Behavior of the eigenphase sum near a resonance

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(Received 21 August 1978)

It is shown that for an isolated resonance in a multichannel problem the sum of the eigenphases δ_n satisfies the usual formula appropriate for the elastic phase shift: $\Sigma_n \delta_n = \Delta^0 + \tan^{-1}[\Gamma/2(E_0 - E)]$. The parameter Γ is the total width of the resonance.

It is well known that, for an isolated resonance in single-channel scattering, the energy dependence of the phase-shift, $\delta(E)$, is described by the formula

$$\tan[\delta(E) - \delta^0] = \Gamma/2(E_0 - E), \tag{1}$$

where E_0 and Γ denote the energy and the width of the resonance, respectively. The background, or nonresonant, phase shift δ^0 is assumed to vary slowly with E in the neighborhood of E_0. Alternatively, Eq. (1) can be written in the form

$$e^{2i\delta(E)} = e^{2i\delta^0}\left(\frac{E - E_0 - \frac{1}{2}i\Gamma}{E - E_0 + \frac{1}{2}i\Gamma}\right), \tag{2}$$

which clearly shows that the S matrix has a pole at the complex energy $E_0 - \frac{1}{2}i\Gamma$.

For multichannel scattering, Macek[1] has derived a generalization of Eq. (1) to describe the energy dependence of the eigenphases, $\delta_n(E)$, namely,

$$2(E - E_0) = \sum_{m=1}^{N} \Gamma_m \cot[\delta_m^0 - \delta_n(E)], \quad n = 1, \ldots, N. \tag{3}$$

In Eq. (3) Γ_m is the partial width representing the decay of the resonance into the mth eigenchannel of the background S matrix, S^0. These eigenchannels, and the corresponding background eigenphases δ_m^0 are defined by the unitary transformation U which diagonalizes S^0:

$$U^\dagger S^0 U = e^{2i\delta^0}. \tag{4}$$

As usual, it is assumed that S^0, and therefore δ_m^0, are slowly varying functions of E near the resonance energy E_0.

In spite of its simplicity, Macek's formula [Eq. (3)] has not been used extensively in the study of multichannel resonances. This is particularly true in the case of electron-molecule collisions where even elastic scattering is a multichannel problem because the anisotropy of the electron-molecule potential couples the various partial waves. Instead, the authors of recent theoretical papers[2-11] have preferred to discuss the results in terms of the eigenphase sum: $\Delta(E) = \sum_n \delta_n(E)$. In particular, the convergence of the computed eigenphase sum has been used often to study the convergence of the partial-wave expansion in close-coupling calculations.[2-7] It has been also stated[2] that, for multichannel resonances, the eigenphase sum increases by π as the energy passes through the resonance energy. Although this behavior is not obvious *a priori*, it can be verified empirically from published eigenphases, e.g., in the case of inelastic electron-helium scattering.[12] The situation has not been clarified by the various procedures which have been employed to extract molecular resonance parameters from computed eigenphases. For example, in the case of N_2^-, Burke and Chandra[3] fitted the $^2\Pi_g$ eigenphase sum to the single-channel formula in Eq. (1) to obtain the total width. However, Buckley and Burke[10] used only the resonant, $l = 2$, eigenphase in a later calculation on N_2^-. Yet another proposed resonance formula[2] appears more appropriate for many overlapping resonances than for an isolated resonance in a multichannel problem. Thus, the theoretical situation is clearly unsatisfactory.

It is the purpose of this note to derive the energy dependence of the eigenphase sum near an isolated multichannel resonance. To my knowledge, no such derivation exists in the atomic and molecular physics literature, although it was considered previously.[13] As I will show, the eigenphase sum, $\Delta(E)$, satisfies the "single-channel" formula

$$\Delta(E) \equiv \sum_n \delta_n(E) = \Delta^0 + \tan^{-1}\frac{\Gamma}{2(E_0 - E)}, \tag{5}$$

where Γ is the *total* width of the resonance, and Δ^0 is the sum of the background eigenphases, i.e., $\Delta^0 = \sum_n \delta_n^0$.

It is convenient to start with the multichannel S matrix which can be diagonalized to yield the eigenphases:

$$e^{2i\delta} = \mathcal{V}^\dagger S \mathcal{V}. \tag{6}$$

Since $\mathcal{V}$ is a unitary matrix, and $e^{2i\delta}$ is a diagonal matrix with nonzero elements $e^{2i\delta_n}$, the eigenphase sum Δ can be obtained from the relation

$$e^{2i\Delta} \equiv e^{2i\Sigma_n \delta_n} = \det S. \tag{7}$$

Using formal resonance theory[14,15] one can show that for an isolated resonance the S matrix has the form[1]

$$S = UAU^\dagger, \tag{8}$$

where the energy dependence of the matrix elements A_{nm} is given by

$$A_{nm} = e^{i\delta_n^0}[\delta_{nm} - i(\Gamma_n\Gamma_m)^{1/2}/(E - E_0 + \tfrac{1}{2}i\Gamma)]e^{i\delta_m^0}. \tag{9}$$

As in Eq. (3), Γ_n is the partial width describing the decay of the resonance into the nth eigenchannel of S^0. The total width Γ is a simple sum of the partial widths

$$\Gamma = \sum_n \Gamma_n, \tag{10}$$

and it is independent of the definition of the individual channels. The background eigenphases δ_n^0 are defined by Eq. (4). Since the matrix U is a slowly varying function of E, Eqs. (8) and (9) imply that for an isolated resonance the multichannel S matrix has a pole at the complex energy $E_0 - \frac{1}{2}i\Gamma$.

To proceed further, one utilizes the unitarity of U to combine Eqs. (7) and (8) in the form

$$e^{2i\Delta} = \det A. \tag{11}$$

The determinant of A can be evaluated by first noting that the matrix A has the form

$$A = e^{2i\delta^0} - iC\tilde{C}, \tag{12}$$

where $e^{2i\delta^0}$ is a diagonal matrix. The matrix C is an $N\times 1$ rectangular matrix (vector) with elements

$$C_n = e^{i\delta_n^0}[\Gamma_n/(E - E_0 + \tfrac{1}{2}i\Gamma)]^{1/2}, \tag{13}$$

and its transpose is denoted by $\tilde{C}$. The so-called diagonal expansion of $\det A$ is given by[16]

$$\det A = \det(e^{2i\delta^0}) + \sum_{n=1}^{N} \prod_{m\neq n}^{N} e^{2i\delta_m^0} M_{nn} + \sum_{n<m}^{N}\sum^{N} \prod_{\substack{p\neq m\\ p\neq n}}^{N} e^{2i\delta_p^0} M_{nm,nm} + \cdots + \det(-iC\tilde{C}), \tag{14}$$

where $M_{nn}, M_{mn,mn}, \ldots$ are the principal minors of orders $1, 2, \ldots$ of the $N\times N$ matrix $-iC\tilde{C}$. Equation (14) can be simplified using the result[16] that a matrix which is a product of $N\times 1$ and $1\times N$ rectangular matrices has a zero determinant when $N>1$. Thus $\det(C\tilde{C})=0$. Furthermore, since every principal minor of $C\tilde{C}$ has the form $\det(F\tilde{F})$, where F is an $N'\times 1$ matrix, every minor except M_{nn} (for which $N'=1$) is zero. Using Eq. (13), M_{nn} can be written explicitly in the form

$$M_{nn} = -ie^{2i\delta_n^0}\Gamma_n(E - E_0 + \tfrac{1}{2}i\Gamma)^{-1}. \tag{15}$$

With these results, Eq. (14) reduces to the expression

$$\det A = e^{2i\Sigma_n\delta_n^0}\left(1 - i\sum_{n=1}^{N}\Gamma_n(E - E_0 + \tfrac{1}{2}i\Gamma)^{-1}\right). \tag{16}$$

Finally, combining Eqs. (10), (11), and (14) yields the desired result:

$$e^{2i\Delta} = e^{2i\Delta^0}(E - E_0 - \tfrac{1}{2}i\Gamma)/(E - E_0 + \tfrac{1}{2}i\Gamma), \tag{17}$$

which is completely equivalent to the expression in Eq. (5).

The formulas in Eqs. (5) and (17) describe the energy dependence of the eigenphase sum near an isolated resonance. It is clear that the resonant part of the eigenphase sum, $\Delta(E) - \Delta^0$ increases by π as the energy varies from $E<E_0$ to $E>E_0$. The present analysis suggests that it is the eigenphase sum which should be fitted to the usual single-channel resonance formula [Eq. (5)] in order to extract the resonance energy and the *total width* from the computed eigenphases. Alternatively, the energy dependence of each eigenphase can be fitted to Macek's formula [Eq. (3)] to ob-

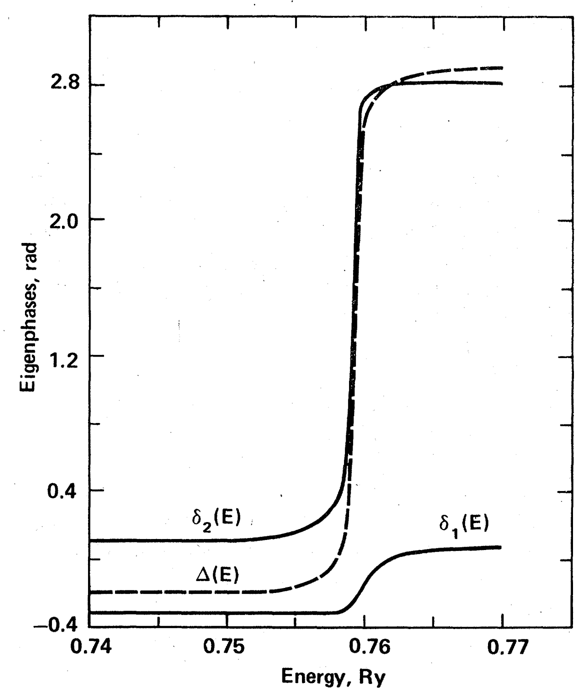

FIG. 1. $^1\Pi_u$ eigenphases and the corresponding eigenphase sum calculated by Robb (Ref. 17) for elastic e-H_2^+ scattering at $R=2.0$ bohrs. The solid lines give the eigenphases for the $l=1$ and $l=3$ channels, the dashed line gives their sum.

tain the individual partial widths.

To illustrate the behavior described by the expressions in Eqs. (3) and (5), Fig. 1 shows the $^1\Pi_u$ eigenphases, and the corresponding eigenphase sum, which have been calculated by Robb[17] for elastic e-H_2^+ scattering at an internuclear separation of 2.0 bohrs. Fitting[18] the energy dependence of the two eigenphases to Eq. (3) gives $E_0 = 0.7591$ Ry, $\Gamma_1 = 8.0 \times 10^{-5}$ Ry, and $\Gamma_2 = 5.10 \times 10^{-4}$ Ry. On the other hand, fitting the eigenphase sum to the expression in Eq. (5) yields the same resonance energy and a total width of 5.90×10^{-4} Ry. These results provide numerical verification of the conclusions that (i) the eigenphase sum satisfies the "single-channel" formula in Eq. (5), and (ii) the width parameter occurring in Eq. (5) [or Eq. (15)] is indeed the total width of the resonance. In addition, Fig. 1 shows that the eigenphase sum $\Delta(E)$ increases by slightly less than π, from -0.20 to 2.89, as E varies from 0.75 to 0.77 Ry. In contrast, the resonant eigenphase $\delta_2(E)$ increases by only 2.69 rad in the same interval. Thus, treating this $^1\Pi_u$ resonance as a single-channel problem would certainly yield incorrect response parameters.

Finally, it should be noted that, throughout the paper I have assumed the background eigenphases to be slowly varying functions of E. This assumption is usually valid for narrow resonances. In some cases, such as broad resonances or electron-polar molecule scattering, it is necessary to consider the relationship between the energy-dependent resonance parameters obtained from Feshbach's theory[15] and the complex pole of the total S matrix.[19]

Note added in proof. After this Comment was accepted for publication, Dr. R. K. Nesbet informed me that the main result of this paper, Eq. (17), was given, without proof, in his review article on electron-atom collisions in Adv. At. and Mol. Phys. 13, 315 (1977). Nesbet and Lyons [Phys. Rev. A 4, 1812 (1971)] discussed the application of Eqs. (1) and (3) to multichannel resonances in e–H-atom scattering.

ACKNOWLEDGMENTS

I am indebted to Dr. W. D. Robb for stimulating the development reported here by providing his unpublished $^1\Pi_u$ eigenphases for elastic e-H_2^+ collisions. I also thank Dr. T. Rescigno for several useful discussions. Work performed under the auspices of the U. S. Department of Energy at Lawrence Livermore Laboratory under Contract No. W-7405-Eng-48.

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