(E)=e^{-2i\phi(E)}\frac{1+iP(E)R_p(E)}{1-iP(E)R_p(E)} \ , \tag{5}$$

where $R_p(E)$ is written as the sum

$$R_p(E)=R^{\rm ext}(E)+R^{\rm int}(E) \tag{6a}$$

of a function $R^{\rm ext}(E)$ which is a smooth function of energy in the domain $[E_l,E_u]$ and of the "internal R function"

$$R^{\rm int}(E)=\sum_{\lambda=1}^{N}\gamma_\lambda^2/(E_\lambda-E) \ , \tag{6b}$$

where the sum over λ runs over the N resonances observed in the experimental domain. We now spell out and substantiate our main objections against approximating $S(E+iI)$ by $S_p(E+iI)$.

(a) Brown's theorem is not valid for expression (5) because of the hard sphere factor $\exp[-2i\phi(E)]$. This was shown on p. 1920 of Ref. 2. We do not elaborate on this difficulty because we expressed on p. 1921 of Ref. 2 our agreement with the practice of not replacing E by $E+iI$ in $\phi(E)$ adopted by all authors (see, e.g., Refs. 5 and 7) except MacDonald and Birse.[1,3,4]

(b) $S_p(E+iI)$ can be significantly different from $S(E+iI)$ even when $S_p(E)$ fulfills the requirements for the applicability of Brown's theorem. We substantiate this statement by the following simple but nevertheless realistic example,

$$S_p(E)=\frac{1+iP[a+bE+R^{\rm int}(E)]}{1-iP[a+bE+R^{\rm int}(E)]} \ , \tag{7}$$

where P is a constant. The conditions of applicability of Brown's theorem are fulfilled if $b\geq 0$. Let us write

$S_p(E+iI)$ in the familiar form

$$S_p(E+iI)=\frac{1+iP[\bar{R}_p(E)+i\pi s_p(E)]}{1-iP[\bar{R}_p(E)+i\pi s_p(E)]} \quad ; \tag{8}$$

the corresponding "strength function" $s_p(E)$ is given by

$$s_p(E)=\frac{bI}{\pi}+I\sum_{\lambda=1}^{N}\frac{\gamma_\lambda^2}{(E_\lambda-E)^2+I^2} \quad . \tag{9}$$

The first term on the right-hand side of Eq. (9) can be dubbed "spurious" since it is not related to the usual strength function $\langle\gamma_\lambda^2\rangle/d$; it can be as large as the second term as we show in Sec. II; it is furthermore proportional to the averaging interval I. This first term is the main origin of the problem exhibited in Fig. 10 of Ref. 2. Its appearance reflects the drawback that "the Lorentzian weight overemphasizes the importance of distant states."[8] In the present context, it introduces a sensitivity upon the detailed parametrization of the background $R^{\text{ext}}(E)$ which arises from resonances which lie far from the experimental domain and on which one thus has little information.

(c) Two accurate parametrizations $S_p^{(1)}(E)$ and $S_p^{(2)}(E)$ which both fulfill the conditions of applicability of Brown's theorem can lead to quantities $S_p^{(1)}(E+iI)$ and $S_p^{(2)}(E+iI)$ which are significantly different. This fact derives from the sensitivity of $S_p^{(1)}(E)$ to the parametrization of $R^{\text{ext}}(E)$. It will be illustrated by a realistic example in Sec. II. Here, we consider the simple example of a background due to the tail of a resonance which lies far from $[E_l,E_u]$. We thus take

$$S_p(E)=1-i\Gamma_0/(E-E_0+\tfrac{1}{2}i\Gamma_0) \quad .$$

For $E\approx 0$, $|E_0|\gg\Gamma_0$, the quantity $S_p(E)$ only depends upon *one* parameter, namely the ratio Γ_0/E_0. The strength function s_p as defined by Eq. (8) is given by $(2\pi)^{-1}\times\Gamma_0 I/E_0^2$; it depends upon *two* parameters, namely Γ_0/E_0 and E_0, i.e., upon one parameter on which the measured resonance tail is not sensitive; it is proportional to I.

In order to identify and avoid these pitfalls associated with the application of Brown's definition to a parametrization of the scattering function, we defined in Ref. 2 the average S function by the integral

$$\langle S_p(\langle E\rangle)\rangle=\int_{E_l}^{E_u}dE'F(E,E';I)S_p(E') \tag{10}$$

that we evaluated by numerical integration. Since this definition involves only the values of $S_p(E)$ for E *inside* the experimental domain, it is not sensitive to the choice of a specific parametrization of the data. The average energy $\langle E\rangle$ on the left-hand side of Eq. (10) was introduced in order to reduce the spurious energy dependence due to end-point effects. These end-point distortions limit the usefulness of the definition (10) in the domain where $|E-E_u|$ or $|E-E_l|$ is comparable to I; but the average (10) is quite reliable in the middle of the experimental domain. We found that expression (10) is quite stable with respect to variations of the weight factor F. This is a requirement for the meaningfulness of the standard optical model, since empirical optical-model potentials do not refer to a specific weight factor. The definition (10) enabled us to identify the origin of the problems associated with the practical application of Brown's theorem and to propose for $\langle S_p(\langle E\rangle)\rangle$ an algebraic expression whose accuracy has been demonstrated in the case when the strength function $\langle\gamma^2\rangle/d$ can be considered as constant in the experimental domain.

Application to $n+{}^{32}S$

The high-resolution data on the scattering of $p_{3/2}$ neutrons by ^{32}S in the domain [0, 1100 keV] were analyzed by Johnson and Winters[9] with the parametric expressions (5)–(6b). MacDonald and Birse[1,3] criticize this parametrization and advocate the use of the parametrization

$$S_p^{(2)}(E)=e^{-2i\phi(E)}\frac{1+i[S(E)-B+iP(E)]R_p^{(2)}(E)}{1-i[S(E)-B+iP(E)]R_p^{(2)}(E)} \quad , \tag{11}$$

$$R_p^{(2)}(E)=R_2^{\text{ext}}(E)+R_2^{\text{int}}(E) \quad , \tag{12}$$

with the choice $B=-1$ for the R-matrix boundary condition parameter. The choice of the boundary condition parameter is actually irrelevant as far as our discussion in Sec. I is concerned since the conditions of applicability of Brown's theorem are fulfilled in both cases provided that one leaves untouched the common hard sphere factor $\exp[-2i\phi(E)]$ as usual. We have nevertheless verified numerically that the numerical value of $\langle S_p(\langle E\rangle)\rangle$ [Eq. (10)] as well as its algebraic approximation yields practically the same values of the compound elastic and shape elastic cross sections for the parametrization (5) as well as with the parametrization (11) for both $B=-1$ and for $B=S(E=600\text{ keV})$.

The quantity $R_2^{\text{ext}}(E)$ obtained by MacDonald[3] from the parametrization (11) and (12) with $B=-1$ is represented by the open dots in Fig. 1. A least-squares fit with the expression

$$R_2^{\text{ext}}(E)=\alpha_2+\beta_2E-s_2\ln\frac{E_u-E}{E-E_l} \quad , \tag{13}$$

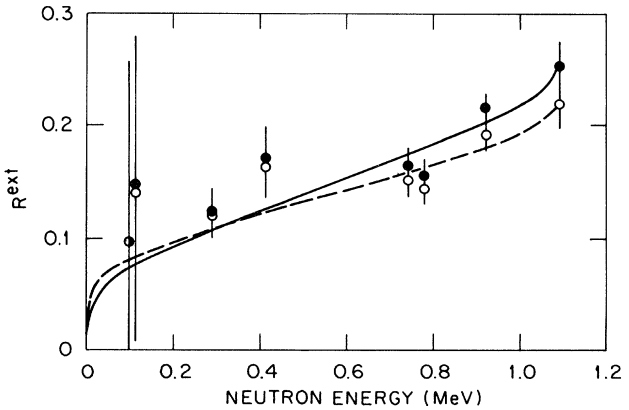

FIG. 1. Energy dependence of $R^{\text{ext}}(E)$ for the scattering of $p_{3/2}$ neutrons by ^{32}S. The full dots correspond to the parametrization (5) of Johnson and Winters (Ref. 9) and the open dots to the parametrization (11) of MacDonald and Birse (Refs. 1 and 3). The curves are least-squares fits with the parametric form (13).

with $s_2=0.010$, yields $\alpha_2=0.010$, $\beta_2=(0.066\pm0.032)$ MeV^{-1}. The first term on the right-hand side of Eq. (9) shows that the corresponding strength function $s_p(E)$ of Eq. (8) contains the I-dependent spurious contribution $\pi^{-1}\beta_2 I$. For the typical averaging interval $I=300$ keV this spurious contribution is equal to 0.006, and is comparable to the physical strength function $\langle\gamma^2\rangle/d=0.010\pm0.001$.[2-4,9] MacDonald and Birse did not encounter this spurious contribution in Fig. 1 of Ref. 1 because they happened to fit the open dots in Fig. 1 with expression (13), *where they set* $\beta_2=0$ and take $\alpha_2=0.150$, $s_2=0.011$.[3] The resulting disappearance of the spurious contribution $\pi^{-1}\beta_2 I$ illustrates our statement (c) in Sec. I. An even more striking illustration of this statement emerges if one notices that a good fit to the open dots in Fig. 1 is obtained by setting $\alpha_2=0.09$, $\beta_2=0.10$ MeV^{-1}, $s_2=0$. The corresponding spurious I-dependent contribution to the strength function reaches 0.009 for $I=300$ keV; it is thus practically equal to the physical strength function $\langle\gamma^2\rangle/d$.

MacDonald and Birse[1] also claim that the optical-model potential of Johnson and Winters[10] does not fit the "standard" average that we had calculated from Eq. (10). We first recall that the energy dependence of the quantities $\bar{R}$ and s calculated from this numerical average could be affected by end-point effects. Nevertheless, Fig. 12 of Ref. 2 shows that these "standard" quantities $\bar{R}$ and s are very close to the quantities $\tilde{R}$ and $\tilde{s}$ which have been adopted by Johnson and Winters to construct the shape elastic and compound elastic cross sections represented by the full curves in Fig. 3 of Ref. 10. Hence, the agreement between the predictions of their optical-model potential and the physical observables computed from the "standard" quantities $\bar{R}$ and s of Ref. 2 is as good as that displayed in Fig. 3 of Ref. 10.

Definition of the optical-model potential

We reiterate that our criticism of the use of Brown's theorem for the calculation of the average of a scattering function derived form the analysis of high-resolution neutron scattering data does *not* apply to the identification of $S(E+iI)$ with the average of the exact $S(E)$ in the theoretical literature. There, indeed, one is not hampered by the finiteness of the experimental domain. Therefore, we have no basic objection to the use of the modified optical-model wave equation advocated by MacDonald and Birse.[4] The following brief comments aim at clarifying some points and are a reminder of the existence of some earlier works not mentioned in Refs. 3 and 4. The one-body component $\psi_E(\vec{r})$ of the full scattering wave function satisfies the Schrödinger equation (we set $\hbar^2/2m=1$)

$$[E-\nabla^2-\mathscr{V}(E)]\psi_E(\vec{r})=0 \ , \tag{14}$$

where the "mass operator" $\mathscr{V}(E)$ is nonlocal and strongly depends upon energy; it is real for E smaller than the lowest inelastic threshold. Its explicit expression has been given by Lipperheide[11] in the framework of Feshbach's theory of nuclear ractions.[12] Optical-model analyses use the Schrödinger equation

$$[E-\nabla^2-V(E)-iW(E)]u_E(\vec{r})=0 \ . \tag{15}$$

Lipperheide[13] proposed the following identification,

$$V(E)+iW(E)\approx\mathscr{V}(E+iI) \ , \tag{16}$$

which has been widely used in the theoretical literature. Relation (16) is an approximation because the scattering function obtained by substituting $\mathscr{V}(E+iI)$ in Eq. (15) is not equal to $S(E+iI)$, where $S(E)$ is the exact scattering function. Equation (14) shows that the scattering function $S(E+iI)$ is obtained if one uses the wave equation

$$[E+iI-\nabla^2-\mathscr{V}(E+iI)]\psi_{E+iI}(\vec{r})=0 \ . \tag{17}$$

MacDonald and Birse[3,4] thus propose to analyze the energy-average data with the wave equation

$$[E+iI-\nabla^2-\hat{V}(E)-i\hat{W}(E)]\hat{u}_E(\vec{r})=0 \ . \tag{18}$$

It might be of interest to investigate numerically to what extent the potential $V+iW$ differs from $\hat{V}+i\hat{W}$ when both are required to yield the same model scattering function. This would provide a numerical check of the arguments presented on pp. 502 and 503 of Ref. 14 and according to which the difference between the two potentials is quite small, i.e., is much smaller than the accuracy presently reached in theoretical calculations of $\mathscr{V}(E+iI)$. This is the relevant criterion since the only merit of the wave equation (18) is that $\hat{V}(E)+i\hat{W}(E)$ can be identified with $\mathscr{V}(E+iI)$. The main drawback of Eq. (18) is that the corresponding "optical-model wave function" $\psi_{E+iI}(\vec{r})$ increases exponentially for large $|\vec{r}|$. In an infinite medium, $\psi_{E+iI}(\vec{r})$ is a plane wave whose amplitude is damped even in the absence of interaction.

In summary, we have rebutted the criticisms of MacDonald and Birse[1] and spelled out and substantiated the arguments presented in Ref. 2 against the use of an infinite range Lorentzian weight factor for averaging the scattering function obtained by fitting high-resolution low-energy neutron scattering data. The basic origin of the objections is that the tail of the Lorentzian weight factor overemphasizes the importance of the values taken by the scattering function outside the energy domain covered by the experimental data.

[1] W. M. MacDonald and M. C. Birse, Phys. Rev. C 29, 1560 (1983) (preceding paper).
[2] C. H. Johnson, N. M. Larson, C. Mahaux, and R. R. Winters, Phys. Rev. C 27, 1913 (1983).
[3] W. M. MacDonald, Nucl. Phys. A395, 221 (1983).
[4] W. M. MacDonald and M. C. Birse, Nucl. Phys. A403, 99 (1983).
[5] G. E. Brown, Rev. Mod. Phys. 31, 893 (1959).
[6] A. M. Lane and R. G. Thomas, Rev. Mod. Phys. 30, 257 (1968).
[7] J. E. Lynn, *The Theory of Neutron Resonance Reactions* (Clarendon, Oxford, 1968).
[8] H. Feshbach, private communication quoted on p. 73 of N. Austern, *Direct Nuclear Reaction Theories* (Wiley, New York, 1970).
[9] C. H. Johnson and R. R. Winters, Phys. Rev. C 21, 2190 (1980).
[10] C. H. Johnson and R. R. Winters, Phys. Rev. C 27, 416 (1983).
[11] R. Lipperheide, Nucl. Phys. 89, 97 (1966).
[12] H. Feshbach, Ann. Phys. (N.Y.) 5, 357 (1958); 19, 287 (1962).
[13] R. Lipperheide, Z. Phys. 202, 58 (1967).
[14] J. Hüfner, C. Mahaux, and H. A. Weidenmüller, Nucl. Phys. A105, 489 (1967).