Comments

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

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In a recent paper, Johnson, Larson, Mahaux, and Winters have claimed that the use of the Lorentz-weighted average to determine optical model phase shifts from low-energy neutron scattering data is invalid. We show that this conclusion is unjustified since the R-matrix parametrization fails to describe the exact S matrix as $|E|\to\infty$. We also show that the inconsistent numerical averaging precedure used by those authors leads to values of $\bar{R}$ and s which do not agree with those obtained from an optical potential fitted to the same data. Correct use of the Lorentz-weighted average avoids these problems.

We have recently shown[1] that the theorem by Brown[2] on the Lorentz-weighted average of the S matrix for elastic neutron scattering,

$$\langle S(E)\rangle_I = S(E+iI) \ , \tag{1}$$

can be used to determine phase shifts of the optical model potential (OMP) directly from high-resolution measurements of resonant cross sections. One of us (W.M.M.) has used this theory to determine parameters for an OMP for $n+{}^{32}S$ by using R-matrix parameters fitted to high-resolution data.[3] In a recent paper on energy averaging the S matrix, Johnson, Larson, Mahaux, and Winters[4] attack the basis for our approach by claiming that Eq. (1) is an approximation which is not valid if one uses the R-matrix parametrization to calculate $S(E+iI)$. JLMW illustrate the failure of "contour integration methods" by some numerical comparisons with their own "standard average." In this Comment we shall show that both the analytical and numerical results obtained by JLMW are incorrect and result from (1) the failure of the R-matrix parametrization as $|E|\to\infty$ and (2) an incorrect analytic continuation of the R-matrix parametrization into the complex energy plane.

The theorem of Brown stated in Eq. (1) above is an exact relation, not an approximation as stated by JLMW and implied by their Eq. (1.2) and their symbolic proof in Eq. (3.15). The proof we have given in the appendix of Ref. 1 shows that Eq. (1) follows from Cauchy's theorem of residues and the analyticity in the entire upper half of the physical energy sheet of the S matrix for physical potentials, viz. potentials which are continuous functions of radius and decrease exponentially at infinity.[5] For physical potentials, $|S(\mathscr{E})-1|\to 0$ as $|\mathscr{E}|\to\infty$. Excluded as physical potentials are the square well and any other potential which is truncated at some radius a_c; the truncation *introduces* into the S matrix an essential singularity at infinity so that $|S-1|\to\exp[2a_c\mathrm{Im}(k)]$ as $\mathrm{Im}(k)\to+\infty$. Since the R-matrix representation is obtained by cutting off the nuclear potential at some channel radius, it therefore necessarily fails to represent the physical S matrix as $|E|\to\infty$. Thus, the discussion of Eq. (1) given by JLMW is incorrect.

Nevertheless, contrary to JLMW, the R-matrix representation can be an excellent approximation to $S(\mathscr{E})$ for complex energies in the *finite* part of the physical energy sheet if the potential is sufficiently small outside the channel radius. In fact, the R-matrix representation for the elastic neutron channel is simply a fancy way of writing the equation for the S matrix which results from matching the interior radial wave equation $u_{jl}(r)$ to the asymptotic solution $I_l(r)-S_{jl}O_l(r)$,

$$S_{jl}(k)=\frac{u_{jl}'(a_c)I_l(a_c)-u_{jl}(a_c)I_l'(a_c)}{u_{jl}'(a_c)O_l(a_c)-u_{jl}(a_c)O_l'(a_c)} \ . \tag{2}$$

Introducing the definitions $L_l(k)\equiv a_cO_l'(a_c)/O_l(a_c)$, $\phi_l\equiv\arg I_l(a_c)$, and $R_{jl}\equiv u_{jl}(a_c)/au_{jl}'(a_c)$ gives the R-matrix representation

$$S_{jl}(k)=e^{2i\phi_l}\frac{1-L_l^*(k^*)R_{jl}(a_c)}{1-L_l(k)R_{jl}(a_c)} \ . \tag{3}$$

We have here allowed for a complex k and given a form which is suitable for analytic continuation into the complex k plane. However, as noted above, Eq. (2) or (3) cannot be used to discuss the *asymptotic* behavior of S_{jl} as $|k\to\infty$ because the limit $a_c\to\infty$ must be taken first. In taking the latter limit for a physical potential an exponentially divergent factor from $\exp(2i\phi_l)$ displayed in Eq. (3.16) by JLMW is canceled by an exponentially damped factor from the ratio in Eq. (3) above. Therefore, the exact asymptotic behavior of S_{jl} is not governed by the phase factor studied by JLMW.

JLMW have obtained the numerical results on $S(E+iI)$ presented in their Fig. 8 by using an incorrect analytic continuation of Eq. (3) to complex energies. This error arises from their use of Eq. (3.1), an approximation to Eq. (3) which has already been shown[6] to introduce an extra energy dependence into the values for R_{ext} obtained by Johnson and Winters.[7,8] To see how this comes about, we first use the result proved by Wigner[9] that a real linear fractional transformation of R_{jl} gives again an R function. Let $R_{jl}^0 = R_{jl}/(1-B_l R_{jl})$ and get

$$S_{jl}(k)=e^{2i\phi_l}\frac{1-[\mathscr{L}_l^*(k^*)-B_l]R_{jl}^0}{1-[\mathscr{L}_l(k)-B_l]R_{jl}^0} \ . \qquad (4)$$

The quantity

$$\mathscr{L}_l^0(k) \equiv \mathscr{L}_l(k) - B_l \equiv [S_l(k)-B_l] + iP_l(k)$$

is an analytic function of k whose real part can be made to vanish at some momentum k_0 corresponding to energy E_0. For low-energy reactions, the choice is $k_0=0$, corresponding to the threshold for neutron emission, which gives $B_l=-l$. However, some authors completely drop the real part of $\mathscr{L}_l^0(k)$, the subtracted shift function $S_l^0(k)=S_l(k)-B_l$. This is Eq. (3.1) of JLMW, where the function $R(E)$ is the quantity we have denoted as R_{jl}^0. Dropping $S_l^0(k)$ is a poor *approximation* for real energies; at complex energies the neglect of $S_l^0(k)$ gives an erroneous analytic continuation of the S matrix. It is sometimes argued that S_l^0 can be made exactly equal to zero by using an energy-dependent $B_l=S_l(k)$. However, the resulting R_{jl}^0 is *not* an R function, i.e., it is not an analytic function with poles *only* on the real axis. The use of Eq. (3.2) of JLMW for this R_{jl}^0 is not correct, and the use of this equation would give an erroneous continuation of R_{jl}^0, and therefore the S matrix, into the complex plane.

Neglect of the energy dependence of the shift function by Johnson and Winters[7] has also led to the strange results for $\bar{R},s$ presented in Fig. 10 of JLMW. As noted already,[6] the R^{ext} values found by Johnson and Winters include a strong energy dependence introduced by their neglect of the energy-dependent shift function in transforming from single-level parameters to R-matrix parameters. This spurious energy dependence shows up in their $\bar{R}+i\pi s = R(E+iI)$ as a very strong dependence on I. By contrast, MacDonald[3] derived γ_λ^2, E_λ, and R^{ext} values by including the shift function in the transformation from single-level parameters of Halperin, Johnson, Winters, and Macklin.[10] Shown in Fig. 1 are the $\bar{R}$ and s given by his $R(E+iI)$. The curves for $I=0.4$ MeV show less fluctuation than those for $I=0.3$ MeV, but no larger change in magnitude results from changing I.

The $\bar{R},s$ found by JLMW using their standard average are shown in our Fig. 2. Both $\bar{R}$ and s show a strong energy dependence which is in striking contrast to the $\bar{R}$ and s shown in Fig. 1. This raises the following question: Are these *energy dependences* really *both* compatible with the

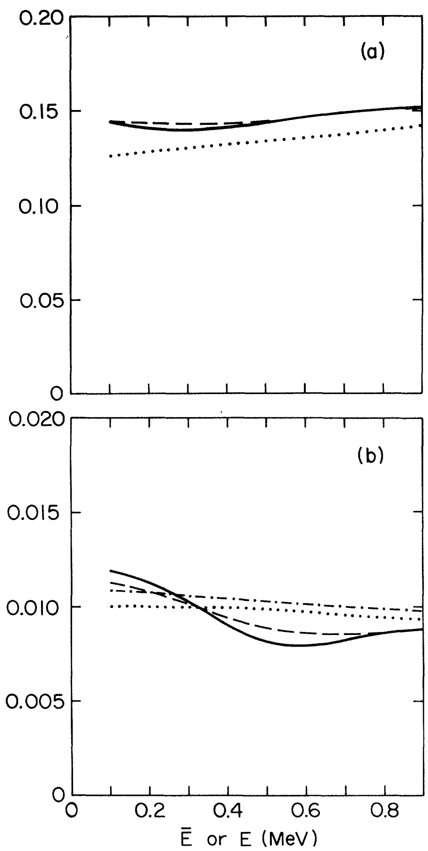

FIG. 1. The $\bar{R},s$ from $R(E+iI)=\bar{R}+i\pi s$ using the R-matrix parametrization given in Ref. (3) are compared with the corresponding quantities for the OMP found in Ref. (3). (a) $\bar{R}$ for the OMP ($\cdots$) for both $I=0.3$ and 0.4 MeV compared to $\bar{R}$ from $S(E+iI)$ for $I=0.3$ MeV (——) and $I=0.4$ MeV (— — —). (b) s for the OMP for $I=0.3$ MeV ($\cdots$) and for $I=0.4$ MeV (— · — · —) compared to s from $S(E+iI)$ for $I=0.3$ MeV (——) and $I=0.4$ MeV (— — —).

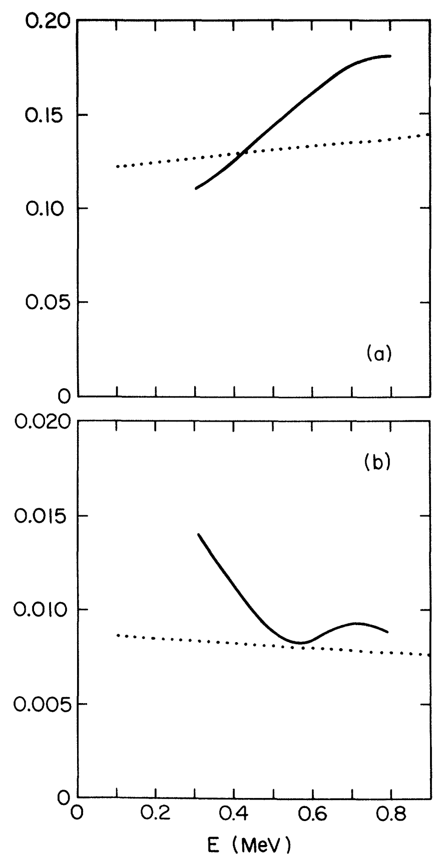

FIG. 2. The $\bar{R},s$ given by the "standard" average of JLMW (——) are compared with the $\bar{R},s$ given by the OMP of Ref. (8) ($\cdots$).

respective optical model potentials found by MacDonald[3] and by Johnson and Winters?[8] To answer the question, it is perfectly straightforward to calculate the R_{jl}^0 of an OMP for *either* real or complex energies by integrating the radial Schrödinger equation for u_{jl} out to a specified channel radius and using the expressions for R_{jl} and R_{jl}^0 given before Eqs. (3) and (4) above. Here again the functions $\bar{R},s$ are simply the real and imaginary parts of R_{jl}^0.

In Fig. 1 we have added the $\bar{R},s$ for the OMP of MacDonald[3] found by evaluating $R_{jl}^0(E+iI)$ along both $I=0.3$ MeV and $I=0.4$ MeV. The $\bar{R}$ curves are indistinguishable; the two s curves are separated by an almost constant amount equal to about 0.005. One must not expect the $\bar{R},s$ given by the OMP to agree exactly in magnitude with the $\bar{R},s$ obtained from the experimentally determined R_{jl}^0 because the OMP was not truncated at the channel radius. The OMP outside the 6.4 Fermi channel radius contributes significantly to its S matrix. We note, however, that both sets of $\bar{R}$ show the same energy dependence. The experimentally determined s fluctuates more than that of the s from the OMP, but the dependences agree rather well given the small number of levels.

In Fig. 2 we have added the $\bar{R},s$ curves found from $\bar{R}+i\pi s=R_{jl}^0(E)$ by using the OMP of Johnson and Winters[8] to calculate the R function at real energies. There is a massive disagreement between the energy dependence of $\bar{R}$ from the "standard" average and from the OMP. Moreover, we have used the OMP to calculate $\bar{R}$ at different channel radii and found that its energy dependence does not change significantly. The fluctuation of s is also much larger than that of the curves in Fig. 1(b) and the mean value in the range $E=0.3$–0.8 MeV is well above the value given by their OMP. Note also that the small differences in strengths between the OMP's given in Refs. 3 and 8, show up as shifts in the magnitudes of $\bar{R},s$ but that their energy dependences are changed very little. We conclude that the energy dependences of $\bar{R},s$ found by JLMW disagree with those of the OMP given by Johnson and Winters. Therefore, the so-called "standard" average of JLMW does not give the S matrix for their OMP.

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