Spurious singularities in the Schwinger variational method

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We analyze a type of spurious resonance recently identified [see, for example, B. Apagyi, P. Lévay, and K. Ladányi, Phys. Rev. A **37**, 4577 (1988)] in the Schwinger variational method. It is found that this type of anomaly is associated with ill conditioning of the potential matrix $\underline{V}$, and that this fact allows the identification and removal of any such resonances by straightforward numerical procedures. We therefore anticipate that such anomalies will have little relevance to practical applications of the Schwinger method.

I. INTRODUCTION

Apagyi and his co-workers[1–3] have recently examined the application of the Schwinger variational method[4] to several simple problems, and have found spurious resonances in two cases, specifically ^1S electron scattering by the H atom in the static-exchange approximation[1] and scattering by a local potential which changes sign.[2] Since anomalous behavior has not been previously reported in applications of the Schwinger method, these results deserve study both for their own interest and as they may affect practical applications of the Schwinger principle.

The anomalous resonances seen by Apagyi and his co-workers[1–3] are closely associated with zero eigenvalues of the $N \times N$ matrix representation $\underline{V}$ of the potential, in the sense that they are seen only when $\underline{V}$ is either ill conditioned or actually singular. Such an association was explicitly noted by Apagyi, Lévay, and Ladányi[1] for the $^1S\, e^- - \mathrm{H}$ atom problem, and can be readily verified for the local potential[2] as well. We have found that this observation is the key to understanding the numerical origin of these resonances; furthermore, we show here that resonances of this type can be readily distinguished from physical resonances and can, in fact, be avoided entirely by the use of fairly standard computational techniques. In spite of their possible theoretical interest, therefore, anomalies of this type should be of little practical significance.

In the present paper we first review some relevant aspects of the Schwinger variational method and discuss how anomalous resonances may arise in it. We then show how spurious resonances associated with the behavior of $\underline{V}$ can be identified and eliminated. A simple numerical example illustrates the main points presented, followed by a brief discussion and conclusions.

II. THEORY

To simplify the discussion, we consider s-wave elastic scattering using standing-wave boundary conditions and real basis functions. The Schwinger principle for a linear trial function[5]

$$\psi(kr)=\sum_{i=1}^{N} x_i \chi_i(r) \tag{2.1}$$

then takes the form

$$\tan\delta = -\frac{2}{k}\mathbf{b}^T\cdot\mathbf{x} \ , \tag{2.2}$$

where $\mathbf{x}$ is the solution of the linear system

$$\underline{A}\mathbf{x}=\mathbf{b} \ , \tag{2.3}$$

with

$$A_{ij}=\langle \chi_i | V - VG^{(P)}V | \chi_j \rangle \tag{2.4}$$

and

$$b_i=\langle \chi_i | V | \sin(kr) \rangle \ , \tag{2.5}$$

for i and j running from 1 to N. In (2.4), $G^{(P)}$ is the principal-value free Green's function for $l=0$.

If $\underline{A}$ is nonsingular, we solve Eq. (2.3) in the form

$$\mathbf{x}=\underline{A}^{-1}\mathbf{b} \ , \tag{2.6}$$

and we then may write

$$\tan\delta = -\frac{2}{k}\mathbf{b}^T\underline{A}^{-1}\mathbf{b} \ . \tag{2.7}$$

Since a resonance is signaled by $\tan\delta=\infty$, it is clearly a necessary condition for a resonance that $\underline{A}$ be singular. However, it is important to understand that this is not a *sufficient* condition for a resonance to exist. For instance, suppose that

$$\underline{A}\mathbf{z}=0 \tag{2.8}$$

is satisfied for exactly one nontrivial $\mathbf{z}$, but also that

$$\mathbf{b}^T\cdot\mathbf{z}=0 \ . \tag{2.9}$$

Then, according to the Fredholm alternative, solutions to Eq. (2.3) exist[6] and take the general form

$$\mathbf{x}=\mathbf{x}'+\beta\mathbf{z} \ , \tag{2.10}$$

where $\mathbf{x}'$ is orthogonal to $\mathbf{z}$ and β is arbitrary. If we then use Eq. (2.2) to evaluate $\tan\delta$, we obtain

$$\tan\delta = -\frac{2}{k}\mathbf{b}^T\cdot\mathbf{x}' \ , \tag{2.11}$$

in light of Eq. (2.9). Equation (2.11) for $\tan\delta$ is independent of $\mathbf{z}$ and finite, and consequently, there is no resonance. For a true resonance to exist, we therefore have the additional condition

$$\mathbf{b}^T\cdot\mathbf{z}\neq 0 \ . \tag{2.12}$$

When Eqs. (2.8) and (2.12) together hold, then the inhomogeneous equation (2.3) has no solution,[6] and we are justified in taking $\tan\delta=\infty$.

It is worth observing that the well-known[7,8] equivalence between the Schwinger principle for linear trial functions and the use of a separable approximation for the potential,

$$V_{\text{sep}}(r)=\sum_{i,j=1}^{N} V(r)|\chi_i\rangle[\underline{V}^{-1}]_{ij}\langle\chi_j|V(r) \ , \tag{2.13}$$

provides a simple physical interpretation of these elementary facts. From the separable-potential point of view, Eqs. (2.8) and (2.9) characterize the presence of a bound state in the continuum, in contrast to a true resonance. Such a bound state is asymptotically decaying, and thus does not affect the phase shift. On the other hand, the solution associated with $\mathbf{z}$ is degenerate with a scattering solution (associated with $\mathbf{x}'$), so that the phase shift is still well defined and is, in fact, given by Eq. (2.11). These issues have been discussed in some detail by Gourdin and Martin[9] and in particular by Martin;[10] the latter reference also makes the key observation that any slight alteration in a separable potential which supports a bound state in the continuum is likely to convert that bound state into a resonance. Since a bound state in the continuum is an artifact of the separable approximation to the potential, so also are any such resonances associated with it. Here, then, we have a category of spurious resonances associated with separable potentials, or, equivalently, with the Schwinger variational method.

The preceding discussion immediately suggests a means of identifying and dealing with any such resonances. Since they are very closely related to actual bound states, we anticipate that Eq. (2.9) will be very nearly satisfied for such resonances, i.e., that the overlap of the normalized vectors $\mathbf{b}$ and $\mathbf{z}$,

$$\lambda=\frac{\mathbf{b}^T\cdot\mathbf{z}}{\|\mathbf{b}\|\,\|\mathbf{z}\|} \ , \tag{2.14}$$

will be small. In such a case we are justified in proceeding as if Eq. (2.9) held exactly, that is, by requiring that the solution $\mathbf{x}$ to Eq. (2.3) be orthogonal to $\mathbf{z}$. Such an approach is simply the standard procedure in solving inhomogeneous equations when a solution to the corresponding homogeneous system exists,[11] with the difference that we do not necessarily require that $\underline{A}$ be numerically singular, or that λ be numerically zero, for it to be appropriate to proceed in this manner.

As already mentioned, the anomalies seen by Apagyi and his co-workers[1-3] are associated with singular behavior of the matrix $\underline{V}$. Since the separable potential, Eq. (2.13), is not even defined when $\underline{V}$ is singular, the resonances they observe cannot be directly associated with positive-energy bound states. However, in terms of the linear equations, these resonances originate in a closely analogous manner. Assuming for convenience that our N-term basis in Eqs. (2.4) and (2.5) is a subset of a complete orthonormal set of functions, those equations may be written as

$$A_{ij}=\sum_{m=1}^{\infty}\langle\chi_i|1-VG^{(P)}|\chi_m\rangle\langle\chi_m|V|\chi_j\rangle \tag{2.4'}$$

and

$$b_i=\sum_{m=1}^{\infty}\langle\chi_i|V|\chi_m\rangle\langle\chi_m|\sin(kr)\rangle \ . \tag{2.5'}$$

Moreover, since we can only expect meaningful results when the basis adequately represents the potential, for any useful basis Eqs. (2.4') and (2.5') must very nearly be satisfied even when the m sum is truncated at $m=N$. Put another way, we must have

$$\underline{A}=\underline{A}'\underline{V}+\underline{\Delta} \tag{2.15}$$

and

$$\mathbf{b}=\underline{V}\mathbf{b}'+\boldsymbol{\delta} \ , \tag{2.16}$$

with

$$\|\underline{\Delta}\|\ll\|\underline{A}\| \tag{2.17}$$

and

$$\|\boldsymbol{\delta}\|\ll\|\mathbf{b}\| \ , \tag{2.18}$$

the matrix $\underline{A}'$ and vector $\mathbf{b}'$ being given by

$$A'_{ij}=\langle\chi_i|1-VG^{(P)}|\chi_j\rangle \tag{2.19}$$

and

$$b'_i=\langle\chi_i|\sin(kr)\rangle \ , \tag{2.20}$$

respectively, for $i,j=1,\ldots,N$. When an eigenvalue of $\underline{V}$ equals zero, we then have for the corresponding normalized eigenvector ζ

$$\underline{A}\zeta=\underline{\Delta}\zeta \tag{2.21}$$

and

$$\mathbf{b}^T\cdot\zeta=\boldsymbol{\delta}^T\cdot\zeta \ . \tag{2.22}$$

Because $\underline{\Delta}$ and $\boldsymbol{\delta}$ have small norms, we see that ζ very nearly satisfies Eqs. (2.8) and (2.9). It is thus quite possible that, by making slight modifications to the basis or by tuning the scattering energy (which modifies $\underline{A}$ and $\mathbf{b}$), we may find a vector $\mathbf{z}$, close to or identical to ζ, that satisfies Eq. (2.8) exactly. We thereby produce a "resonance," unless Eq. (2.9) happens to be satisfied simultaneously, which is unlikely. However, the quantity λ given by Eq. (2.14) will be approximately equal to $\|\boldsymbol{\delta}\|/\|\mathbf{b}\|$. As we have shown, this ratio must be small for any adequate basis, and goes to zero as the basis representation of the potential improves. It is therefore clear that such a resonance is of the type we have been discussing, arising when there is a solution to the homogeneous equation, Eq. (2.8), nearly orthogonal to the inhomogeneous term in Eq. (2.3). As already mentioned, the natural way to deal with such cases is to require the solution to be orthogonal to the "resonant" state. In this particular instance, we have not only the smallness of λ but the conditioning of the matrix $\underline{V}$ as diagnostics of possible anomalous behavior, so that there should be no danger of confusing such artifacts with true resonances.

III. NUMERICAL EXAMPLE

In this section we briefly illustrate the ideas developed in Sec. II for the simple example of s-wave scattering by the potential

$$V(r) = -e^{-2r}\left[1-\frac{1}{r}\right] \tag{3.1}$$

using Slater-type basis functions

$$\phi_m(r) = r^m e^{-\alpha r}, \quad m=1,\ldots,N . \tag{3.2}$$

Lévay and Apagyi found for this problem that anomalous resonances arose in the Schwinger method for certain combinations of the basis set parameters and the scattering energy. Their results for a seven-term basis are reproduced in Fig. 1, which shows the variation of $\tan\delta$ with the parameter α for $k=\frac{1}{2}$. The anomalous behavior near $\alpha=3.7$ is obvious. In Fig. 2, we show how the smallest eigenvalues of the matrices $\underline{A}$ and $\underline{V}$ vary over the same range of α. When a resonance is induced $\underline{A}$ of course is singular. We see that $\underline{V}$ is also singular very near by, identifying the origin of the anomalous behavior. Also shown in Fig. 2 is the quantity

$$\lambda' = \frac{\mathbf{b}^T\cdot\mathbf{x}}{\|\mathbf{b}\|\,\|\mathbf{x}\|} , \tag{3.3}$$

corresponding to the λ of Eq. (2.14), which according to Eq. (2.22) should very nearly vanish for an anomalous

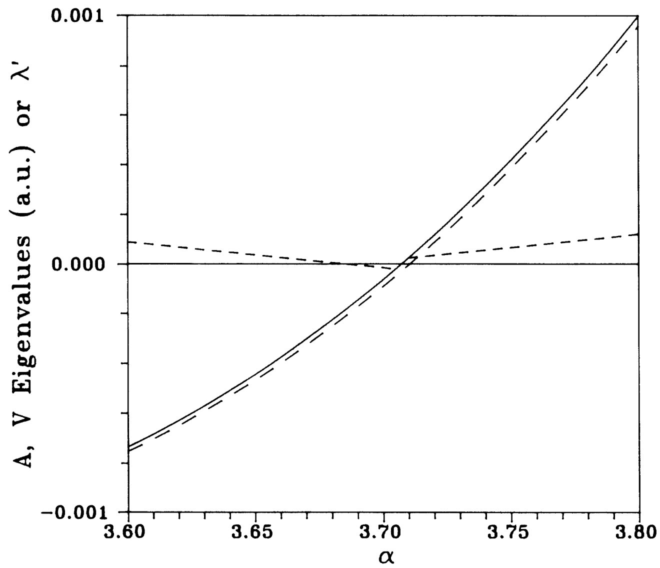

FIG. 2. Variation with α of the smallest eigenvalues of $\underline{A}$ (solid line) and $\underline{V}$ (long dashes), and of the overlap λ' of Eq. (3.3) (short dashes), for the same case as Fig. 1. Note that all three quantities pass through zero at almost the same value of α, indicating the anomalous origin of the "resonance" signaled by the zero eigenvalue of $\underline{A}$. The discontinuity in λ' arises from an abrupt change of sign at the location of the spurious resonance.

resonance. This condition is clearly satisfied in the present case.

Since, as discussed in Sec. II, the behavior of $\underline{V}$ and λ' illustrated in Fig. 2 provides a means of identifying the resonant behavior shown in Fig. 1 near $\alpha=3.7$ as spurious, it is appropriate to eliminate the linear combination

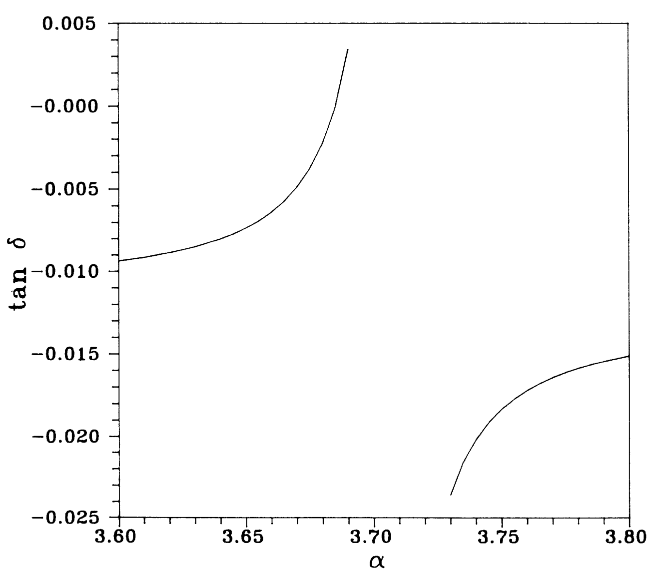

FIG. 1. Variation of $\tan\delta$ with the basis parameter α for the model problem defined by Eq. (3.1), for a fixed value $k=\frac{1}{2}$ and basis size $N=7$. The correct value of $\tan\delta$ is approximately -0.0104.

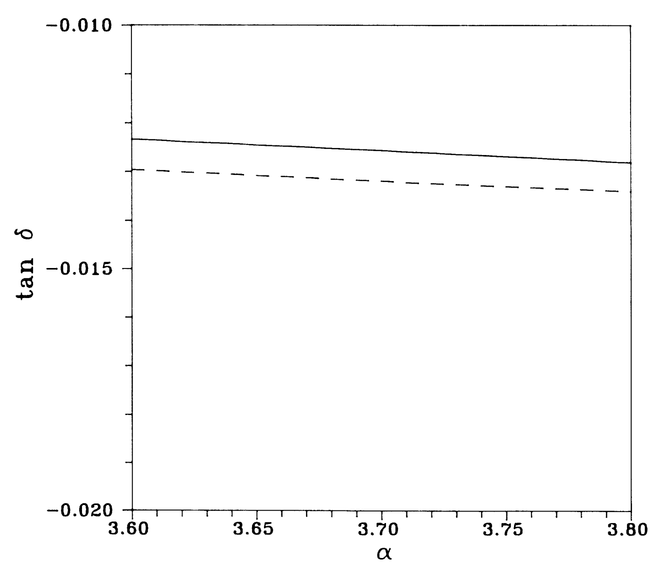

FIG. 3. Variation of $\tan\delta$ with α as in Fig. 1, but with the eigenvector of $\underline{A}$ corresponding to the near-zero eigenvalue excluded from the solution space by singular value decomposition (solid line). For comparison, results for $\tan\delta$ using a basis size $N=6$ are also shown (dashed line).

causing the anomalous behavior from the solution space. This is conveniently accomplished by singular value decomposition,[11] with the result shown in Fig. 3. Clearly the behavior of tanδ is much improved. In fact, the results are comparable to those obtained for $N=6$, i.e., using one basis function fewer from the outset, also shown in Fig. 3. We thus can be confident that the procedure outlined here is capable of dealing with such anomalies if and when they arise.

IV. DISCUSSION AND CONCLUSIONS

We have seen that the anomalous resonances observed[1–3] in the Schwinger variational method can be understood as artifacts induced by the behavior of the potential matrix $\underline{V}$, and that they are similar to a type of anomaly identified earlier[9,10] as arising for nonlocal approximate potentials in general. Fortunately, the "parentage" of these anomalies implies numerical criteria for identifying them. Still more importantly, we have shown that the nature of the anomalous solutions to Eq. (2.8) implies that, to a very accurate approximation, there simultaneously exist solutions to Eq. (2.3) which provide finite, and in our example reasonable, values for tanδ. It should also be clear from the foregoing discussion that such anomalies, unless deliberately sought out, should be quite rare in practice, arising as they do from a highly artificial choice of basis set. Indeed, the apparent absence of such anomalies in the many practical applications of the Schwinger method since its formulation[4] provides a strong indication of their unlikelihood. We conclude that the behavior seen by Apagyi and his co-workers, although of some theoretical interest, has little relevance to the usefulness of the Schwinger variational method as a computational tool.

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