Anomaly-Free Variational Method for Inelastic Scattering

R. K. Nesbet
IBM *Research Laboratory, San Jose, California* 95114
(Received 30 September 1968)

Analysis, given in an earlier paper, of standard variational methods for elastic scattering is extended to the case of several open channels. As in the case of elastic scattering, and contrary to widespread expectation, the spurious singularities inherent in the Kohn formalism are shown, for the general multichannel case, not to arise from the singularities of the linear inhomogeneous system of equations common to standard variational methods. The Kohn formula for elements of the R or K matrix, and its analog for the R^{-1} matrix, are shown to vary smoothly, without poles, as the energy parameter goes through eigenvalues of this system of equations. The spurious singularities arise from isolated zeroes of determinants that occur in the denominator of the Kohn formula and of its analog (the inverse Kohn formula) for R^{-1}. The singularities in these formulas do not in general coincide, and a criterion is proposed for alternative use of these formulas, resulting in a procedure free of spurious singularities. This analysis is illustrated by calculations on a soluble two-channel-model problem. An incidental result of the present formalism is a proof that the approximate R matrix given by the Kohn formula is symmetric and real if the basis functions used are real.

I. INTRODUCTION

Several standard variational methods in elastic-scattering theory, together with a new method proposed by Harris,[1] have recently been analyzed, especially with regard to their behavior near singularities of the inhomogeneous system of linear equations common to the various methods.[2] This analysis reached the somewhat unexpected conclusion that these singularities exactly cancel out of the Kohn formula[3] for the tangent of the phase shift, which can be expressed as a ratio of two functions with coincident simple poles at singular values of the energy E (or wave vector k). The spurious singularities inherent in the Kohn formula, discussed most fully by Schwartz,[4] then must arise from some other aspect of the formalism. It was shown[2] that the Kohn formula can be expressed as a ratio whose denominator, denoted by M_{11} in the single-channel problem, has isolated zeroes at values of E that are artifacts of the variational method, since they depend on the particular choice of basis functions used for linear expansion of a trial wave function. These zeroes are the sources of the spurious singularities in the Kohn formula. The corresponding formula for the cotangent of the phase shift, due to Hulthén and Rubinow,[5] which will be called the inverse Kohn formula here, can also be expressed as a ratio whose denominator, denoted by M_{00} in the single-channel problem, has isolated zeroes that depend on the choice of basis function set. These zeroes cause spurious singularities in the inverse Kohn formula. Since the zeroes of M_{00} and M_{11} do not, in general, coincide, the ratio $|M_{00}/M_{11}|$ can be used as a criterion to choose either the Kohn or inverse Kohn formula, thus giving an anomaly-free variational procedure.

In the present paper these results are generalized to the theory of inelastic scattering. The principal result is the formulation of a variational procedure that avoids all spurious singularities, works with real numbers only, and obtains the reactance matrix R or its inverse R^{-1} by use of a suitable generalization of the Kohn or inverse Kohn methods, respectively.[6] The inhomogeneous linear system of large dimension common to variational methods is solved only once for each energy in the present method, in contrast to iterated solution of such equations inherent in some earlier methods.

The proposed method is applied to a soluble model problem, and results are compared with earlier calculations on this model reported by Huck,[7] who used methods proposed by Moiseiwitsch[8] and by Rubinow.[5] The present results indicate that the method proposed here converges rapidly, is free of spurious singularities, and compares favorably in terms of computational effort with earlier methods.

It is intended to apply this method to electron-atom scattering, using a Bethe-Goldstone formalism proposed earlier to deal with the many-particle aspect of such calculations.[9]

II. VARIATIONAL FORMALISM

Consider the system of equations

$$\sum_q (H_{pq} - E\delta_{pq})\psi_q = 0, \tag{1}$$

where indices p and q represent separate open channels and run from 1 to N, the number of channels. The Hamiltonian H_{pq} is a matrix of operators and ψ_p is a vector whose components are wave functions. For a spherically symmetric system, it is

convenient to make a partial-wave expansion, and to associate a wave number k_p and angular momentum l_p with each channel index p. An example leading to equations of this form occurs in electron-atom scattering, where the scattering atom has several bound states with energy E_p less than E. Each such bound state defines at least one channel. If the state is not spherically symmetric, there might be several channels with different l values but the same value of k. In Hartree atomic units

$$\tfrac{1}{2}k_p^2 = E - E_p, \tag{2}$$

where E_p is the energy of the bound state associated with channel p for the scattered electron. Equations (1) are obtained by taking matrix elements of the many-electron Hamiltonian between the various bound-state wave functions of the scattering atom, and by expanding the wave function of the scattered electron in partial waves. Alternatively, the functions ψ_p can be taken to be many-particle functions defined by their asymptotic behavior as antisymmetrized products of a bound-state eigenfunction and a one-electron continuum function appropriate to parameters k_p and l_p.

If the channel wave functions ψ_p are considered as one-electron functions, the partial-wave decomposition leads to equations of the form considered here for the separate radial functions. It is convenient to multiply each wave function by r, so that each ψ_p vanishes at $r=0$, and can be chosen to have the asymptotic form

$$\psi_p \sim \alpha_{0p} S_p + \alpha_{1p} C_p, \tag{3}$$

$$\text{where} \quad S_p \sim \sin(k_p r - \tfrac{1}{2} l_p \pi), \qquad C_p \sim \cos(k_p r - \tfrac{1}{2} l_p \pi). \tag{4}$$

In general, the coefficients α will be complex. The form of S_p and C_p in the region of small r is arbitrary, except that both functions should vanish as r^{l+1}; the exact form to be chosen is a matter of computational convenience. Given specific forms for these functions, the function ψ_p can be approximated by the linear expansion

$$\psi_p = \phi_p + \alpha_{0p} S_p + \alpha_{1p} C_p, \tag{5}$$

$$\text{where} \quad \phi_p = \sum_{a=1}^{n_p} \eta_a^p c_a^p. \tag{6}$$

The functions η_a^p are normalizable basis functions chosen from a countable set that becomes complete (for finite r) as n_p is increased. Then ϕ_p is also normalizable and does not affect the asymptotic behavior of ψ_p.

Scattering cross sections depend only on the relative values of the coefficients α. In practice the dimensions n_p of the normalizable basis function sets will be increased until the coefficients α are seen to converge to a desired accuracy. In order to avoid the use of complex numbers, the reactance matrix R[6] (or K in another common usage), which is real and symmetric in the channel indices, can be computed directly. The scattering and transition matrices are given, respectively, by[6]

$$S = (1 + iR)/(1 - iR), \tag{7}$$

$$T = -2R/(1 - iR). \tag{8}$$

The partial cross section for a transition from channel p to channel q is, in atomic units,

$$Q_{pq} = (\pi/k_p^2)|T_{pq}|^2 = (4\pi/k_p^2)|[R/(1 - iR)]_{pq}|^2. \tag{9}$$

If the coefficients of one of N degenerate solutions ψ^σ of Eqs. (1) at given E are chosen to satisfy the condition,

$$\alpha_{0q}^{\ \sigma} = \delta_{q\sigma}, \quad q = 1, \ldots, N, \tag{10}$$

for each $\sigma = 1, \ldots, N$, then the computed values of $\alpha_{1q}^{\ \sigma}$ will be denoted by

$$\gamma_{\sigma q} = \alpha_{1q}^{\ \sigma}. \tag{11}$$

The elements of the R matrix are defined in terms of these coefficients to be[6]

$$R_{pq} = (k_q/k_p)^{1/2} \gamma_{pq}. \tag{12}$$

An alternative set of definitions leads directly to the matrix R^{-1}, which must also be real and symmetric. If the coefficients are required to satisfy,

$$\alpha_{1q}^{\ \sigma} = \delta_{q\sigma}, \quad q = 1, \ldots, N \tag{13}$$

for each $\sigma = 1, \ldots, N$, then the computed values of $\alpha_{0q}^{\ \sigma}$ will be denoted by

$$\beta_{\sigma q} = \alpha_{0q}^{\ \sigma}. \tag{14}$$

The elements of R^{-1} are given by

$$R_{pq}^{-1} = (k_q/k_p)^{1/2} \beta_{pq}. \tag{15}$$

The coefficients in Eq. (6) are determined by the condition that Eqs. (1) should have no components in the Hilbert spaces spanned by the basis functions η_a^p. This leads to the system of linear equations of dimension $\sum_p n_p$, for $p = 1, \ldots, N$ and $a = 1, \ldots, n_p$,

$$\sum_s \sum_b M_{ab}^{ps} c_b^s = -\sum_q (\alpha_{0q} M_{aS}^{pq} + \alpha_{1q} M_{aC}^{pq}), \tag{16}$$

where $$M_{ab}^{pq} = (\eta_a^p | H_{pq} - E\delta_{pq} | \eta_b^q), \tag{17}$$

$$M_{aS}^{pq} = (\eta_a^p | H_{pq} - E\delta_{pq} | S_q), \tag{18}$$

$$M_{aC}^{pq} = (\eta_a^p | H_{pq} - E\delta_{pq} | C_q). \tag{19}$$

The computations for an N-channel problem can be greatly simplified, following the procedure used by Schwartz for the single-channel problem,[4] by observing that the coefficients c_b^q obtained by solving Eqs. (16) depend linearly on the coefficients α. In particular,

$$c_b^s = \sum_q (\alpha_{0q} c_{bS}^{sq} + \alpha_{1q} c_{bC}^{sq}), \tag{20}$$

where, for $p = 1, \ldots, N$ and $a = 1, \ldots, n_p$,

$$\begin{aligned} \sum_s \sum_b M_{ab}^{ps} c_{bS}^{sq} &= -M_{aS}^{pq}, \\ \sum_s \sum_b M_{ab}^{ps} c_{bC}^{sq} &= -M_{aC}^{pq}. \end{aligned} \tag{21}$$

Solution of these equations reduces to successive solution of $2N$ inhomogeneous linear systems of dimension $\sum_p n_p$ with a common homogeneous matrix M_{ab}^{pq}, for each of the $2N$ inhomogeneous vectors $-M_{aS}^{pq}$ and $-M_{aC}^{pq}$. The solution of these equations, of large dimensionality, is a common starting point for all variational methods of determining the coefficients α. Equations (20) and (21) imply that Eqs. (16) are satisfied identically for any arbitrary values of these coefficients. Since Eqs. (21)do not involve the α's, they must be solved only once for a given value of E, regardless of the specific method used subsequently to determine the α's. Most of the computational effort in any practical calculation occurs in the solution of Eqs. (21).

Through Eqs. (21), each independent asymptotic function, S_q or C_q, picks up a normalizable complement denoted by ϕ_{Sq} or ϕ_{Cq}, with components ϕ_{Sq}^s or ϕ_{Cq}^s in each of the channels. This leads to a set of functions corresponding to particular solutions of the linear system of Eq. (21), with components in channel s given by

$$\begin{aligned} \psi_{0q}^s &= \phi_{Sq}^s + S_q \delta_{qs}, \\ \text{or} \quad \psi_{1q}^s &= \phi_{Cq}^s + C_q \delta_{qs}, \quad s = 1, \ldots, N, \end{aligned} \tag{22}$$

$$\begin{aligned} \text{where} \quad \phi_{Sq}^s &= \sum_b \eta_b^s c_{bS}^{sq}, \\ \text{and} \quad \phi_{Cq}^s &= \sum_b \eta_b^s c_{bC}^{sq}, \quad s = 1, \ldots, N. \end{aligned} \tag{23}$$

Equations (21) imply, for $p, q = 1, \ldots, N$ and $a = 1, \ldots, n_p$,

$$\begin{aligned} \sum_s (\eta_a^p | H_{ps} - E\delta_{ps} | \psi_{0q}^s) &= 0, \\ \sum_s (\eta_a^p | H_{ps} - E\delta_{ps} | \psi_{1q}^s) &= 0. \end{aligned} \tag{24}$$

The variational methods to be considered here can be described in terms of the matrix elements

$$\begin{aligned} M_{00}^{pq} &= \sum_r \sum_s (\psi_{0p}^r | H_{rs} - E\delta_{rs} | \psi_{0q}^s) \\ &= \sum_s (S_p | H_{ps} - E\delta_{ps} | \psi_{0q}^s), \\ M_{01}^{pq} &= \sum_r \sum_s (\psi_{0p}^r | H_{rs} - E\delta_{rs} | \psi_{1q}^s) \\ &= \sum_s (S_p | H_{ps} - E\delta_{ps} | \psi_{1q}^s), \\ M_{10}^{pq} &= \sum_r \sum_s (\psi_{1p}^r | H_{rs} - E\delta_{rs} | \psi_{0q}^s) \\ &= \sum_s (C_p | H_{ps} - E\delta_{ps} | \psi_{0q}^s), \\ M_{11}^{pq} &= \sum_r \sum_s (\psi_{1p}^r | H_{rs} - E\delta_{rs} | \psi_{1q}^s) \\ &= \sum_s (C_p | H_{ps} - E\delta_{ps} | \psi_{1q}^s). \end{aligned} \tag{25}$$

The last term in each of these equations follows from Eqs. (24), since the normalizable part ϕ_{Sp}^r or ϕ_{Cp}^r of each of the functions ψ_{0p}^r or ψ_{1p}^r is a linear combination of the basis functions η_a^r, and, by Eqs. (24), does not contribute to the matrix elements defined by Eqs. (25). In terms of the matrix elements and coefficients defined by Eqs. (17), (18), (19), and (21) above,

$$\begin{aligned} M_{00}^{pq} &= M_{SS}^{pq} + \sum_r \sum_a M_{Sa}^{pr} c_{aS}^{rq} = M_{SS}^{pq} \\ &\quad - \sum_{rs} \sum_{ab} M_{Sa}^{pr} (M^{-1})_{ab}^{rs} M_{bS}^{sq}, \\ M_{01}^{pq} &= M_{SC}^{pq} + \sum_r \sum_a M_{Sa}^{pr} c_{aC}^{rq} = M_{SC}^{pq} \\ &\quad - \sum_{rs} \sum_{ab} M_{Sa}^{pr} (M^{-1})_{ab}^{rs} M_{bC}^{sq}, \\ M_{10}^{pq} &= M_{CS}^{pq} + \sum_r \sum_a M_{Ca}^{pr} c_{aS}^{rq} = M_{CS}^{pq} \\ &\quad - \sum_{rs} \sum_{ab} M_{Ca}^{pr} (M^{-1})_{ab}^{rs} M_{bS}^{sq}, \end{aligned} \tag{26}$$

$$M_{11}{}^{pq} = M_{CC}{}^{pq} + \sum_r \sum_a M_{Ca}{}^{pr} c_{aC}{}^{rq} = M_{CC}{}^{pq} - \sum_{rs} \sum_{ab} M_{Ca}{}^{pr} (M^{-1})_{ab}{}^{rs} M_{bC}{}^{sq}.$$

Because the operator H is Hermitian with respect to normalizable functions, the matrix elements defined by Eqs. (26) are real and, except for $M_{01}{}^{pp}$ and $M_{10}{}^{pp}$, symmetric in the index pairs

$$\binom{p}{i} \text{ or } \binom{q}{j},$$

where $i, j = 0, 1$. The exceptional case is

$$M_{01}{}^{pp} - M_{10}{}^{pp} = M_{SC}{}^{pp} - M_{CS}{}^{pp} = \tfrac{1}{2}k_p, \quad p = 1, \ldots, N, \tag{27}$$

if the functions S_p and C_p satisfy Eqs. (4). This result follows upon integrating the kinetic-energy integral by parts and evaluating the resulting surface integral. Equation (27) can also be written in the form

$$M_{ij}{}^{pq} = M_{ji}{}^{qp} + \tfrac{1}{2}k_p \delta_{pq}(\delta_{i0}\delta_{j1} - \delta_{i1}\delta_{j0}), \quad ij = 0, 1; \quad p, q = 1, \ldots, N. \tag{28}$$

Up to this point in the analysis the coefficients $\alpha_{ip} (i = 0, 1;\ p = 1, \ldots, N)$ of Eq. (5) are as yet undetermined, although the coefficients $c_a{}^p$ defined by Eq. (6) are determined as linear functions of the α's by Eqs. (20) and (21). For a variational calculation this implies a trial function ψ^ν with component in channel s given by

$$\psi_{\nu s} = \sum_i \sum_q \alpha_{iq} \psi_{iq}{}^s, \tag{29}$$

where the functions $\psi_{iq}{}^s$ are defined by Eqs. (22).

Consider the variational functional

$$I_{\sigma\nu} = (\psi^\sigma | H - E | \psi^\nu) = \sum_{rs} (\psi_{\sigma r} | H_{rs} - E\delta_{rs} | \psi_{\nu s}). \tag{30}$$

If ψ^ν were an exact solution of the Schrödinger equation, Eq. (1), then $I_{\sigma\nu}$ would vanish for arbitrary $\psi\sigma$. This condition, for $I_{\nu\nu}$, is required as a constraint on ψ^ν in the Hulthén variational method.[10] If Eq. (1) were satisfied, the integrals

$$I_{i\nu}{}^p = \sum_{rs} (\psi_{ip}{}^r | H_{rs} - E\delta_{rs} | \psi_{\nu s}) \tag{31}$$

would vanish for each value of $i = 0, 1$ and $p = 1, \ldots, N$. In terms of the matrix elements defined previously,

$$I_{i\nu}{}^p = \sum_j \sum_q M_{ij}{}^{pq} \alpha_{jq}{}^\nu. \tag{32}$$

The matrix elements $M_{ij}{}^{pq}$, defined by Eqs. (25), above, are real if the basis functions $\eta_a{}^p$ are chosen to be real. While each of the integrals $I_{i\nu}{}^p$ would vanish for an exact solution ψ^ν of Eq. (1), setting all of these integrals equal to zero would give $2N$ homogeneous equations to determine the $2N$ unknown coefficients α in the variational trial function ψ^ν. In general, for a finite set of basis functions $\eta_a{}^p$, these equations will be inconsistent. The various variational methods that can be applied to this problem represent different procedures for combining these equations to reduce their number and obtain a consistent set.

From Eqs. (25), (29), and (31), the variational functional can be expressed in the form

$$I_{\sigma\nu} = \sum_{ij} \sum_{pq} \alpha_{ip}{}^{\sigma *} M_{ij}{}^{pq} \alpha_{jq}{}^\nu = \sum_i \sum_p \alpha_{ip}{}^{\sigma *} I_{i\nu}{}^p. \tag{33}$$

Alternatively, from Eq. (28),

$$I_{\sigma\nu} = \sum_{ij} \sum_{pq} \alpha_{ip}{}^{\sigma *} [M_{ji}{}^{qp} + \tfrac{1}{2}k_p \delta_{pq} \times (\delta_{i0}\delta_{j1} - \delta_{i1}\delta_{j0})] \alpha_{jq}{}^\nu = \sum_j \sum_q [I_{j\sigma}{}^{q*} + \tfrac{1}{2}k_q \times (\delta_{j1}\alpha_{0q}{}^{\sigma *} - \delta_{j0}\alpha_{1q}{}^{\sigma *})] \alpha_{jq}{}^\nu. \tag{34}$$

From these equations, if the coefficients α^σ and α^ν are independent,

$$\frac{\partial I_{\sigma\nu}}{\partial \alpha_{ip}{}^{\sigma *}} = I_{i\nu}{}^p \tag{35}$$

and

$$\frac{\partial I_{\sigma\nu}}{\partial \alpha_{jq}{}^\nu} = I_{j\sigma}{}^{q*} + \tfrac{1}{2}k_q (\delta_{j1}\alpha_{0q}{}^{\sigma *} - \delta_{j0}\alpha_{1q}{}^{\sigma *}). \tag{36}$$

The first-order variation of $I_{\sigma\nu}$ is given in general by

$$\delta I_{\sigma\nu} = \sum_i \sum_p \delta\alpha_{ip}{}^{\sigma *} I_{i\nu}{}^p + \sum_j \sum_q I_{j\sigma}{}^{q*} \delta\alpha_{jq}{}^\nu + \sum_q \tfrac{1}{2}k_q (\alpha_{0q}{}^{\sigma *} \delta\alpha_{1q}{}^\nu - \alpha_{1q}{}^{\sigma *} \delta\alpha_{0q}{}^\nu). \tag{37}$$

For exact solutions ψ^σ and ψ^ν, since all of the integrals $I_{i\nu}{}^p$ or $I_{j\sigma}{}^{q*}$ vanish, this reduces to

$$\delta I_{\sigma\nu} = \sum_q \tfrac{1}{2}k_q (\alpha_{0q}{}^{\sigma *} \delta\alpha_{1q}{}^\nu - \alpha_{1q}{}^{\sigma *} \delta\alpha_{0q}{}^\nu). \tag{38}$$

III. THE KOHN AND INVERSE KOHN VARIATIONAL METHODS

Equation (37) for the first variation of the variational functional simplifies considerably if the R matrix is computed directly, using Eqs. (10), (11), and (12). All coefficients α are real. Because the values of $\alpha_{0p}{}^{\sigma}$ or $\alpha_{0q}{}^{\nu}$ are fixed (0 or 1), their variations vanish, and Eq. (37) reduces to

$$\delta I_{\sigma\nu} = \sum_p I_{1\nu}{}^p \delta\alpha_{1p}{}^{\sigma} + \sum_q I_{1\sigma}{}^q \delta\alpha_{1q}{}^{\nu} + \tfrac{1}{2} k_\sigma \delta\alpha_{1\sigma}{}^{\nu}, \tag{39}$$

$$= \sum_p I_{1\nu}{}^p \delta\gamma_{\sigma p} + \sum_q I_{1\sigma}{}^q \delta\gamma_{\nu q} + \tfrac{1}{2} k_\sigma \delta\gamma_{\nu\sigma}. \tag{40}$$

The integrals $I_{1\nu}{}^p$ that occur in this equation can all simultaneously be reduced to zero by an appropriate choice of the coefficients $\gamma_{\nu q}$, equivalent to elements of the R matrix except for simple factors given in Eq. (12). These values of the coefficients will be denoted by $\gamma_{\nu q}{}^{(0)}$ and satisfy the equations, from Eq. (32),

$$\sum_q M_{11}{}^{pq} \gamma_{\nu q}{}^{(0)} = -M_{10}{}^{p\nu}, \qquad \nu = 1, \ldots, N; \quad p = 1, \ldots, N. \tag{41}$$

For each index ν, this is a set of N inhomogeneous linear equations for N unknowns $\gamma_{\nu q}{}^{(0)}$. The system of equations has finite solutions unless

$$\det(M_{11}{}^{pq}) = 0. \tag{42}$$

In the present context, the Kohn variational method,[3] as applied to elements of the R matrix,[6] makes use of Eq. (40) to compute first-order corrections to the $\gamma_{\nu q}{}^{(0)}$. From Eq. (40), if the integrals $I_{1\nu}{}^p$ or $I_{1\sigma}{}^q$ vanish,

$$\delta(I_{\sigma\nu} - \tfrac{1}{2} k_\sigma \gamma_{\nu\sigma}) = 0. \tag{43}$$

This gives approximately stationary values of the coefficients

$$\gamma_{\nu q} = \gamma_{\nu q}{}^{(0)} - (2/k_q) I_{q\nu}(\gamma_{\nu q}{}^{(0)}). \tag{44}$$

From Eqs. (10) and (33), when all $I_{1\nu}{}^p$ vanish,

$$I_{q\nu}(\gamma_{\nu q}{}^{(0)}) = \sum_i \sum_p \alpha_{ip}{}^q I_{i\nu}{}^p = \sum_p \alpha_{0p}{}^q I_{0\nu}{}^p = I_{0\nu}{}^q(\gamma_{\nu q}{}^{(0)}). \tag{45}$$

Then Eq. (44), the Kohn formula, reduces to

$$\gamma_{\nu q} = \gamma_{\nu q}{}^{(0)} - (2/k_q) I_{0\nu}{}^q(\gamma_{\nu q}{}^{(0)}) \tag{46}$$

$$= \gamma_{\nu q}{}^{(0)} - (2/k_q)(M_{00}{}^{q\nu} + \sum_p M_{01}{}^{qp} \gamma_{\nu p}{}^{(0)}). \tag{47}$$

Equation (32) has been used here to give an explicit formula in terms of the matrix elements $M_{ij}{}^{pq}$.

A similar method can be used to compute elements of the R^{-1} matrix. This will be called the inverse Kohn method here, although in the single-channel problem it reduces to a method proposed by Hulthén and by Rubinow, sometimes referred to as the second Hulthén method.[5] In terms of Eqs. (13), (14), and (15), the first variation of the variational functional $I_{\sigma\nu}$ becomes

$$\delta I_{\sigma\nu} = \sum_p I_{0\nu}{}^p \delta\beta_{\sigma p} + \sum_q I_{0\sigma}{}^q \delta\beta_{\nu q} - \tfrac{1}{2} k_\sigma \delta\beta_{\nu\sigma}. \tag{48}$$

The integrals $I_{0\nu}{}^p$ or $I_{0\sigma}{}^q$ in this equation can all be reduced to zero by solution of the inhomogeneous linear equations

$$\sum_q M_{00}{}^{pq} \beta_{\nu q}{}^{(0)} = -M_{01}{}^{p\nu}, \qquad \nu = 1, \ldots, N; \quad p = 1, \ldots, N \tag{49}$$

This system of equations has finite solutions for the coefficients $\beta_{\nu q}{}^{(0)}$, related to elements of the R^{-1} matrix by Eq. (15), unless

$$\det(M_{00}{}^{pq}) = 0. \tag{50}$$

From Eq. (37), if the integrals $I_{0\nu}{}^p$ or $I_{0\sigma}{}^p$ vanish,

$$\delta(I_{\sigma\nu} + \tfrac{1}{2} k_\sigma \beta_{\nu\sigma}) = 0. \tag{51}$$

This gives approximately stationary values of the coefficients

$$\beta_{\nu q} = \beta_{\nu q}{}^{(0)} + (2/k_q) I_{q\nu}(\beta_{\nu q}{}^{(0)}). \tag{52}$$

From Eqs. (13) and (33), when all $I_{0\nu}{}^p$ vanish,

$$I_{q\nu}(\beta_{\nu q}{}^{(0)}) = \sum_i \sum_p \alpha_{ip}{}^q I_{i\nu}{}^p = \sum_p \alpha_{1p}{}^q I_{1\nu}{}^p = I_{1\nu}{}^q(\beta_{\nu q}{}^{(0)}). \tag{53}$$

Then Eq. (52), the inverse Kohn formula, reduces to

$$\beta_{\nu q} = \beta_{\nu q}^{(0)} + (2/k_q) I_{1\nu}^{q}(\beta_{\nu q}^{(0)}) = \beta_{\nu q}^{(0)} + (2/k_q)(M_{11}^{q} + \sum_p M_{10}^{qp} \beta_{\nu p}^{(0)}) . \quad (54)$$

Equation (32) has been used to give an explicit formula in terms of the matrix elements M_{ij}^{pq}.

IV. AVOIDANCE OF SPURIOUS SINGULARITIES

When applied to a single-channel problem, the Kohn formula, Eq. (47), becomes a formula for the tangent of the elastic phase shift. Spurious singularities, in the form of isolated poles whose position as a function of E or k depends on the choice of normalizable basis set, occur in this formula and have been studied by Schwartz.[4] While these singularities were attributed by Schwartz to the singular points of Eqs. (21), where the determinant of M_{ab} vanishes, it has been shown more recently that the Kohn formula remains smooth at such points, since it can be written as the ratio of two functions with coincident simple poles at these points.[2] The spurious singularities arise instead from the zeroes of M_{11}, the single-channel form of Eq. (42). These points do not, in general, coincide with the zeroes of M_{00}, so the inverse Kohn formula, in which M_{00} occurs as a denominator, can be used to give smooth results whenever $|M_{00}/M_{11}|$ exceeds unity.[2] This apparently gives an anomaly free variational method for the single-channel problem.

With the formalism developed here, these results can easily be generalized to the multichannel problem. Equations (26) show that each of the matrix elements M_{ij}^{pq} has a simple pole at an eigenvalue E_α of the Hamiltonian matrix H_{ab}^{pq}, where the determinant of M_{ab}^{pq} vanishes. These eigenvalues will be assumed to be nondegenerate, as they appear to be in simple examples using an arbitrary finite basis function set.

The eigenvalues E_α and eigenvectors, with components $c_{b\alpha}^{s}$, of the homogeneous part of Eqs. (21) satisfy the equations

$$\sum_s \sum_b H_{ab}^{ps} c_{b\alpha}^{s} = E_\alpha c_{a\alpha}^{p} . \quad (55)$$

The eigenvectors can be assumed to be orthonormal. It should be noted that each eigenvector has components in all channels, so the index α does not specify any particular channel. There are $\sum_p n_p$ independent eigenvectors, each of which corresponds to a normalized function with component in channel p.

$$\phi_\alpha^{p} = \sum_{a=1}^{n_p} \eta_a^{p} c_{a\alpha}^{p} . \quad (56)$$

The ϕ_α are eigenfunctions of the Hamiltonian within the Hilbert space spanned by the basis functions η_a^p. The functions ϕ_{Sq}^{s} and ϕ_{Cq}^{s} of Eq. (23) can be expanded in terms of the function ϕ_α and eigenvalues E_α in the form

$$\phi_{Sq}^{s} = \sum_\alpha \phi_\alpha^{s} (E - E_\alpha)^{-1} M_{\alpha S}^{q} ,$$

$$\phi_{Cq}^{s} = \sum_\alpha \phi_\alpha^{s} (E - E_\alpha)^{-1} M_{\alpha C}^{q} , \quad (57)$$

where $M_{\alpha S}^{q} = \sum_p (\phi_\alpha^{p} | H_{pq} - E\delta_{pq} | S_q) ,$

$$M_{\alpha C}^{q} = \sum_p (\phi_\alpha^{p} | H_{pq} - E\delta_{pq} | C_q) . \quad (58)$$

These matrix elements are real and symmetric if the basis functions η_a^p, S_q, and C_q are all real. The matrix elements M_{ij}^{pq}, defined by Eqs. (25), reduce to

$$M_{00}^{pq} = M_{SS}^{pq} + \sum_\alpha M_{S\alpha}^{p} (E - E_\alpha)^{-1} M_{\alpha S}^{q} ,$$

$$M_{01}^{pq} = M_{SC}^{pq} + \sum_\alpha M_{S\alpha}^{p} (E - E_\alpha)^{-1} M_{\alpha C}^{q} ,$$

$$M_{10}^{pq} = M_{CS}^{pq} + \sum_\alpha M_{C\alpha}^{p} (E - E_\alpha)^{-1} M_{\alpha S}^{q} ,$$

$$M_{11}^{pq} = M_{CC}^{pq} + \sum_\alpha M_{C\alpha}^{p} (E - E_\alpha)^{-1} M_{\alpha C}^{q} . \quad (59)$$

These matrix elements obviously have coincident simple poles at the eigenvalues E_α. As E approaches a particular eigenvalue E_μ,

$$(E - E_\mu) M_{00}^{pq} \to M_{S\mu}^{p} M_{\mu S}^{q} ,$$

$$(E - E_\mu) M_{01}^{pq} \to M_{S\mu}^{p} M_{\mu C}^{q} ,$$

$$(E - E_\mu) M_{10}^{pq} \to M_{C\mu}^{p} M_{\mu S}^{q} ,$$

$$(E - E_\mu) M_{11}^{pq} \to M_{C\mu}^{p} M_{\mu C}^{q} . \quad (60)$$

These formulas will be used here to show that the coefficients $\gamma_{\nu q}$, determined by Eqs. (41), or by the Kohn formula, Eq. (47), can be expressed as ratios of quantities with coincident simple notes

at an eigenvalue E_μ, and hence that these eigenvalues do not introduce spurious poles in the computed R matrix elements. A similar result holds for the coefficients $\beta_{\nu q}$ and the inverse Kohn formula for elements of the R^{-1} matrix.

The solution of Eqs. (41) and the Kohn formula, Eq. (47), can be expressed in terms of determinants of submatrices of the matrix $M_{ij}{}^{pq}$, where $i, j = 0, 1$ and $p, q = 1, \ldots, N$. A convenient notation for such submatrices is

$$\left(\begin{matrix} pq & \cdots \\ ij & \cdots \end{matrix}\middle|\begin{matrix} rs & \cdots \\ kl & \cdots \end{matrix}\right)_n = \begin{vmatrix} M_{ik}{}^{pr} & M_{il}{}^{ps} & \cdots \\ M_{jk}{}^{qr} & M_{jl}{}^{qs} & \cdots \\ \cdots & \cdots & \end{vmatrix}, \quad (61)$$

where n, the order of the submatrix, is the number of pairs of upper and lower indices in each part of the bracket symbol.

In this notation, the solution of Eqs. (41) is

$$\gamma_{\nu q}{}^{(0)} = -\frac{\left(\begin{matrix} 1 & q & N \\ \cdots & \cdots & \\ 1 & 1 & 1 \end{matrix}\middle|\begin{matrix} 1 & \nu & N \\ \cdots & \cdots & \\ 1 & 0 & 1 \end{matrix}\right)_N}{\left(\begin{matrix} 1 & q & N \\ \cdots & \cdots & \\ 1 & 1 & 1 \end{matrix}\middle|\begin{matrix} 1 & q & N \\ \cdots & \cdots & \\ 1 & 1 & 1 \end{matrix}\right)_N}. \quad (62)$$

If it is recognized that the second term in Eq. (47) is equivalent to the expansion by minors of a determinant of order $N+1$, this equation, the Kohn formula, can be expressed in the form

$$\gamma_{\nu q} = \gamma_{\nu q}{}^{(0)} - \frac{2}{k_q}\frac{\left(\begin{matrix} q & 1 & N \\ & \cdots & \\ 0 & 1 & 1 \end{matrix}\middle|\begin{matrix} \nu & 1 & N \\ & \cdots & \\ 0 & 1 & 1 \end{matrix}\right)_{N+1}}{\left(\begin{matrix} 1 & N \\ \cdots & \\ 1 & 1 \end{matrix}\middle|\begin{matrix} 1 & N \\ \cdots & \\ 1 & 1 \end{matrix}\right)_N}. \quad (63)$$

Similar formulas can be written for $\beta_{\nu q}{}^{(0)}$, the solution of Eqs. (49), and for the inverse Kohn formula, Eq. (54), for $\beta_{\nu q}$.

To examine the behavior of a determinant of the kind indicated by Eq. (61), near an eigenvalue E_μ of the finite matrix $H_{ab}{}^{pq}$, Eqs. (59) can be used to write Eq. (61) in the form

$$\left(\begin{matrix} pq & \cdots \\ ij & \cdots \end{matrix}\middle|\begin{matrix} rs & \cdots \\ kl & \cdots \end{matrix}\right)_n = (E - E_\mu)^{-n} M_{i\mu}{}^{p} M_{j\mu}{}^{q} \times \cdots M_{\mu k}{}^{r} M_{\mu l}{}^{s} \cdots \det_n[f_{ij}{}^{pq}(E)], \quad (64)$$

where

$$f_{ij}{}^{pq}(E) = (E - E_\mu) M_{ij}{}^{pq}(E) / M_{i\mu}{}^{p} M_{\mu j}{}^{q}, \quad (65)$$

and the symbol $\det_n$ denotes a determinant of order n. Here $M_{i\mu}{}^{p}$ denotes $M_{S\mu}{}^{p}$ if $i = 0$ and $M_{C\mu}{}^{p}$ if $i = 1$. From Eqs. (60), as E approaches E_μ,

$$f_{ij}{}^{pq}(E) \to 1. \quad (66)$$

Then $\det_n[f_{ij}{}^{pq}(E_\mu)]$ is the determinant of a matrix of order n, all of whose elements are unity. Such a matrix is of rank one. A theorem proved in matrix theory[11] states that if $\Delta(\lambda)$ is the determinant of a matrix of order n, whose elements are functions of λ, and if for some λ_S the matrix becomes singular, of rank r, then $(\lambda - \lambda_S)^{n-r}$ is a factor of $\Delta(\lambda)$. It follows immediately from this theorem since $f_{ij}{}^{pq}(E_\mu)$ is a matrix of rank one, that $(E - E_\mu)^{n-1}$ is a factor of $\det_n[f_{ij}{}^{pq}(E)]$. Hence any determinant of the form given by Eq. (64) or Eq. (61) has a simple pole at E_μ, unless one or more of the matrix elements $M_{i\mu}{}^{p}$ should vanish at E_μ. Because ϕ_μ is a normalized function, these matrix elements are finite. In the example considered later in this paper, they do not vanish at E_μ, and there appears to be no general reason for such matrix elements to vanish when a finite set of basis functions is used. It can be concluded that determinants of submatrices of $M_{ij}{}^{pq}$, of any order $n \leq 2N$, will in general have simple poles at each eigenvalue E_μ.

Since $\gamma_{\nu q}{}^{(0)}$ and the Kohn formula for $\gamma_{\nu q}$ can be expressed as ratios of such determinants, as in Eqs. (62) and (63), the poles at E_μ cancel exactly and these coefficients vary smoothly as E passes through an eigenvalue. A similar result holds for $\beta_{\nu q}{}^{(0)}$ and for the inverse Kohn formula for $\beta_{\nu q}$.

The determinant of $M_{11}{}^{pq}$ is the denominator in both Eqs. (62) and (63), which can be expressed as a ratio. Since there is no general reason why $|M_{11}{}^{pq}(E)|$ should not have isolated zeroes, as a function of E, these points will be spurious singularities of the Kohn formula, as the zeroes of $M_{11}(E)$ are in the single channel problem.[2] The zeroes of $|M_{00}{}^{pq}(E)|$ are spurious singularities of the inverse Kohn formula, Eq. (54), as the zeroes of $M_{00}(E)$ are in the single-channel problem. There is no general reason, in the present formalism, why these zeroes should coincide, and they are found to be distinct in the example considered below. It can be expected, in analogy to the anomaly-free procedure proposed for the single-channel problem, that spurious singularities can be avoided completely by using the Kohn formula only when the ratio of determinants

$$|M_{00}{}^{pq}| / |M_{11}{}^{pq}| \quad (67)$$

is less than unity, and by using the inverse Kohn formula when this ratio is greater than unity.

The formalism developed here can be used to show that the R matrix, computed from Eq. (12) and from the Kohn formula, Eq. (47), is symmetric. This is not in general true if the coefficients $\gamma_{\nu q}^{(0)}$ are used in Eq. (12). From Eqs. (47) and (28),

$$R_{pq} = -[2/(k_p k_q)^{\frac{1}{2}}][M_{00}^{qp} + \sum_s (M_{01}^{qs} - \tfrac{1}{2}k_q \delta_{qs})\gamma_{ps}^{(0)}] \quad (68)$$

$$= -[2/(k_p k_q)^{1/2}] \times (M_{00}^{qp} + \sum_s M_{10}^{sq}\gamma_{ps}^{(0)}) \quad (69)$$

$$= -[2/(k_p k_q)^{1/2}] \times \frac{\begin{vmatrix} M_{00}^{qp} & M_{10}^{1q} & \cdots & M_{10}^{qq} & \cdots \\ M_{10}^{1p} & M_{11}^{11} & & M_{11}^{1q} & \cdots \\ \cdots & & & & \\ M_{10}^{pp} & M_{11}^{p1} & & M_{11}^{pq} & \end{vmatrix}}{\begin{vmatrix} M_{11}^{11} & \cdots & M_{11}^{1q} & \cdots \\ \cdots & & & \\ M_{11}^{p1} & & M_{11}^{1q} & \\ \cdots & & & \end{vmatrix}} . \quad (70)$$

The determinant in the numerator of this equation is carried into itself by first interchanging rows and columns, and then exchanging indices p and q and transposing all of the matrix elements M_{11}^{rs}, which by Eq. (28) are symmetric in their indices. Since interchanging rows and columns does not change the value of a determinant, Eq. (70) is symmetric in the indices p, q. A similar result holds for the R^{-1} matrix computed from the inverse Kohn formula, Eq. (54).

V. CALCULATIONS FOR A TWO-CHANNEL MODEL PROBLEM

A simple two-channel model problem, with exact solutions computable in terms of elementary functions, has previously been used as an example of variational methods by Huck.[7] The Hamiltonian operator is

$$H_{11} = -\tfrac{1}{2}d^2/dr^2 ,$$

$$H_{12} = H_{21} = \tfrac{1}{2}C, \quad r<a; \quad = 0, r \geq a ,$$

$$H_{22} = -\tfrac{1}{2}d^2/dr^2 + \Delta E . \quad (71)$$

Following Huck, the values $a = 1$, $\Delta E = 0.375$ were assumed, with all quantities in atomic units. The channel wave functions are required to satisfy the boundary conditions

$$\psi_p(0) = 0 ,$$

$$\psi_p \sim \alpha_{0p}\sin k_p r + \alpha_{1p}\cos k_p r, \quad p = 1, 2; \quad (72)$$

where $\tfrac{1}{2}k_1^2 - \tfrac{1}{2}k_2^2 = \Delta E = 0.375$. (73)

For variational calculations, the normalizable basis functions used in each channel were

$$\eta_a = r^q e^{-2.5r}, \quad a = 1, \ldots, n. \quad (74)$$

The specific asymptotic functions used were

$$S_p = \sin k_p r ,$$

$$C_p = (1 - e^{-r})\cos k_p r, \quad p = 1, 2 . \quad (75)$$

The order of the basis set in each channel, n, varied between 1 and 5.

For $C^2 > k_1^2 k_2^2$, the general solution of Eqs. (71) can be expressed in the form, for $r < a$,

$$\psi_1(r) = A\sin mr + B\sinh pr$$

$$\psi_2(r) = \alpha\sin mr + \beta\sinh pr , \quad (76)$$

where

$$2m^2 = [(k_1^2 - k_2^2)^2 + 4C^2]^{1/2} + (k_1^2 + k_2^2)$$

$$2p^2 = [(k_1^2 - k_2^2)^2 + 4C^2]^{1/2} - (k_1^2 + k_2^2) , \quad (77)$$

and

$$\frac{\alpha}{A} = \left(\frac{k_1^2 - m^2}{k_2^2 - m^2}\right)^{1/2}, \quad \frac{\beta}{B} = \left(\frac{k_1^2 + p^2}{k_2 + p^2}\right)^{1/2} . \quad (78)$$

The constants A and B are chosen to satisfy Eqs. (10), giving a direct determination of the elements of the R matrix through Eqs. (11) and (12).

From Eq. (9), if Q_{pq} is the cross section for a transition from channel p to channel q, the various cross sections expressed as functions of elements of the R matrix, in units πa_0^2, are

$$Q_{11}/\pi = (4/k_1^2) \times \frac{R_{11}^2 + (R_{12}R_{21} - R_{11}R_{22})^2}{(R_{11}+R_{22})^2 + (1+R_{12}R_{21}-R_{11}R_{22})^2},$$

$$Q_{12}/\pi = (4/k_1^2) \times \frac{R_{12}^2}{(R_{11}+R_{22})^2 + (1+R_{12}R_{21}-R_{11}R_{22})^2},$$

$$Q_{21}/\pi = (4/k_2^2) \times \frac{R_{21}^2}{(R_{11}+R_{22})^2 + (1+R_{12}R_{21}-R_{11}R_{22})^2}, \tag{79}$$

$$Q_{22}/\pi = (4/k_2^2) \times \frac{R_{22}^2 + (R_{12}R_{21} - R_{11}R_{22})^2}{(R_{11}+R_{22})^2 + (1+R_{12}R_{21}-R_{11}R_{22})^2}.$$

In the exact solution, as well as the Kohn and inverse Kohn variational formulas, the matrix elements R_{12} and R_{21} are equal. Similar formulas, used with the inverse Kohn formula, hold for the cross sections as functions of elements of the R^{-1} matrix.

Matrix elements of the operators in Eq. (71), between any two of the functions defined by Eqs. (74) and (75), can be expressed in terms of elementary functions and evaluated in closed form. Computations were carried out by diagonalizing the matrix $H_{ab}{}^{pq}$, through the eigenvalue equations, Eqs. (55) and then by evaluating Eqs. (59) explicitly. The Kohn or inverse Kohn formulas, Eqs. (47) and (54), respectively, were used alternatively according to the criterion given by Eq. (67). This procedure, as discussed in Sec. IV, above, avoids spurious singularities inherent in these formulas.

Results for $C^2 = 2(2)12$ and for $n = 1(1)5$ are given in Table I. The variational procedure appears to converge rapidly and smoothly. Detailed numerical results are given by Huck, with the values of k_1 and k_2 used here, only for $C^2 = 10.0$. He finds 0.767 for the exact value of Q_{12}, in agreement with the present result, and obtains values 0.937, 0.937, 0.927, 0.797, and 0.711 for five different variational calculations.[7] The present method, both in terms of the computational labor required and of the rapidity of convergence, appears to be superior to the methods used by Huck.

TABLE I. Elastic and inelastic cross sections, in πa_0^2 atomic units, for $k_1 = 1.0$, $k_2 = 0.5$. Comparison of variational and exact results for different values of n, the number of basis functions in each channel.

	C_2	2.0	4.0	6.0	8.0	10.0	12.0
Q_{11}	$n=1$	0.153 516	0.577 469	1.101 00	1.559 67	1.896 62	2.124 57
	2	0.201 946	0.779 186	1.417 33	1.881 10	2.154 04	2.300 03
	3	0.223 666	0.793 405	1.429 23	1.871 35	2.118 38	2.242 59
	4	0.206 931	0.780 991	1.420 35	1.884 87	2.159 84	2.308 05
	5	0.208 917	0.788 733	1.429 91	1.892 89	2.164 61	2.309 69
	exact	0.211 324	0.796 646	1.440 18	1.900 53	2.167 91	2.309 04
Q_{12}	1	0.363 195	0.674 684	0.846 888	0.888 440	0.853 299	0.786 291
	2	0.380 416	0.725 170	0.868 641	0.854 035	0.772 634	0.678 856
	3	0.386 459	0.743 678	0.885 588	0.862 239	0.774 109	0.676 967
	4	0.387 109	0.722 779	0.865 142	0.851 725	0.772 211	0.680 029
	5	0.387 974	0.723 923	0.865 797	0.850 480	0.769 720	0.677 009
	exact	0.388 993	0.726 203	0.866 754	0.849 444	0.767 462	0.674 333
Q_{21}	1	1.452 78	2.698 74	3.387 55	3.553 76	3.413 19	3.145 16
	2	1.521 66	2.900 68	3.474 56	3.416 14	3.090 53	2.715 42
	3	1.545 84	2.974 71	3.542 35	3.448 96	3.096 44	2.707 87
	4	1.548 44	2.891 12	3.460 57	3.406 90	3.088 84	2.720 12
	5	1.551 89	2.895 69	3.463 19	3.401 92	3.078 88	2.708 04
	exact	1.555 97	2.904 81	3.467 02	3.397 77	3.069 85	2.697 33
Q_{22}	1	0.207 837	0.781 447	1.489 22	2.108 63	2.562 98	2.869 69
	2	0.230 592	0.938 986	1.706 52	2.266 11	2.594 44	2.769 82
	3	0.238 877	1.021 33	1.837 94	2.404 00	2.718 61	2.874 91
	4	0.246 214	0.929 030	1.681 59	2.231 17	2.556 25	2.731 16
	5	0.247 654	0.932 284	1.689 31	2.236 48	2.557 22	2.728 10
	exact	0.249 583	0.940 700	1.700 28	2.243 33	2.558 44	2.724 45

As a verification of the analysis given in Sec. IV, above, which indicates that the Kohn and inverse Kohn formulas should vary smoothly through the singularities of Eqs. (21), computed cross sections near two of these singularities are tabulated in Table II. These results speak for themselves.

TABLE II. Behavior of computed cross sections near eigenvalues of the Hamiltonian matrix. The eigenvalues considered, for $C^2 = 6.0$ and $n = 5$, occur at ($E = 0.535\,275$, $k_1 = 1.034\,67$, $k_2 = 0.566\,171$) and at ($E = 0.876\,882$, $k_1 = 1.324\,30$, $k_2 = 1.001\,88$).

	k_1	1.033 03	1.034 13	1.035 22	1.036 32
	k_2	0.563 171	0.565 171	0.567 171	0.569 171
Q_{11}	$n=5$	1.253 80	1.250 65	1.244 38	1.237 95
	exact	1.261 34	1.256 10	1.250 90	1.245 71
Q_{12}	$n=5$	0.834 744	0.833 519	0.832 448	0.831 408
	exact	0.835 648	0.834 523	0.833 394	0.832 254
Q_{21}	$n=5$	2.808 68	2.790 64	2.773 28	2.756 22
	exact	2.811 72	2.794 00	2.776 44	2.759 03
Q_{22}	$n=5$	1.481 06	1.474 93	1.469 03	1.462 91
	exact	1.489 59	1.483 43	1.477 30	1.471 18
	k_1	1.322 03	1.323 54	1.325 05	1.326 57
	k_2	0.998 88	1.000 88	1.002 88	1.004 88
Q_{11}	$n=5$	0.538 701	0.536 211	0.534 771	0.532 798
	exact	0.540 973	0.539 010	0.537 056	0.535 110
Q_{12}	$n=5$	0.547 283	0.546 102	0.544 836	0.543 643
	exact	0.547 517	0.546 312	0.545 110	0.543 909
Q_{21}	$n=5$	0.958 666	0.954 959	0.951 119	0.947 426
	exact	0.959 074	0.955 325	0.951 596	0.947 889
Q_{22}	$n=5$	0.639 360	0.636 927	0.634 504	0.632 239
	exact	0.640 938	0.638 624	0.636 321	0.634 029

TABLE III. Behavior of computed cross sections near a spurious singularity in the Kohn formula, where $|M_{11}^{pq}|$ passes through zero. K denotes Kohen, K^{-1} denotes inverse Kohn. $C^2 = 6.0$ and $n = 5$.

	k_1	0.923 255	0.925 000	0.926 769	0.928 561
	k_2	0.320	0.325	0.330	0.335
	$\lvert M_{00}^{pq}\rvert$	−0.017 444	−0.018 189	−0.018 963	−0.019 766
	$\lvert M_{11}^{pq}\rvert$	0.000 864	0.000 418	−0.000 039	−0.000 507
Q_{11}	K	2.121 37	2.110 46	1.749 52	2.020 86
	K^{-1}	2.109 37	2.086 26	2.063 43	2.040 88
	exact	2.127 21	2.103 86	2.080 79	2.057 99
Q_{12}	K	0.867 206	0.868 909	0.889 486	0.876 935
	K^{-1}	0.867 661	0.870 315	0.872 767	0.875 018
	exact	0.868 997	0.871 640	0.874 082	0.876 324
Q_{21}	K	7.218 82	7.038 68	7.015 42	6.737 50
	K^{-1}	7.222 60	7.050 07	6.883 56	6.722 77
	exact	7.233 72	7.060 80	6.893 93	6.732 80
Q_{22}	K	2.493 14	2.464 16	2.461 87	2.416 48
	K^{-1}	2.491 00	2.463 78	2.436 90	2.410 31
	exact	2.509 68	2.482 17	2.454 99	2.428 13

The analysis given in Sec. IV indicates that spurious singularities occur in the Kohn formula at zeroes of the determinant $|M_{11}^{pq}|$ and in the inverse Kohn formula at zeroes of $|M_{00}^{pq}|$. Examples of the resulting erratic behavior of computed cross sections are shown in Tables III and IV. It is clear from these tables that the use of Eq. (67) as a criterion for choice between the Kohn and inverse Kohn formulas provides a satisfactory procedure for avoiding these spurious singularities.

ACKNOWLEDGMENT

The calculations reported here were carried out on the IBM CALL/360 terminal system, using programs written in the BASIC language.

TABLE IV. Behavior of computed cross sections near a spurious singularity in the inverse Kohn formula, where $|M_{00}^{pq}|$ passes through zero. K denotes Kohn, K^{-1} denotes inverse Kohn. $C^2 = 6.0$ and $n = 5$.

	k_1	1.088 85	1.091 89	1.094 94	1.098 01
	k_2	0.660	0.665	0.670	0.675
	$\|M_{00}^{pq}\|$	0.008 127	0.003 783	−0.000 321	−0.004 224
	$\|M_{11}^{pq}\|$	−0.054 485	−0.056 256	−0.058 033	−0.059 825
Q_{11}	K	1.026 87	1.016 64	1.006 53	0.996 537
	K^{-1}	1.045 73	1.055 37	0.611 520	0.964 826
	exact	1.034 42	1.024 05	1.013 80	1.003 67
Q_{12}	K	0.774 245	0.770 885	0.767 507	0.764 115
	K^{-1}	0.773 203	0.768 493	0.764 856	0.765 946
	exact	0.774 960	0.771 582	0.768 187	0.764 779
Q_{21}	K	2.107 31	2.078 28	2.049 82	2.021 92
	K^{-1}	2.104 47	2.071 83	2.042 74	2.026 76
	exact	2.109 25	2.080 16	2.051 63	2.023 67
Q_{22}	K	1.215 35	1.203 33	1.191 43	1.179 67
	K^{-1}	1.215 59	1.202 60	1.161 77	1.181 08
	exact	1.222 29	1.210 08	1.198 00	1.186 07

[1] F. E. Harris, Phys. Rev. Letters 19, 173 (1967); H. H. Michels and F. E. Harris, Phys. Rev. Letters 19, 885 (1967).

[2] R. K. Nesbet, Phys. Rev. 175, 134 (1968); H. Morawitz, unpublished.

[3] W. Kohn, Phys. Rev. 74, 1763 (1948).

[4] C. Schwartz, Ann. Phys. (N. Y.) 16, 36 (1961).

[5] L. Hulthén, Arkiv. Mat. Astron. Fysik 35A, No. 25 (1948); S. I. Rubinow, Phys. Rev. 98, 183 (1955); K. L. Williams, Proc. Phys. Soc. (London) 91, 807 (1967).

[6] N. F. Mott and H. S. W. Massey, The Theory of Atomic Collisions (Oxford University Press, New York, 1965), pp. 369–379.

[7] R. J. Huck, Proc. Phys. Soc. (London) A70, 369 (1957).

[8] B. L. Moiseiwitsch, Phys. Rev. 82, 753 (1951).

[9] R. K. Nesbet, Phys. Rev. 156, 99 (1967).

[10] L. Hulthén, Kgl. Fysiograf Sällskap. Lund Forh. 14, No. 21 (1944).

[11] R. A. Frazer, W. J. Duncan, and A. R. Collar, Elementary Matrices (Cambridge University Press, New York, 1947), p. 17.