Anomalous singularities in the complex Kohn variational principle of quantum scattering theory

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Variational principles for symmetric complex scattering matrices (e.g., the S matrix or the T matrix) based on the Kohn variational principle have been thought to be free from anomalous singularities. We demonstrate that singularities do exist for these variational principles by considering single and multichannel model problems based on exponential interaction potentials. The singularities are found by considering simultaneous variations in two nonlinear parameters in the variational calculation (e.g., the energy and the cutoff function for the irregular continuum functions). The singularities are found when the cutoff function for the irregular continuum functions extends over a range of the radial coordinate where the square-integrable basis set does not have sufficient flexibility. Effects of these singularities generally should not appear in applications of the complex Kohn method where a fixed variational basis set is considered and only the energy is varied.

I. INTRODUCTION

The use of variational principles can be a very powerful approach for solving the equations of quantum scattering theory. Variational principles can be constructed for a wide variety of quantities of interest, including the scattering wave function, the scattering amplitudes, and any overlap matrix element with the scattering wave function.[1] In molecular physics, variational principles have been applied to electron-atom[2] and electron-molecule[3,4] scattering and to chemical reaction dynamics.[5-7]

Variational principles have been based both on the differential and integral forms of the Schrödinger equation. Each approach has its own advantages and disadvantages for numerical computations based on the ease of implementation, computation time required, numerical stability, and the occurrence of anomalous features.

One of the earliest methods to be used in significant computational studies was the Kohn method which is based on the differential equation form of the Schrödinger equation.[8] As was discovered by Schwartz,[9] this method has severe problems with anomalous singularities. For a given choice of variational basis set, the K matrix obtained from the Kohn method contains a series of anomalous singularities, and the number of these singularities increases as the size of the basis set increases, although the width of the singularities becomes smaller as the number of basis functions increases.[2] Nesbet and co-workers[2] have developed a variety of approaches for circumventing these anomalous singularities including the optimized anomaly-free (OAF), minimum norm (MN), and restricted interpolated anomaly-free (RIAF) methods. These methods are successful in avoiding singularities but are not particularly satisfying solutions to the problem due to their *ad hoc* nature. Several of these methods are based on the observation that by employing different asymptotic boundary conditions in the variational trial function, the singularities could be shifted to different energies. Thus by choosing different boundary conditions at different energies, the anomalous singularities could be avoided.

It was subsequently noted that by choosing complex boundary conditions, the singularities could be shifted to complex energies and thus could be avoided for scattering calculations at real energies.[10] This observation forms the basis for an alternative approach for employing the Kohn principle, which is based on the use of boundary conditions appropriate for the S matrix or T matrix.[4-6,11] These methods involve the inversion of complex symmetric matrices instead of real symmetric matrices as in traditional Kohn-based methods which employ standing-wave boundary conditions. It has been shown that these methods generally are free from singularities of the type associated with the Kohn variational principle. Thus, for a given choice of variational basis set, no anomalous singularities are found as variations in the energy are considered.[4-6,11,12]

A second type of variational principle is the Schwinger-type variational principle.[3,13] These variational methods are based on the integral equation form of the Schrödinger equation. These methods include the asymptotic boundary conditions through the use of a Green's function. It can be shown that the results obtained from these principles for a given interaction potential are identical to those obtained from the exact solution of a corresponding model-separable-potential problem. Then, as long as the model potential is free of anomalous features, the corresponding results from the variational principle will also be free of anomalous features. However, as has been demonstrated by Apagyi *et al.*,[14] if a poor choice of variational basis set is made, the Schwinger variational principle will yield anomalous results.[15] One disadvantage of the Schwinger-type variational principles is that matrix elements of the Green's function are often more difficult to compute than the Hamiltonian matrix elements which are required in the Kohn-type methods.

In this paper we will examine anomalous features in the complex Kohn methods by considering a model-potential scattering problem. We have considered both a one-channel problem with an attractive exponential potential and a five-channel problem where all diagonal and off-diagonal coupling potentials are exponential but with different strengths. This multichannel model potential is similar to the Huck problem, which has been used previously to test variational principles,[16,17] but does not contain the discontinuity in the potential which complicates the variational basis needed in Kohn-type methods.[17] We will show that anomalous features exist in the complex Kohn method, but that they are not found when reasonable variational trial functions are chosen.

II. COMPLEX KOHN VARIATIONAL PRINCIPLES

A variety of Kohn-type variational principles can be obtained by imposing different boundary conditions on the trial variational function. Using a notation similar to that of Nesbet,[2] we will write state functions as $|\psi_p^{(+)}\rangle$ where this state function is expanded in terms of radial channel function $\psi_{qp}^{(+)}(r)$ for $q=1,\ldots,N$, where N is the number of channels. The asymptotic form of state function $|\psi_p^{(+)}\rangle$ is then (using atomic units)

$$\psi_{qp}^{(+)}(r) \sim \phi_{0p}(r)\delta_{qp} + \phi_{1q}(r)L_{qp} \ , \tag{1}$$

where $\phi_{ip}(r)$ are radial functions which are regular at the origin and which behave asymptotically as

$$\phi_{0p}(r) \sim k_p^{-1/2}[u_{00}\sin\theta_p(r) + u_{01}\cos\theta_p(r)] \ , \tag{2}$$

$$\phi_{1p}(r) \sim k_p^{-1/2}[u_{10}\sin\theta_p(r) + u_{11}\cos\theta_p(r)] \ , \tag{3}$$

where $\theta_p(r) = k_p r - \frac{1}{2} l_p \pi$ when the potentials die more rapidly than $1/r$ as $r \to \infty$ and where k_p and l_p are the asymptotic momentum and angular momentum of the pth channel. Note that asymptotically the Wronskian of $\phi_{0p}(r)$ and $\phi_{1p}(r)$ is given by

$$W(\phi_{0p}, \phi_{1p}) \sim u_{01}u_{10} - u_{00}u_{11} = -\det\underline{u} \ . \tag{4}$$

Now a variational estimate of the elements of the matrix $\underline{L}$ can be obtained from a Kohn-type variational principle with trial functions $|\tilde{\psi}_q^{(+)}\rangle$ and $|\tilde{\psi}_p^{(+)}\rangle$ of the form

$$L_{qp} = L[|\tilde{\psi}_q^{(+)}\rangle, |\tilde{\psi}_p^{(+)}\rangle] = \tilde{L}_{qp} - \frac{2}{\det\underline{u}}\langle \tilde{\psi}_q^{(-)}|H-E|\tilde{\psi}_p^{(+)}\rangle \ , \tag{5}$$

where $\tilde{L}_{qp}$ gives the asymptotic form of $|\tilde{\psi}_p^{(+)}\rangle$ in terms of appropriately defined radial functions and the radial functions of $|\tilde{\psi}_q^{(-)}\rangle$ are just the complex conjugates of the radial functions of $|\tilde{\psi}_q^{(+)}\rangle$. Equation (5) can be turned into a matrix variational expression by expanding the trial functions as linear combinations of basis functions of the form

$$|\tilde{\psi}_p^{(+)}\rangle = \sum_\mu c_{\mu p}|\Phi_\mu\rangle + |\phi_p^0\rangle + \sum_s |\phi_s^1\rangle \tilde{L}_{sp} \ , \tag{6}$$

where the radial functions of the functions $|\phi_p^i\rangle$ are given by $\phi_{sp}^i(r) = \delta_{sp}\phi_{ip}(r)$ and where $|\Phi_\mu\rangle$ is a square-integrable function, so that its radial functions go to zero asymptotically. Then, requiring the matrix elements of $\underline{L}$ to be variationally stable with respect to the expansion coefficients $c_{\mu p}$ and $\tilde{L}_{sp}$ yields the following expression for $\underline{L}$:

$$\underline{L} = -\frac{2}{\det\underline{u}}(\underline{m}_{00} - \underline{m}_{10}^T \underline{m}_{11}^{-1}\underline{m}_{10}) \ , \tag{7}$$

where the superscript T stands for matrix transpose and where the matrix elements of the matrices $\underline{m}_{ij}$ are defined by

$$(\underline{m}_{ij})_{pq} = M_{pq}^{ij} - \sum_\mu \sum_\nu M_{ip,\mu}(M)_{\mu\nu}^{-1} M_{\nu,iq} \ , \tag{8}$$

where

$$M_{\mu\nu} = \langle \Phi_\mu|H-E|\Phi_\nu\rangle \ , \tag{9}$$

$$M_{\mu,ip} = \langle \Phi_\mu|H-E|\phi_p^i\rangle \ , \tag{10}$$

$$M_{pq}^{ij} = \langle \phi_p^i|H-E|\phi_q^j\rangle \ , \tag{11}$$

and where the radial functions are not complex conjugated for the functions on the left sides of these integrals. A variety of different L's can be computed by making different choices for $\underline{u}$. For example,

$$\underline{L} = \underline{K} \quad \text{for } \underline{u} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} , \tag{12}$$

$$\underline{L} = \underline{K}^{-1} \quad \text{for } \underline{u} = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} , \tag{13}$$

$$\underline{L} = \underline{S} \quad \text{for } \underline{u} = \begin{bmatrix} i & -1 \\ i & 1 \end{bmatrix} , \tag{14}$$

and

$$\underline{L} = -\pi\underline{T} \quad \text{for } \underline{u} = \begin{bmatrix} 1 & 0 \\ i & 1 \end{bmatrix} . \tag{15}$$

After a particular scattering matrix $\underline{L}$ has been computed, the corresponding K matrix can be obtained using

$$\underline{K} = (u_{01} + u_{11}\underline{L})(u_{00} + u_{10}\underline{L})^{-1} \ . \tag{16}$$

III. SINGULARITIES IN KOHN-TYPE VARIATIONAL EXPRESSIONS

As has been shown by Nesbet[2] anomalous singularities will occur in $\underline{L}$ when $\det\underline{m}_{11}=0$ not when $\det M_{\mu\nu}=0$. Thus different choices of u will yield singularities at different values of the scattering energy or of the parameters of the variational basis set. For methods based on a choice for $\underline{u}$ where all of its matrix elements are real, $\det\underline{m}_{11}$ will also be a real number. Then sets of parameters (e.g., nonlinear parameters in the basis sets and the scattering energy) which yield $\det\underline{m}_{11}=0$ can be found by varying only one parameter. Thus for a given basis set in the K-matrix Kohn method, anomalous singularities can be found by varying only the energy. In fact, it can be shown[2] that there will be a singularity at some energy between each successive pair of energies where $\det M_{\mu\nu}=0$.

When complex Kohn variational principles are used, such as the T-matrix or S-matrix versions given above, the matrix $\underline{m}_{11}$ becomes a complex symmetric matrix. In general, there is no reason why a complex symmetric matrix cannot have a zero determinant, although the determinant will usually be a complex number. Thus one would expect $\det\underline{m}_{11}$ to have zeros but that the zeros of $\det\underline{m}_{11}$ would only be found when two parameters are varied at the same time, since both the real and imaginary parts of $\det \underline{m}_{11}$ must be zero at the same time. Then for a given choice of basis set and cutoff function, one would not expect to find singularities in the complex Kohn method when only variations in the energy are considered. One however would expect to find singularities when two parameters are varied, e.g., energy and cutoff parameter. As an example, consider the S-matrix Kohn method, where $\underline{m}_{11}$ is given by

$$\underline{m}_{11}^{(S)}=(\underline{m}_{11}^{(K)}-\underline{m}_{00}^{(K)})+i(\underline{m}_{01}^{(K)}+\underline{m}_{10}^{(K)}) \ , \tag{17}$$

and where $\underline{m}_{ij}^{(K)}$ are the matrices obtained with $\underline{u}=1$. Then in a one-channel problem, the S-matrix Kohn method will be singular when $m_{11}^{(K)}=m_{00}^{(K)}$ and $m_{01}^{(K)}=-m_{10}^{(K)}$ simultaneously.

IV. MODEL-POTENTIAL CALCULATIONS

We have chosen a simple model scattering problem to investigate singularities in the complex Kohn method. The differential equation for the radial wave function of $|\psi_p\rangle$ in channel q is

$$\left[-\frac{1}{2}\frac{d^2}{dr^2}+(E-\tilde{E}_q)\right]\psi_{qp}(r)+\sum_{s=1}^{N} V_{qs}(r)\psi_{sp}(r)=0 \ , \tag{18}$$

where

$$V_{qs}(r)=A_{qs}e^{-\gamma r} \ . \tag{19}$$

The square-integrable variational basis set is composed of the functions $\{|\Phi_j^\lambda\rangle:\lambda=1,\ldots,M \text{ and } j=1,\ldots,N\}$, where M is the number of functions in each channel, and where the radial wave functions are of the form

$$\Phi_{ij}^{\lambda}(r)=\delta_{ij}r^{\lambda}e^{-\alpha r} \ . \tag{20}$$

The continuum trial functions $|\phi_p^i\rangle$ have radial functions given by

$$\phi_{sp}^{i}(r)=\delta_{sp}k_p^{-1/2}[u_{i0}\sin k_p r+u_{i1}(1-e^{-\beta r})\cos k_p r] \ , \tag{21}$$

where the channel momentum is given by

$$k_q=[2(E-\tilde{E}_q)]^{1/2} \ . \tag{22}$$

For this study we will consider both a one-channel ($N=1$) problem with $A_{11}=-1$ and $\tilde{E}_1=0$, i.e., an attractive exponential potential, and a five-channel problem ($N=5$) with the potential coupling coefficients given by

$$A=\begin{bmatrix} -2.00 & 0.40 & 0.30 & 0.20 & 0.10 \\ 0.40 & -1.75 & 0.40 & 0.30 & 0.20 \\ 0.30 & 0.40 & -1.50 & 0.40 & 0.30 \\ 0.20 & 0.30 & 0.40 & -1.25 & 0.40 \\ 0.10 & 0.20 & 0.30 & 0.40 & -1.00 \end{bmatrix} , \tag{23}$$

and $\tilde{E}=(-1,-0.75,-0.5,-0.25,0)$. For all model potentials considered here, we will take the exponent in the interaction potential to be $\gamma=1$.

For a given model potential and fixed basis set size, i.e., for fixed N, M, A, γ, and $\tilde{E}$, there are then three free parameters α, β, and E in our calculation. From the discussion given in Sec. III we would then expect to be able to locate zeros of $\det \underline{m}_{11}$ and thus singularities in $\underline{L}$ by varying any two of these parameters and keeping the other parameter fixed.

We will investigate the singularities in the complex Kohn method by considering the behavior of the S-matrix Kohn method. Unless otherwise noted, all results presented here will be obtained with the S-matrix Kohn method. Note that the T-matrix Kohn method will have singularities at the same values of α, β, and E as does the S-matrix method since $\underline{m}_{11}$ is the same for both methods.

In Fig. 1 we present the value of $1/|\det \underline{m}_{11}|$ as a function of β and E with $\alpha=2$ for the $N=1$ and $M=2$ model. In the region of parameter space presented in Fig. 1, we find one zero in $\det \underline{m}_{11}$ which is located at ($E=0.562$, $\beta=0.188$). The other feature present in this figure is the zero in $1/|\det m_{11}|$ which occurs at around $E=0.32$. This energy corresponds to an energy where $\det M_{\mu\nu}=0$. The location of the singularities of the S-matrix Kohn method forms lines in the three-dimensional parameter space with coordinates α, β, and E. In Fig. 2 we plot the projection of the line of singularities onto the β versus E plane. We can see that the position of the singularities remains restricted to relatively small values of β, and thus if a larger value of β were chosen, e.g., $\beta=1$, then there would not be a value of E and α for which there is a singularity in S.

To examine the effects of the zero in $\det \underline{m}_{11}$ on the S matrix in the one-channel problem, we will consider the phase shift δ and the amplitude σ of the S matrix element, where

$$S=\sigma e^{i2\delta} \ . \tag{24}$$

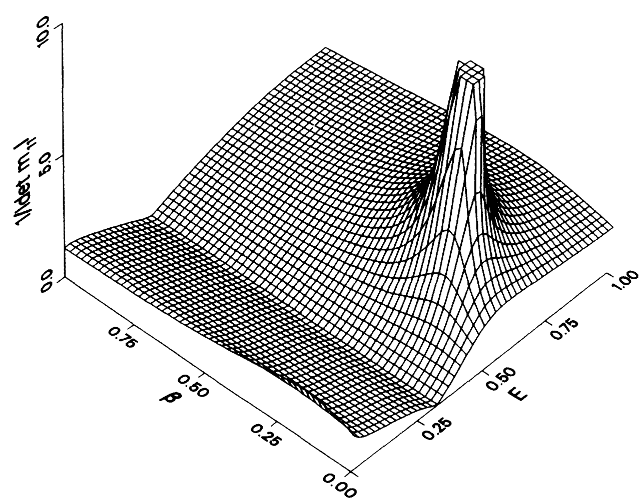

FIG. 1. Singularity in $1/|\det \underline{m}_{11}|$ of the S-matrix Kohn method when considered as a function of E and β with $N=1$, $M=2$, and $\alpha=2$. The values near the singularities have been truncated at $1/|\det \underline{m}_{11}|=10$.

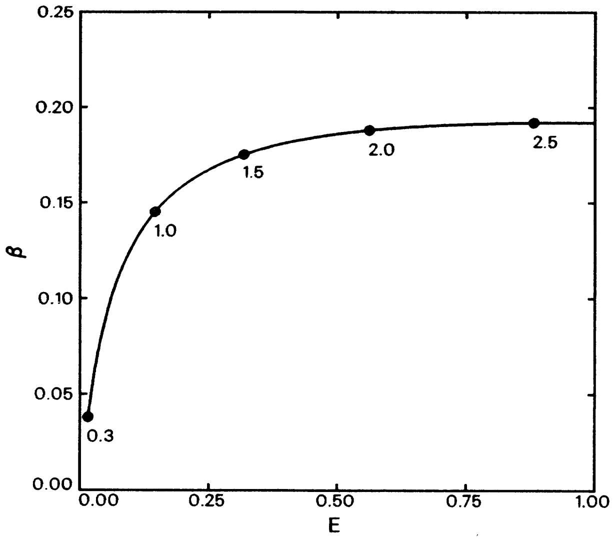

FIG. 2. Position of the singularity in $1/|\det \underline{m}_{11}|$ of the S-matrix Kohn method in the β vs E plane as a function of α with $N=1$ and $M=2$. The value of α is indicated at representative points along the curve.

In Fig. 3 we present the value of δ as a function of E and β with $\alpha=2$. We see that exactly on the singularity, $\beta=0.188$, there is a jump in phase of $\pi/2$ which is just what would be expected if $1/S$ were to pass through the origin. We can also see that the singularity in S is not highly localized with respect to variations in E or β.

In Fig. 4 we present the results of a calculation using the K-matrix Kohn method, the S-matrix Kohn, and the interpolated anomaly-free (IAF) method of Nesbet[2] for the $N=1$, $M=2$ model with $\alpha=2$ and $\beta=0.188$. This

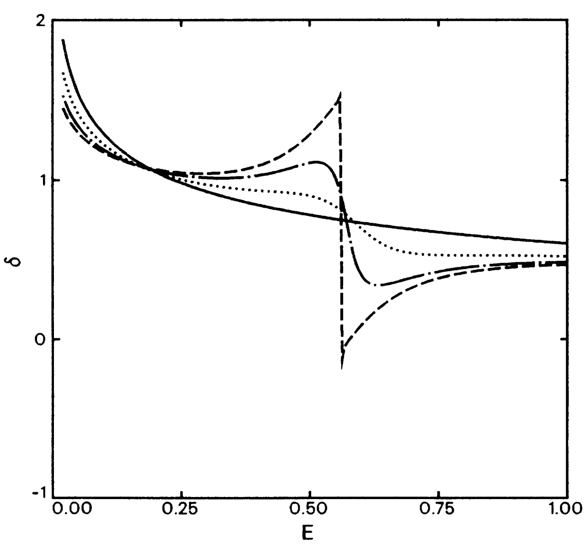

FIG. 3. Phase shift for the $N=1$ model potential near the $E=0.562$, $\beta=0.188$ singularity of the S-matrix Kohn method with the $M=2$ basis set. — — —, $\beta=0.188$, $M=2$; —·—·—·, $\beta=0.22$, $M=2$; · · · ·, $\beta=0.30$, $M=2$; ——, accurate value obtained with $\beta=1$ and $M=8$. For all curves $\alpha=2$.

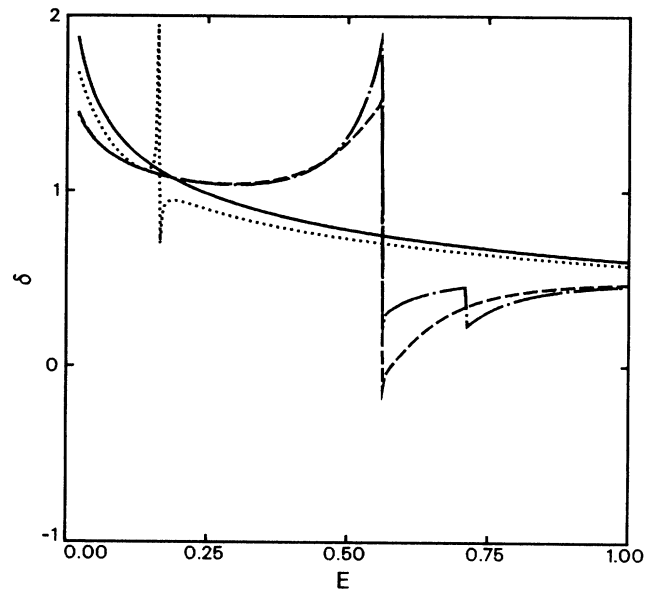

FIG. 4. Phase shift for the $N=1$ model potential with $M=2$, $\beta=0.188$, and $\alpha=2$ using different variational methods. — — —, S-matrix Kohn; —·—·—·, IAF Kohn; · · · ·, K-matrix Kohn; ——, accurate values obtained with the S-matrix Kohn method using $\beta=1$ and $M=8$.

choice of parameters forces the S-matrix Kohn result to go through the singularity at $E=0.562$. We can see that the K-matrix Kohn method is not affected by the singularity in the S-matrix method, however the IAF method gives results which are very close to the S-matrix method, including having a singularity at the same value of the energy.

In the IAF method for a one-channel problem, the matrix $\underline{u}$, is given by

$$\underline{u}=\begin{bmatrix} \cos\chi & \sin\chi \\ -\sin\chi & \cos\chi \end{bmatrix} . \tag{25}$$

Then the angle χ is chosen to maximize $|\det m_{11}|$. For the one-channel case this can be done analytically to yield

$$\chi=\tfrac{1}{2}\tan^{-1}\left[\frac{m_{01}^{(K)}+m_{10}^{(K)}}{m_{00}^{(K)}-m_{11}^{(K)}}\right] . \tag{26}$$

Thus the IAF will be indeterminate and thus have a discontinuity as seen in Fig. 4 under exactly the same conditions as when S-matrix method is singular, i.e., when $m_{11}^{(K)}=m_{00}^{(K)}$ and $m_{01}^{(K)}=-m_{10}^{(K)}$ simultaneously.

From Fig. 4 we can conclude that there is nothing intrinsically wrong with choosing $\beta=0.188$ and $\alpha=2$ since the K-matrix Kohn method gives good results with these same parameters in the region of the singularities in the S-matrix and IAF methods. However, the K-matrix Kohn method does exhibit a singularity of the usual Kohn type at a different energy. It seems that for these parameters, neither the S-matrix Kohn method nor the IAF method yields the best choice for the transformation matrix $\underline{u}$ near $E=0.562$.

One method for detecting the presence of singularities in the S matrix is by checking the unitarity of the S matrix, or in our model one-channel case, by examining the difference between σ and 1. In Fig. 5 we plot the $(1/\sigma)-1$ and the error in δ as a function of E. The error in the unitarity of S is certainly evident near the singularity; however, away from the singular energy, S becomes nearly unitary again. In Fig. 6 we consider the dependence on β of the error in σ and δ. As was indicated in Fig. 3, we see that as the value of β becomes larger, the S matrix becomes unitary and the phase shift becomes correct.

The occurrence of a singularity with $\beta=0.188$ when the exponent of the square-integrable basis functions is $\alpha=2.0$ would seem to indicate that singularities occur when the cutoff function and the basis set span different regions of the radial coordinate. To test this hypothesis, we searched for singularities when $\beta \gg \alpha$. We found such a singularity at $\beta=30.50$, $E=0.361$, and $\alpha=2$. In Fig. 7 we present the phase shift as a function of E and β for large values of β near this singularity. The results are very similar to those presented in Fig. 3, with the effects of the singularity slowly decaying away as β approaches values which bring the cutoff function into a region of coordinate space which is covered by the square-integrable basis set.

The location and number of singularities is also dependent on the size of the square-integrable basis set. In Fig. 8 we present a plot of $1/|\det \underline{m}_{11}|$ as a function of E and β with $\alpha=2$ for the one-channel problem with eight basis functions, i.e., $M=8$. Three singularities were found in this region of parameter space ($0 \le \beta \le 1$ and $0 \le E \le 1$) at $E=0.060$, $\beta=0.079$; $E=0.252$, $\beta=0.075$; and $E=0.635$, $\beta=0.073$. In comparison to Fig. 1, we see that with $M=8$ there are more singularities, there are more energies where $\det M_{\mu\nu}=0$, and the values of β for which there are singularities have also become smaller. In Fig. 9 we see the effect of these singularities on the computed phase shift. From these results we conclude that improving the basis set moves the singularities further from a region of parameter space in which a typical calculation would be performed. Also, improving the basis set does not make the resonances narrower with respect to any of the parameters. This is in contrast to the behavior of the singularities in the K-matrix Kohn method which become

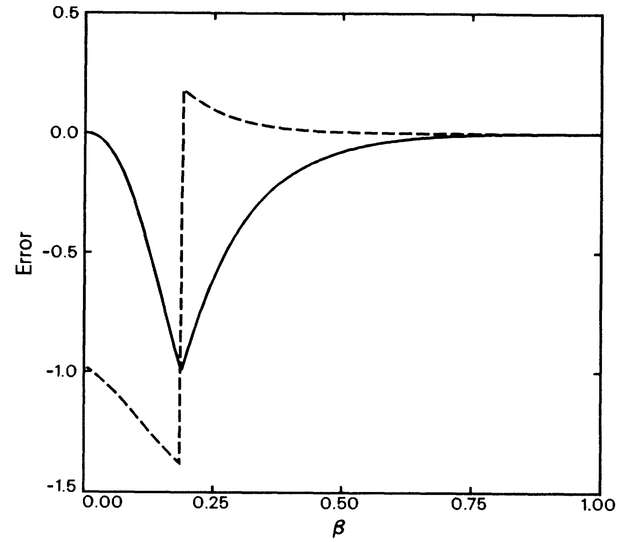

FIG. 6. Error in the S-matrix element obtained from the S-matrix Kohn method for $N=1$, $M=2$, $\alpha=2$, $E=0.562$ as a function of β. ——, error $1/\sigma$; — — —, error in δ. In both cases the error is defined as the difference between the value calculated using $M=2$ and the indicated β and the value obtained with $M=8$ and $\beta=1$.

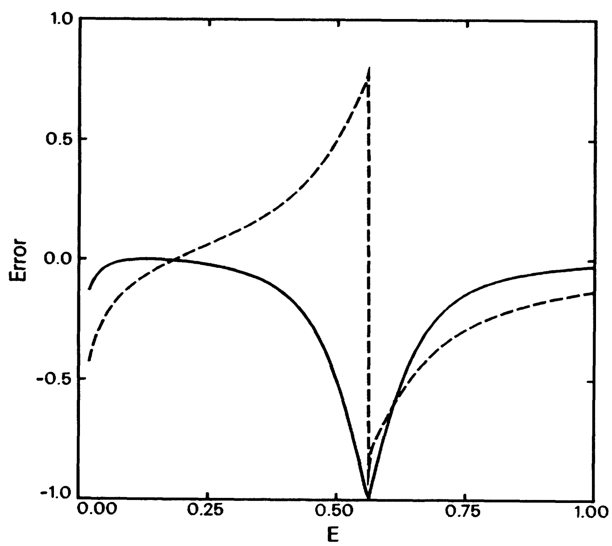

FIG. 5. Error in the S-matrix element obtained from the S-matrix Kohn method for $N=1$, $M=2$, $\alpha=2$, and $\beta=0.188$ as a function of E. ——, error in $1/\sigma$; — — —, error in δ. In both cases the error is defined as the difference between the value calculated using $M=2$ and $\beta=0.188$ and the value obtained with $M=8$ and $\beta=1$.

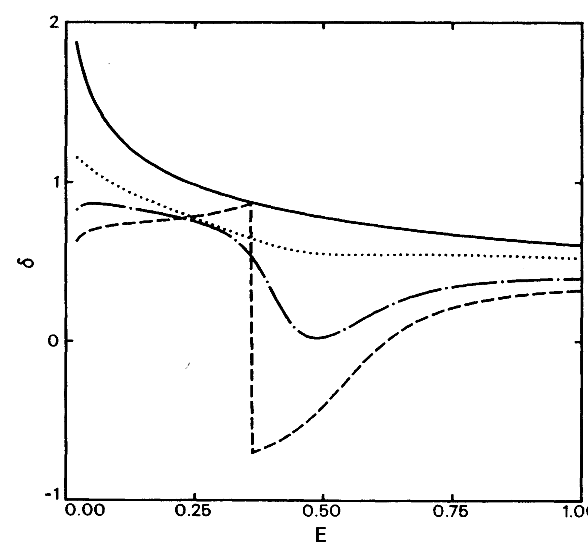

FIG. 7. Phase shift for the $N=1$ model potential near the $E=0.361$, $\beta=30.50$ singularity of the S-matrix Kohn method with the $M=2$ basis set. — — —, $\beta=30.50$, $M=2$; —·—·—·, $\beta=15$, $M=2$; · · · ·, $\beta=10$, $M=2$; ——, accurate value obtained with $\beta=1$ and $M=8$. For all curves $\alpha=2$.

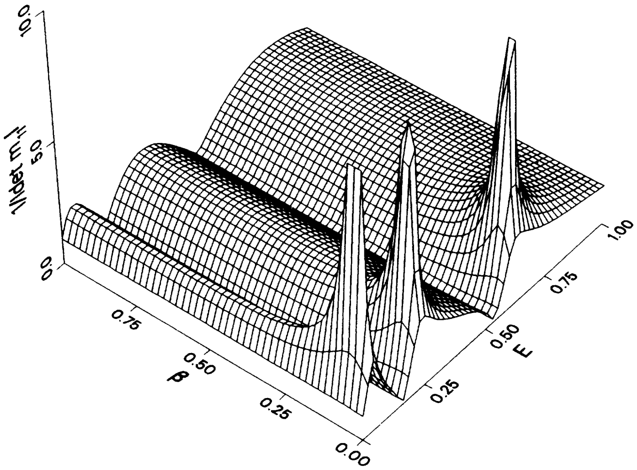

FIG. 8. Singularity in $1/|\det \underline{m}_{11}|$ of the S-matrix Kohn method when considered as a function of E and β with $N=1$, $M=8$, and $\alpha=2$. The values near the singularities have been truncated at $1/|\det \underline{m}_{11}|=10$.

narrower as the quality of the variational basis set improves.[2,9]

Finally, we have considered the effects of including more channels in the calculation on the position of the singularities in S. In Fig. 10 we present $1/|\det \underline{m}_{11}|$ as a function of E and β for $\alpha=2$, $N=5$, and $M=2$. This is a five-channel calculation with two basis functions in each channel for a total of ten square-integrable functions. There are three singularities in the region of parameter space considered in Fig. 10 at $E=0.081$, $\beta=0.238$; $E=0.331$, $\beta=0.213$; and $E=0.571$, $\beta=0.174$. Again, in comparison to Fig. 1, we see that there are more singularities, but that in this case the values of β at which they occur are very similar to those in the $N=1$, $M=2$ calculation. In Fig. 11 the probability $P_{45}=|S_{45}|^2$ is plotted as a function of E and β. In this case we also see that the effects of the singularities continue to persist to quite large values of β.

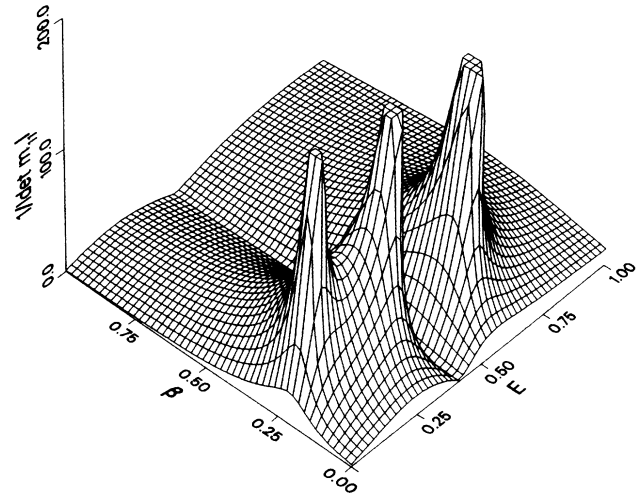

FIG. 10. Singularity in $1/|\det \underline{m}_{11}|$ of the S-matrix Kohn method when considered as a function of E and β with $N=5$, $M=2$, and $\alpha=2$. The values near the singularities have been truncated at $1/|\det \underline{m}_{11}|=200$.

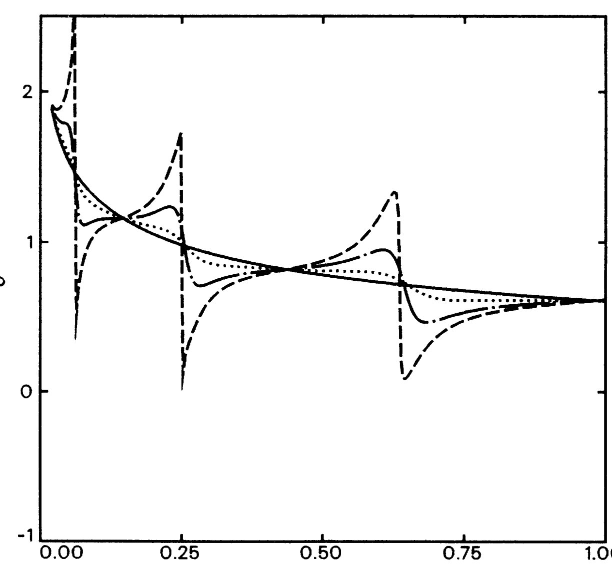

FIG. 9. Phase shift for the $N=1$ model potential of the S-matrix Kohn method near the singularities in the $M=8$ basis set. — — —, $\beta=0.075$, $M=8$; —·—·—·, $\beta=0.10$, $M=8$; · · · ·, $\beta=0.15$, $M=8$; ——, accurate value obtained with $\beta=1$ and $M=8$. For all curves $\alpha=2$.

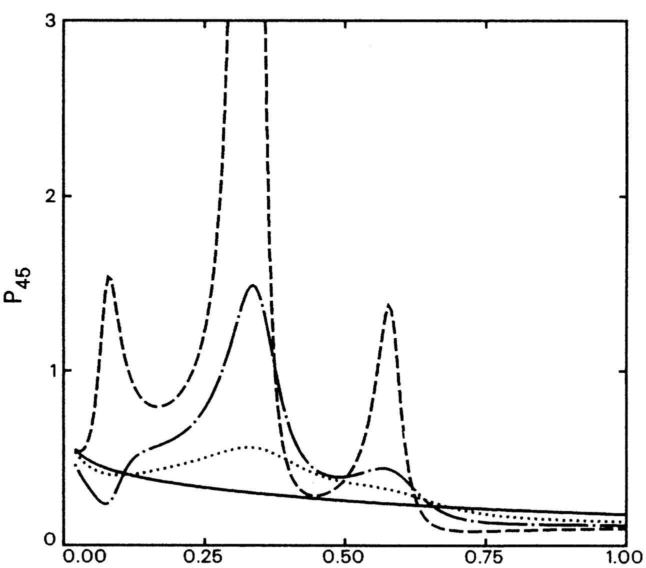

FIG. 11. P_{45} of the S-matrix Kohn method for the $N=5$ model potential near the singularities with the $M=2$ basis set. — — —, $\beta=0.213$, $M=2$; —·—·—·, $\beta=0.28$, $M=2$; · · · ·, $\beta=0.36$, $M=2$; ——, accurate value obtained with $\beta=1$ and $M=8$. For all curves $\alpha=2$.

V. CONCLUSIONS

We have seen that singularities do occur in the complex Kohn method. These singularities have a noticeable effect over substantial ranges of the nonlinear variational parameters and of the energy. In the model problems we have studied here, the singularities occur when the values of the nonlinear variational parameters were such that the cutoff function on the irregular function did not cover the same region of coordinate space as did the square-integrable variational functions. As more channels are introduced the singularities become more numerous, but they remain in the same region parameter space.

The results have at least two implications for applications of the complex Kohn method to more difficult scattering problems. First, the existence of singularities should highlight the fact that one should always consider the effects of changes in the nonlinear variational parameters on the results of the variational principle. Second, the unitarity of the S matrix should be checked for each energy considered in a given calculation. Thus, with a judicious choice of variational basis set and with care in checking the unitarity of S, the complex Kohn method should not be troubled by anomalous singularities.

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