Least-squares method in scattering theory

Barnabás Apagyi
Quantum Theory Group, Institute of Physics, Technical University Budapest, 1521 Budapest, Hungary

Károly Ladányi
Institute of Theoretical Physics, Roland Eötvös University, 1088 Budapest, Hungary

(Received 9 July 1985)

A particular least-squares method is presented for the calculation of inelastic scattering wave functions by an expansion technique. The variational procedure is based on a convenient error functional. The test-function space is spanned by a finite set of square-integrable (Hilbert-space) basis functions. The open-channel orbitals include the Kohn-Hulthén—type oscillatory terms of nonvanishing asymptotic amplitudes. The error functional involves only bound-bound and bound-free matrix elements. Criteria are given to select acceptable approximations. Two-channel calculations show that the zero-order results of this method have an accuracy comparable to the first-order results of earlier calculations. No anomalies are encountered.

I. INTRODUCTION

The calculation of the scattering of a particle by a quantum-mechanical system is inherently a complex problem which covers the whole realm of atomic, nuclear, and strong-interaction physics. Important progress has been made by using variational methods along the lines suggested by Hulthén,[1] Kohn,[2] and Schwinger.[3] Various alternative procedures have been proposed to avoid the anomalies[4,5] or spurious singularities which are encountered in calculations with the Kohn and Hulthén methods. (For reviews of variational procedures and calculations in scattering theory see, e.g., Refs. 6—17.) In particular, several least-squares methods have been suggested and applied both to the calculation of Regge trajectories[18] and to the solution of scattering problems.[19—40]

In the present paper we shall discuss how the least-squares method suggested in Ref. 20 can be extended to the multichannel scattering. Our test-function space will be spanned by a finite set of square-integrable (Hilbert-space) basis functions which can also be applied to the expansion of the closed-channel orbital wave functions. On the other hand, we shall prescribe the correct asymptotic form for the expansion of the channel orbitals. Therefore, the expansion of the open-channel orbitals will include the well-known Kohn-Hulthén—type oscillatory terms of nonvanishing asymptotic amplitudes which cannot be represented as finite superpositions of square-integrable basis functions. Because of our choice of the test-function space, the least-squares method presented here involves only bound-bound and bound-free matrix elements. (All free-free integrals are eliminated.) This method will be referred to as the least-squares variational method involving only square-integrable test functions (LVM-ST).

As a first step of the multichannel LVM-ST, we shall define the measure of the error of the approximate channel orbitals. This error functional must be normalized in order to exclude the trivial solution of the variational problem. By using a convenient normalization and carrying out the variation, we derive the coupled set of inhomogeneous equations which determines all the linear variational parameters including the matrix elements of the reactance matrix K. In addition, we obtain a relatively simple equation for the measure of the error of the dth independent solution. If the number of the test functions is sufficiently large, then the results of the multichannel LVM-ST are "almost free" of anomalies according to the careful analysis presented by Abdel-Raouf.[17]

Most of the variational techniques involve the calculation of free-free matrix elements which are absent from our method. This property of the multichannel LVM-ST has many obvious theoretical and technical advantages. We are therefore motivated to consider some instructive applications. As a test case, we shall treat electron-atom scattering within the framework of the close-coupling formalism. Illustrative numerical calculations have been carried out for the low-energy electron—hydrogen-atom scattering. We shall consider the static exchange approximation and the $1s$-$2s$ close-coupling approximation (including exchange). Both the stability and the convergence of the results will be carefully analyzed and, in addition, we shall investigate the measure of the error of the approximate orbitals.

The results of this paper indicate that the multichannel LVM-ST can be successfully applied to the calculation of scattering processes if the basis functions are chosen according to the following requirements. (i) There must exist a region of the nonlinear scale parameter α (characterizing the basis functions) where a set of the calculated K-matrix elements K_{cd} is stable [i.e., in that region one has $K_{cd}(\alpha) \sim$ const]. (ii) An apparent convergence of these K-matrix elements should be observed as the number of the basis functions is increased. (iii) The measure of the error of the approximate channel orbitals must be sufficiently small. Similar requirements have been already applied to isolate the spurious solutions which may appear in the application of the finite basis-set expansion methods to the Dirac eigenvalue problem.[41]

The organization of this paper is as follows. The next section includes a review of the formalism and notation. Section III is devoted to the multichannel LVM-ST. Our analysis of the numerical results is presented in Sec. IV. Some comments and remarks are left for Sec. V.

II. REVIEW OF FORMALISM AND NOTATION

A. Close-coupling procedure

We consider the scattering of an electron by an n-electron atom. This process is described by an $(n+1)$-electron wave function which will be denoted by $\Psi^{(d)}(q_1,\ldots,q_{n+1})$, where the index d specifies a particular degenerate solution of the Schrödinger equation at total energy E. (The symbol q_i indicates the coordinates x_i and the spin of the ith electron.) In the nonrelativistic limit, the stationary scattering state of the $(n+1)$-electron system can be characterized by the quantum numbers L, S, and parity Π.

Let us consider the expansion of $\Psi^{(d)}$ in terms of a (complete) set of n-electron wave functions $\Phi^{(c)}$. The truncated version of this expansion is given by[13–15]

$$\Psi^{(d)}(q_1,\ldots,q_{n+1}) = \mathscr{A}\sum_{c=1}^{P}\Phi^{(c)}(q_1,\ldots,q_n)\psi^{(cd)}(q_{n+1}) , \quad (2.1)$$

where the operator $\mathscr{A}$ antisymmetrizes the total wave function $\Psi^{(d)}$. The n-electron target-state wave functions $\Phi^{(c)}$ should be carefully selected in order to obtain convergent results at increasing values of P. The expansion (2.1) involves the coefficients $\psi^{(cd)}$ which will be referred to as the one-electron *channel orbital* wave functions. These orbitals are of the form

$$\psi^{(cd)}(q_i)=r_i^{-1}f^{(cd)}(r_i)Y_{lm}(\vartheta_i,\varphi_i)\eta_s(i) , \quad (2.2)$$

with

$$l=l_c,\ \ m=m_c,\ \text{ and } s=s_c\ \ (s_c=\pm\tfrac{1}{2}) . \quad (2.3)$$

Here Y_{lm} is a spherical harmonic, and the *radial* channel orbital wave function $f^{(cd)}$ is characterized by the angular momentum quantum number l_c. (The spin factor is denoted by η_s.)

The close-coupling procedure leads to a coupled system of integro-differential equations for the radial functions $f^{(cd)}(r)$ (see, e.g., Refs. 13–15). These equations can be written as

$$\sum_{c=1}^{P}\hat{D}^{(bc)}f^{(cd)}=0,\ \ b=1,\ldots,P . \quad (2.4)$$

By using atomic units (a.u.) and the notation $\delta^{(bc)}=\delta_{bc}$, the standard form of the operator $\hat{D}^{(bc)}$ becomes[14]

$$\hat{D}^{(bc)}=H^{(bc)}-\epsilon_c\delta^{(bc)} , \quad (2.5)$$

where

$$\epsilon_c=E-E_c , \quad (2.6)$$

$$H^{(bc)}=\left[-\frac{1}{2}\frac{d^2}{dr^2}+\frac{l_c(l_c+1)}{2r^2}\right]\delta^{(bc)}+\hat{U}^{(bc)} , \quad (2.7)$$

$$\hat{U}^{(bc)}=V^{(bc)}(r)+\hat{W}^{(bc)} , \quad (2.8)$$

and

$$\hat{W}^{(bc)}f^{(cd)}=-\int_0^\infty rW^{(bc)}(r,r')r'f^{(cd)}(r')dr' . \quad (2.9)$$

In these equations E is the total energy of the $(n+1)$-electron system, the energy of the target state $\Phi^{(c)}$ is denoted by E_c, the matrix elements $V^{(bc)}(r)$ contain all the contributions of the direct potential terms, and the nonlocal exchange terms are indicated by $\hat{W}^{(bc)}$.

In a nonrelativistic theory, the short-distance behavior of the solution $f^{(cd)}$ is governed by the angular momentum term $l_c(l_c+1)/r^2$. Thus, we have

$$f^{(cd)}(r)\underset{r\to 0}{\sim}r^{l_c+1} . \quad (2.10)$$

We next turn to a discussion of the large-distance properties of the solutions. In the subsequent part of this paper, we restrict ourselves to the case where all the channels of Eqs. (2.4)–(2.5) are open ($\epsilon_c\geq 0$ for $c=1,\ldots,P$). Moreover, we shall consider only short-range interaction terms $\hat{U}^{(bc)}$. In this case, the canonical asymptotic form of the radial channel orbital wave functions $f^{(cd)}$ is the following:

$$f^{(cd)}(r)\to k_c^{-1/2}[\delta_{cd}\sin(k_cr-\tfrac{1}{2}l_c\pi) + K_{cd}\cos(k_cr-\tfrac{1}{2}l_c\pi)] \ \text{ as } r\to\infty , \quad (2.11)$$

with

$$\tfrac{1}{2}k_c^2=\epsilon_c . \quad (2.12)$$

Here K_{cd} is a matrix element of the symmetric reactance matrix K. The transition matrix T is expressed in terms of the reactance matrix by

$$T=K(I-iK)^{-1} , \quad (2.13)$$

and the partial cross section for scattering from channel c to channel d is[15]

$$\sigma_{cd}=\frac{4\pi}{k_c^2}|T_{dc}|^2 . \quad (2.14)$$

In the static exchange approximation ($P=1$), we have

$$K_{11}=\tan\delta , \quad (2.15)$$

where δ is the phase shift.

By using the LS coupling, the K matrix is diagonal in the total quantum numbers L, S, Π, and independent of total M_L and M_S. Therefore, we shall use the notations

$$K_{cd}=K_{cd}^{[LS\Pi]} , \quad (2.16)$$

$$\sigma_{cd}=\sigma_{cd}^{[LS\Pi]} , \quad (2.17)$$

and

$$\delta=\delta^{[LS\Pi]} . \quad (2.18)$$

The parity assignment Π will be omitted in the applications presented in this paper.

Within the framework of the *simple* close-coupling approximation, the wave functions $\Phi^{(c)}$ are identified with the eigenfunctions of the target Hamiltonian. (Instead of this procedure, one may use convenient semiempirical approximations of the operator $H^{(bc)}$.) In the next part of this section, we shall illustrate the structure of the interaction terms $\hat{U}^{(bc)}$ by using the $1s$-$2s$ close-coupling approximation of the low-energy electron–hydrogen-atom scattering.

B. Two-state close-coupling approximation of the e^--H scattering

Let us denote the spatial part of the target state wave functions by $\Phi^{(c)}(x)$. In the $1s$-$2s$ close-coupling approximation we choose

$$\Phi^{(1)}(x)=\Phi_1(r)=\Psi_{1s}(r)\ , \tag{2.19}$$

and

$$\Phi^{(2)}(x)=\Phi_2(r)=\Psi_{2s}(r)\ , \tag{2.20}$$

where Ψ_{1s} and Ψ_{2s} are, respectively, the normalized $1s$ and $2s$ bound-state eigenfunctions of the hydrogen atom.

The contributions of the direct potential terms can be written as[42]

$$V^{(bc)}(r)=\int \Phi^{(b)}(x')\left[\frac{1}{|x-x'|}-\frac{1}{r}\right]\Phi^{(c)}(x')d^3x'\ . \tag{2.21}$$

Straightforward calculation yields[43]

$$V^{(11)}(r)=-\left[\frac{1}{r}+1\right]\exp(-2r)\ , \tag{2.22}$$

$$V^{(12)}(r)=V^{(21)}(r)$$
$$=2^{1/2}\tfrac{4}{27}(1+\tfrac{3}{2}r)\exp(-\tfrac{3}{2}r)\ , \tag{2.23}$$

and

$$V^{(22)}(r)=-\left[\frac{1}{r}+\frac{3}{4}+\frac{r}{4}+\frac{r^2}{8}\right]\exp(-r)\ . \tag{2.24}$$

We now turn to the nonlocal exchange terms of the interaction. One obtains[42]

$$W^{(bc)}(r,r')=(-1)^S 4\pi\Phi_c(r)\left[E-E_c-E_b-\frac{1}{r_>}\right]\Phi_b(r')\ . \tag{2.25}$$

Here we have $S=0$ for singlet scattering processes, and the triplet scattering states are characterized by $S=1$. (The symbol $r_>$ indicates the greater of r,r'.)

The $1s$-$2s$ close-coupling approximation can be obtained by substituting Eqs. (2.22)–(2.25) (and $P=2$, $l_1=l_2=0$) into the coupled system of integro-differential equations (2.4)–(2.9). (At $P=1$, we are led to the static exchange approximation.) These equations can be successfully solved by using the multichannel LVM-ST. Our numerical results are contained in Sec. IV.

III. MULTICHANNEL LVM-ST

We now consider the expansion of the radial channel orbital wave functions $f^{(cd)}(r)$ in terms of a complete set of basis functions $\varphi_i^{(c)}$. The truncated version of this expansion can be written as

$$f^{(cd)'}(r)=\sum_{i=-1}^{N} a_i^{(cd)}\varphi_i^{(c)}(r)\ , \tag{3.1}$$

where the approximate radial functions $f^{(cd)'}(r)$ must satisfy the boundary conditions (2.10) and (2.11). According to these conditions, we shall use

$$\varphi_{-1}^{(c)}(r)=k_c^{1/2}rj_{l_c}(k_cr)\ , \tag{3.2}$$

$$a_{-1}^{(cd)}=\delta^{(cd)}a_{-1}\ , \tag{3.3}$$

$$\varphi_0^{(c)}(r)=k_c^{-1/2}(1-e^{-\beta_c r})^{l_c+1}\cos(k_cr-\tfrac{1}{2}l_c\pi)\ , \tag{3.4}$$

and

$$\varphi_i^{(c)}(r)=A_i^{(c)}r^{l_c+i}e^{-\alpha_c r},\quad i=1,\ldots,N\ . \tag{3.5}$$

Here the coefficients a_{-1} and $a_i^{(cd)}$ $(i=0,\ldots,N)$ are linear variational parameters, and the nonlinear scale parameters are denoted by α_c and β_c. ($A_i^{(c)}$ is a normalization factor.)

By substituting the truncated expansion (3.1) into the coupled set of integro-differential equations (2.4), we may write

$$\sum_{c=1}^{P}\hat{D}^{(bc)}f^{(cd)'}=\Delta^{(bd)}(r),\quad b=1,\ldots,P \tag{3.6}$$

where the deviation $\Delta^{(bd)}$ is related to the error of the approximate radial wave functions $f^{(1d)'},\ldots,f^{(Pd)'}$. Of course, the deviations $\Delta^{(bd)}$ depend on the linear parameters. Thus, we have

$$\Delta^{(bd)}(r)=\Delta^{(bd)}(r;a_{-1},a_0^{(1d)},\ldots,a_N^{(Pd)})\ . \tag{3.7}$$

We now introduce a complete set of square-integrable (Hilbert-space) test functions $\chi_h^{(b)}(r)$. According to the boundary condition (2.10), we choose

$$\chi_h^{(b)}(r)=B_h^{(b)}r^{l_b+h}e^{-\gamma_b r}\quad (h=1,2,\ldots)\ , \tag{3.8}$$

where γ_b is a convenient scale parameter, and the normalization factor is denoted by $B_h^{(b)}$.

As a first step, we consider the components of the deviation vector $\Delta^{(bd)}$ as given by

$$\langle\chi_h^{(b)}\,|\,\Delta^{(bd)}\rangle=\int_0^\infty\chi_h^{(b)}(r)\Delta^{(bd)}(r)dr\ . \tag{3.9}$$

A measure of the error of the approximate radial wave functions $f^{(1d)'},\ldots,f^{(Pd)'}$ will be defined as follows:

$$\lambda^{(d)}[f^{(1d)'},\ldots,f^{(Pd)'}]=\frac{\sum_{b=1}^{P}\sum_{h=1}^{M}w_h^{(b)}\,|\,\langle\chi_h^{(b)}\,|\,\Delta^{(bd)}\rangle\,|^2}{|\,a_{-1}\,|^2}\ , \tag{3.10}$$

where the $w_h^{(b)}$'s are positive weighting factors. We shall use a sufficiently large set of test functions by imposing the requirement

$$M > N+2 \,. \tag{3.11}$$

By variation of the expression (3.10) with respect to the linear parameters a_{-1} and $a_i^{(cd)}$ $(i=0,\ldots,N)$, we obtain a simple eigenvalue problem. As a next step, we normalize the eigenvector by setting

$$a_{-1}=1 \,. \tag{3.12}$$

The final result is the system of inhomogeneous linear equations which determines the coefficients $a_i^{(cd)}$ $(d=1,\ldots,P)$. These equations can be written in the following form:

$$\sum_{c=1}^{P}\sum_{i=0}^{N} \bar{L}_{hi}^{(bc)} a_i^{(cd)} = -\bar{L}_{h,-1}^{(bd)} \,, \qquad b=1,\ldots,P, \quad h=0,\ldots,N \,. \tag{3.13}$$

In addition, we obtain a simple equation for the eigenvalue $\lambda^{(d)}$:

$$\lambda^{(d)} = \bar{L}_{-1-1}^{(dd)} + \sum_{c=1}^{P}\sum_{i=0}^{N} \bar{L}_{-1i}^{(dc)} a_i^{(cd)} \,. \tag{3.14}$$

All the matrix elements of $\bar{L}$ are given by

$$\bar{L}_{hi}^{(bc)} = \sum_{b'=1}^{P}\sum_{h'=1}^{M} w_{h'}^{(b')} \langle \chi_{h'}^{(b')} | \hat{D}^{(b'b)} | \varphi_h^{(b)} \rangle^* \times \langle \chi_{h'}^{(b')} | \hat{D}^{(b'c)} | \varphi_i^{(c)} \rangle \,, \tag{3.15}$$

with

$$\langle \chi_{h'}^{(b')} | \hat{D}^{(b'c)} | \varphi_i^{(c)} \rangle = \int_0^\infty \chi_{h'}^{(b')}(r) \hat{D}^{(b'c)} \varphi_i^{(c)}(r) dr \,. \tag{3.16}$$

According to Eqs. (2.11) and (3.1)—(3.4), the normalization (3.12) implies

$$K_{cd} = a_0^{(cd)} \,. \tag{3.17}$$

In other words, the approximate K-matrix elements are solutions of Eq. (3.13). However, the solutions $a_0^{(cd)}$ are not exactly symmetric. Therefore, we shall apply the symmetrization suggested by Nesbet and Oberoi:[44]

$$\bar{K}_{cd} = \tfrac{1}{2}(a_0^{(cd)} + a_0^{(dc)}) \,. \tag{3.18}$$

In order to control the numerical results, we shall also calculate the values of ΔK_{cd} as defined by

$$\Delta K_{cd} = \tfrac{1}{2}(a_0^{(cd)} - a_0^{(dc)}) \,. \tag{3.19}$$

The matrix $\bar{L}$ is Hermitian and positive semidefinite, and the exact eigenvalue $\lambda^{(d)}$ is zero. One can compute a sequence of the approximate eigenvalues $\lambda^{(d)}(N)$ (and the corresponding linear variational parameters) by choosing finite and increasing values of N $(N=1,\ldots,M-3)$. If the value of M is fixed, then we obtain a sequence of monotonically decreasing approximate eigenvalues $\lambda^{(d)}(N)$ as the number of the basis functions $\varphi_i^{(c)}$ increases. However, this procedure involves a large subspace of test functions if we consider practical applications $(N \ll M)$. In order to simplify the calculations, we shall choose

$$M = N+p, \quad p>2 \tag{3.20}$$

where the value of p will be fixed. Consequently, we can apply a relatively small set of test functions in the lowest approximations. On account of the prescription (3.20), the matrix elements of $\bar{L}$ are not absolutely independent of N [cf. Eq. (3.15)]. Therefore, in general, we should not expect that the sequence of the approximate eigenvalues $\lambda^{(d)}$ *monotonically* approaches to the true eigenvalue $\lambda^{(d)}=0$. In spite of this fact, the computed eigenvalue $\lambda^{(d)}(N)$ may be regarded as a reasonable measure of the error of the approximate radial wave functions $f^{(1d)'}, \ldots, f^{(Pd)'}$.

We now proceed to some remarks. Let us fix the first $N+1$ components of the deviation vector $\Delta^{(bd)}$ at zero:

$$\langle \chi_h^{(b)} | \Delta^{(bd)} \rangle = 0, \quad h=1,\ldots,N+1 \tag{3.21}$$

where $b=1,\ldots,P$. By substituting Eqs. (3.1)—(3.6) and (3.12) into Eq. (3.21), we obtain a system of homogeneous linear equations for the coefficients $a_i^{(cd)}$ $(d=1,\ldots,P)$. Thus, Eq. (3.21) implies

$$\sum_{c=1}^{P}\sum_{i=0}^{N} \langle \chi_h^{(b)} | \hat{D}^{(bc)} | \varphi_i^{(c)} \rangle a_i^{(cd)} = -\langle \chi_h^{(b)} | \hat{D}^{(bd)} | \varphi_{-1}^{(d)} \rangle \,, \qquad b=1,\ldots,P, \quad h=1,\ldots,N+1 \,. \tag{3.22}$$

This system of equations can be regarded as an application of the method of moments to multichannel scattering. In the bound-state region, the method of moments provides an efficient theoretical tool to calculate the energies and eigenfunctions of many-particle systems.[45-47] Moreover, one can frequently get fairly useful approximate solutions of scattering problems by using the simple equations (3.22). (Numerical results are presented in Refs. 20 and 21.) However, like the Hulthén and Kohn methods, the method of moments is not necessarily free of anomalies in the scattering region.

We next compare the method of moments with the multichannel LVM-ST. The method of moments provides a set of *approximate* radial wave functions $f^{(cd)'}(r)$ by using Eqs. (3.1)—(3.5), (3.12), and (3.22). We observe that, at $M=N+1$, the measure of the error (3.10) is zero for the approximate radial wave functions $f^{(cd)'}(r)$ calculated by the method of moments. Let us notice, that Eq. (3.21) can also be satisfied for $h=1,\ldots,N+2$, if the total energy E is a solution of this (artificial) eigenvalue problem. Therefore, in order to have a useful definition of the error $\lambda^{(d)}$, we identify it by the error functional (3.10) which involves the components of the deviation vector $\Delta^{(bd)}$ in a sufficiently large M-dimensional subspace of the test functions $\chi_h^{(b)}(M>N+2)$.

In Sec. IV, we shall apply the multichannel LVM-ST to the simple two-state close-coupling approximation of the low-energy e^--H scattering. The details of this approximation can be found in the second part of Sec. II. As a first step, we shall also investigate the results of the static exchange approximation. Our calculations have been performed by choosing $p=10$ in Eq. (3.20). For simplicity we shall use the weighting factors

$$w_{h'}^{(b')}=1\ . \tag{3.23}$$

In addition, the choice of the nonlinear scale parameters will be restricted by

$$\alpha_c=\beta_c=\gamma_b=\alpha\ . \tag{3.24}$$

The restrictions (3.23) and (3.24) are valid for all possible values of the indices b', h', c, and b.

IV. CALCULATIONS AND RESULTS

A. Static exchange approximation

The system of inhomogeneous linear equations (3.13) has been solved at many values of the nonlinear scale parameter α. We first want to illustrate the behavior of the approximate phase shifts $\delta^{[0S]}(N;\alpha)$ at increasing values of N, where N refers to the size of the basis set. (According to the notations of this paper, $\delta^{[00]}$ and $\delta^{[01]}$ are the $L=0$ singlet and triplet phase shifts, respectively.) Figure 1 shows our computed results at $k_1=0.2$ (a.u.). One can observe a convincing stability of the higher approximations in the region $1.1<\alpha<4$, where the curves $\delta^{[00]}(20;\alpha)$ and $\delta^{[01]}(10;\alpha)$ are almost constant. The convergence of the approximate phase shifts is not necessarily monotonic at increasing values of N. For example, the curve $\delta^{[01]}(3;\alpha)$ oscillates around the plateau of the phase shifts $\delta^{[01]}(10;\alpha)$. However, the amplitude of these oscillations is relatively small. (We have obtained similar oscillations in the region $0<\alpha<1.1$ which is not included in Fig. 1.) Note, that the convergence of the phase shifts $\delta^{[01]}(N;\alpha)$ is much faster than that of the series $\delta^{[00]}(N;\alpha)$.

Let us consider the singlet phase shifts $\delta^{[00]}(N;\alpha)$ at several basis sizes N. Within the region $2.4<\alpha<4$ we find secondary plateaus which disappear in higher approximations. Since a narrow plateau does not necessarily imply an optimal convergence of the higher approximations, it will be instructive to analyze both the convergence of the approximate phase shifts $\delta^{[00]}(N;\alpha)$ and the corresponding measures of the error $\lambda^{(1)}(N;\alpha)$ as given by Eqs. (3.14)–(3.16) and (3.23).

Table I contains the computed values of $\delta^{[00]}(N;\alpha)$ and $\lambda^{(1)}(N;\alpha)$ at $k_1=0.2$ a.u. A series of calculations has been carried out by setting $\alpha=1.1$, 2, and 3. Let us first consider the approximate phase shift $\delta^{[00]}(N;\alpha)$ at $N=4$ and $\alpha=3$. [Figure 1 shows a secondary plateau of the curve $\delta^{[00]}(4;\alpha)$ in the region $2.4<\alpha<3.6$.] The comparison of the measures of the error $\lambda^{(1)}(4;\alpha=3)=2\times10^{-1}$ and $\lambda^{(1)}(4;\alpha=1.1)=3.4\times10^{-7}$ clearly shows the secondary character of the approximation $\delta^{[00]}(4;\alpha=3)$. [At $N=4$ we accept the approximation $\delta^{[00]}(4;\alpha=1.1)$.] A nice convergence of the singlet phase shifts $\delta^{[00]}(N;\alpha)$ is seen at $\alpha=2$. Moreover, we observe a *significant* minimum of the error $\lambda^{(1)}(20;\alpha)$ at $\alpha=2$.

Similar calculations have been carried out for the triplet scattering. In this case, the convergence of our results is excellent in a large region of α. At $\alpha=2$, for example, the

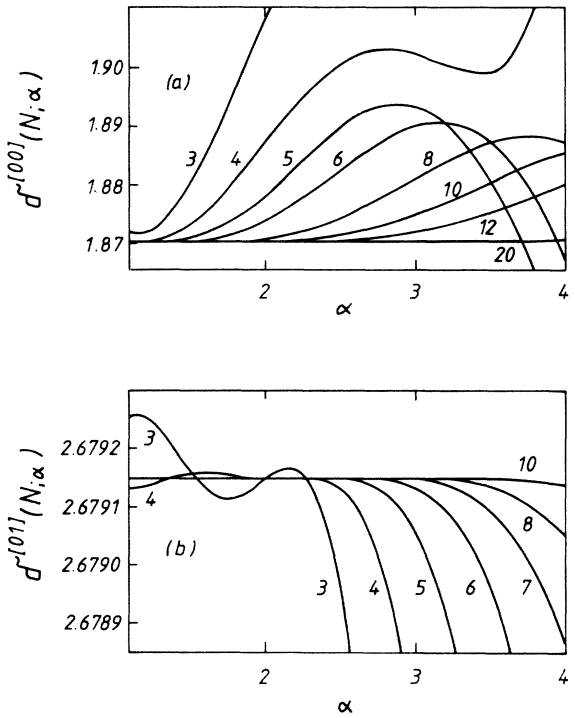

FIG. 1. Computed phase shifts $\delta^{[0S]}$ vs α for $k_1=0.2$ a.u. The curves are numbered to identify the size of the basis set denoted by N in Eq. (3.1). (a) and (b) show the phase shifts $\delta^{[00]}(N;\alpha)$ and $\delta^{[01]}(N;\alpha)$, respectively.

TABLE I. Computed values of $\delta^{[00]}(N;\alpha)$ and $\lambda^{(1)}(N;\alpha)$ at several basis sizes N and several values of α. The value of the wave number k_1 is fixed at $k_1=0.2$ a.u.

N	$\delta^{[00]}(N;1.1)$	$\lambda^{(1)}(N;1.1)$	$\delta^{[00]}(N;2.0)$	$\lambda^{(1)}(N;2.0)$	$\delta^{[00]}(N;3.0)$	$\lambda^{(1)}(N;3.0)$
2	1.860 668 05	1.6×10^{-3}	1.999 381 03	5.5×10^{-1}	2.674 534 77	2.7
4	1.869 883 03	3.4×10^{-7}	1.887 087 92	4.8×10^{-3}	1.902 360 88	2.0×10^{-1}
6	1.870 164 46	3.4×10^{-10}	1.873 608 82	1.5×10^{-5}	1.889 833 51	2.5×10^{-3}
8	1.870 158 08	8.5×10^{-12}	1.870 729 80	2.4×10^{-8}	1.880 878 62	2.0×10^{-5}
10	1.870 156 10	2.0×10^{-13}	1.870 236 16	2.4×10^{-11}	1.874 643 06	1.1×10^{-7}
12	1.870 156 12	2.8×10^{-15}	1.870 166 68	1.8×10^{-14}	1.871 761 75	4.3×10^{-10}
14	1.870 157 05	2.3×10^{-17}	1.870 158 58	1.1×10^{-17}	1.870 670 69	1.4×10^{-12}
16	1.870 157 65	1.3×10^{-19}	1.870 157 82	5.7×10^{-21}	1.870 307 53	3.7×10^{-15}
18	1.870 157 82	5.5×10^{-22}	1.870 157 78	2.4×10^{-24}	1.870 198 00	8.9×10^{-18}
20	1.870 157 82	2.0×10^{-24}	1.870 157 78	8.1×10^{-28}	1.870 167 68	1.9×10^{-20}

TABLE II. Computed phase shifts $\delta^{[00]}$ and $\delta^{[01]}$ for $k_1=0.2$, 0.5, and 1.0 a.u. Comparison of phase shifts relevant to this work (LVM-ST). J is Ref. 48, M is Ref. 43, and HS is Ref. 49.

	$k_1=0.2$ a.u.		$k_1=0.5$ a.u.		$k_1=1.0$ a.u.	
	$\delta^{[00]}$	$\delta^{[01]}$	$\delta^{[00]}$	$\delta^{[01]}$	$\delta^{[00]}$	$\delta^{[01]}$
J			1.031	2.070	0.543	1.391
M			1.030	2.069	0.541	1.389
HS	1.870 158	2.679 15			0.542 894 6	1.390 52
LVM-ST	1.870 1578	2.679 148 733 82	1.031 498 28	2.070 066 636	0.542 894 64	1.390 519 779

computed phase shifts $\delta^{[01]}(6;\alpha)$ and $\delta^{[01]}(20;\alpha)$ are the same up to eight digits.

In Table II we present the computed phase shifts $\delta^{[0S]}(S=0,1)$ for $k_1=0.2$, 0.5, and 1.0 a.u. Our calculations have been carried out by using the LVM-ST ($N=20$). In addition, we show the results calculated by alternative methods. These calculations have been presented by John (J),[48] Moiseiwitsch (M),[43] and by Horáček and Sasakawa (HS).[49]

B. Two-state close-coupling calculations without exchange

We next turn to the $1s$-$2s$ close-coupling calculations without exchange, where the direct potential terms $V^{(bc)}(r)$ are given by Eqs. (2.22)—(2.24). Since the nonlocal exchange terms $\hat{W}^{(bc)}$ [see Eqs. (2.9) and (2.25)] are omitted, we have $K^{[00]}=K^{[01]}=K$ in this model. By solving Eq. (3.13) at $P=2$, we obtain the approximate reactance matrix elements $\bar{K}_{cd}(N;\alpha)$ as defined by Eq. (3.18).

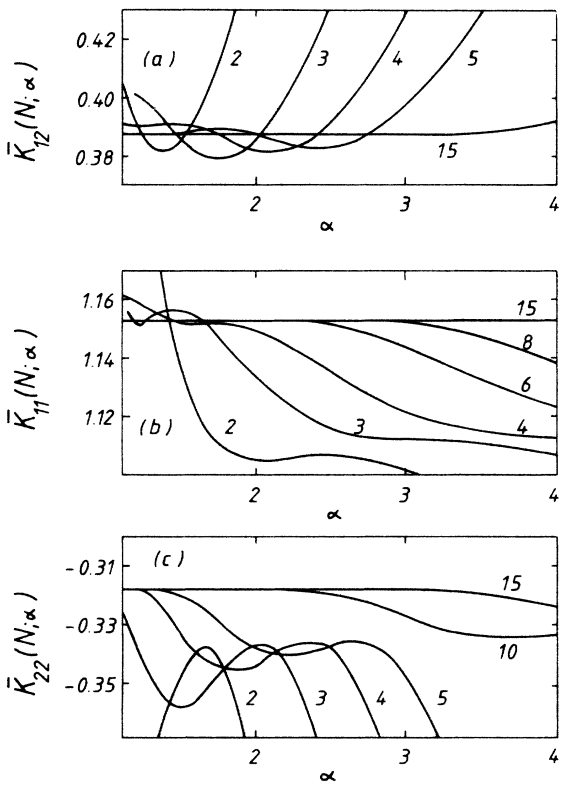

FIG. 2. Computed values of the reactance matrix elements $\bar{K}_{cd}(N;\alpha)$ vs α for $k_1=1.0$ a.u. The curves are numbered to identify the size of the basis set denoted by N in Eq. (3.1). (a), (b), and (c) show, respectively, $\bar{K}_{12}(N;\alpha)$, $\bar{K}_{11}(N;\alpha)$, and $\bar{K}_{22}(N;\alpha)$.

In Fig. 2 we present the functions $\bar{K}_{12}(N;\alpha)$, $\bar{K}_{11}(N;\alpha)$, and $\bar{K}_{22}(N;\alpha)$ for several basis sizes N. These functions have been computed at $k_1=1.0$ a.u. We observe the convincing stability of the approximate matrix elements $\bar{K}_{cd}(15;\alpha)$ in the region $1.1<\alpha<4$. At $N=2,\ldots,5$, on the other hand, the curves show some typical oscillations and secondary plateaus which disappear in higher approximations.

Table III contains the computed values of $\bar{K}_{cd}(N;\alpha=2)$ and $\lambda^{(d)}(N;\alpha=2)$ for several basis sizes N. The wave number k_1 is fixed at $k_1=1.0$ a.u. As a control of the results, we also present the computed values of the matrix element ΔK_{12} as defined in Eq. (3.19). Let us mention, that the measure of the error $\lambda^{(d)}(N;\alpha)$ is not directly related to the approximate reactance matrix element $\bar{K}_{dd}(N;\alpha)$. [The eigenvalue $\lambda^{(d)}(N;\alpha)$ may be regarded as a measure of the error of the dth radial wave functions $f^{(cd)'}(r)$.] The contents of Table III show the convincing convergence properties of the computed matrix elements $\bar{K}_{cd}(N;\alpha=2)$. The reliability of our zero-order results is also indicated by the rapid decrease of $\Delta K_{12}(N;\alpha=2)$ if the basis size N increases.

In Table IV we show the computed values of the $1s\rightarrow 2s$ partial cross sections $\sigma_{12}^{[00]}(\pi a_0^2)$ for $k_1=1.0$, 1.2, 1.5, and 2.0 a.u. Our results have been calculated by the multichannel LVM-ST ($N=20$). We also show the results of Smith, Miller, and Mumford (SMM) (Ref. 50) and Moiseiwitsch (M).[43] The variational linear algebraic procedures VLA^a and VLA^b of Ref. 43 are indicated by M1 and M2, respectively.

C. Two-state close-coupling calculations with exchange

We now present illustrative $1s$-$2s$ close-coupling calculations with exchange. In this case, the interaction matrix $\hat{U}^{(bc)}$ is given by Eqs. (2.8), (2.9), and Eqs. (2.22)—(2.25). We shall only consider the $L=0$ scattering in the singlet spin state ($S=0$). By solving Eq. (3.13) at $P=2$, we obtain the reactance matrix elements $K_{cd}^{[00]}(N)$ as defined by Eq. (3.17). [The symmetric reactance matrix $\bar{K}$ is defined by Eq. (3.18).] For simplicity, we next omit the quantum numbers $L=0$, $S=0$ characterizing the matrix elements $K_{cd}^{[00]}(N)$. The numerical results have been analyzed along the lines discussed in the previous part of this section. Taking into account the requirements (i), (ii), and (iii) (see the last part of Sec. I), we next show our results at $\alpha=1.1$.

TABLE III. Computed values of $\bar{K}_{11}(N;\alpha)$, $\lambda^{(1)}(N;\alpha)$, $\bar{K}_{12}(N;\alpha)$, $\Delta K_{12}(K;\alpha)$, $\bar{K}_{22}(N;\alpha)$, and $\lambda^{(2)}(N;\alpha)$ at several basis sizes N and $\alpha=2$. The value of the wave number k_1 is fixed at $k_1=1.0$ a.u.

N	$\bar{K}_{11}(N;2.0)$	$\lambda^{(1)}(N;2.0)$	$\bar{K}_{12}(N;2.0)$	$\Delta K_{12}(N;2.0)$	$\bar{K}_{22}(N;2.0)$	$\lambda^{(2)}(N;2.0)$
2	1.105 841 9	2.0×10^{-3}	0.449 167 8	5.6×10^{-2}	−0.400 810 7	4.9×10^{-2}
4	1.149 060 1	4.5×10^{-5}	0.382 025 6	3.1×10^{-3}	−0.343 261 5	4.1×10^{-5}
6	1.152 503 1	1.6×10^{-8}	0.388 801 9	2.7×10^{-5}	−0.327 970 2	4.0×10^{-6}
8	1.152 788 2	7.5×10^{-10}	0.387 371 8	-7.4×10^{-5}	−0.319 205 4	2.9×10^{-9}
10	1.153 001 9	4.5×10^{-13}	0.387 172 0	-3.0×10^{-5}	−0.318 945 0	1.0×10^{-11}
12	1.153 012 2	9.6×10^{-16}	0.387 206 7	-7.9×10^{-6}	−0.318 810 5	2.8×10^{-14}
14	1.153 013 8	2.2×10^{-18}	0.387 197 2	-1.7×10^{-6}	−0.318 768 5	2.5×10^{-19}
16	1.153 014 8	1.1×10^{-23}	0.387 196 8	-3.1×10^{-7}	−0.318 769 7	3.3×10^{-20}
18	1.153 014 7	1.8×10^{-24}	0.387 197 0	-5.3×10^{-8}	−0.318 769 2	8.7×10^{-24}
20	1.153 014 7	4.3×10^{-28}	0.387 197 0	-8.3×10^{-9}	−0.318 769 1	7.9×10^{-27}

TABLE IV. Computed partial cross sections $\sigma_{12}^{[00]}(\pi a_0^2)$ for $k_1=1.0$, 1.2, 1.5, and 2.0 a.u. Comparison of partial cross sections relevant to this work (LVM-ST). SMM is Ref. 50 and MB ($B=1,2$) is Ref. 43.

	$\sigma_{12}^{[00]}(\pi a_0^2)$			
	$k_1=1.0$ a.u.	$k_1=1.2$ a.u.	$k_1=1.5$ a.u.	$k_1=2.0$ a.u.
SMM	0.200	0.102	0.0450	0.0154
M1	0.1997	0.1018	0.044 5	0.014 7
M2	0.2001	0.1020	0.044 9	0.015 2
LVM-ST	0.199 983 9	0.102 087 3	0.045 032	0.015 45

TABLE V. Computed values of the matrix elements $K_{cd}(N)$ at several basis sizes N. The value of the wave number k_1 is fixed by $k_1^2=1.21$ a.u. Comparison of K-matrix elements relevant to this work (LVM-ST). The results of Ref. 31 are indicated by KA, MNA, and VLSA ($A=0,1$). $A=0$ and $A=1$ refer to zero-order and first-order results, respectively.

	K0	K1	MN0	MN1	VLS0	VLS1	LVM-ST
$K_{11}(5)$	0.7706	0.3463	0.8364	0.3412	0.6286	0.4881	0.4128
$K_{12}(5)$	0.6130	0.5377	0.7006	0.5461	0.6044	0.6240	0.5834
$K_{21}(5)$	0.6758	0.5377	0.6154	0.5461	0.5159	0.6240	0.5672
$K_{22}(5)$	−1.7581	−1.2058	−0.9920	−1.1175	−1.1491	−1.0795	−1.1195
$K_{11}(10)$	0.3602	0.4386	0.4453	0.4369	0.4347	0.4382	0.4360
$K_{12}(10)$	0.5391	0.5632	0.5598	0.5636	0.5564	0.5636	0.5642
$K_{21}(10)$	0.6069	0.5632	0.5727	0.5636	0.5628	0.5636	0.5644
$K_{22}(10)$	−1.2621	−1.1449	−1.2350	−1.1444	−1.1361	−1.1313	−1.1244
$K_{11}(15)$	0.4452	0.4365	0.4488	0.4365	0.4363	0.4366	0.4365
$K_{12}(15)$	0.5492	0.5631	0.5540	0.5632	0.5642	0.5632	0.5636
$K_{21}(15)$	0.5668	0.5631	0.5441	0.5632	0.5638	0.5632	0.5637
$K_{22}(15)$	−1.0426	−1.1214	−1.0725	−1.1224	−1.1258	−1.1225	−1.1235
$K_{11}(20)$							0.4365
$K_{12}(20)$							0.5636
$K_{21}(20)$							0.5636
$K_{22}(20)$							−1.1235

TABLE VI. Computed values of the matrix elements $K_{cd}(N)$ at several basis sizes N. The value of the wave number k_1 is fixed by $k_1^2=2.25$ a.u. Comparison of K-matrix elements relevant to this work (LVM-ST). The results of Ref. 31 are indicated by KA, MNA, and VLSA ($A=0,1$). $A=0$ and $A=1$ refer to zero-order and first-order results, respectively.

	K0	K1	MN0	MN1	VLS0	VLS1	LVM-ST
$K_{11}(5)$	0.6255	0.2045	0.4705	0.1884	0.3202	0.1562	0.1518
$K_{12}(5)$	1.2506	1.1058	1.2345	1.0988	1.1595	1.1593	1.4344
$K_{21}(5)$	1.2631	1.1058	1.1700	1.0988	1.0363	1.1593	1.4532
$K_{22}(5)$	−4.3952	−3.8049	−4.2980	−3.8058	−4.0496	−3.1718	−4.8747
$K_{11}(10)$	0.3088	0.1758	0.1735	0.2272	0.1864	0.2275	0.1969
$K_{12}(10)$	1.1692	1.3056	1.6942	1.1642	1.2472	1.2414	1.2397
$K_{21}(10)$	1.1885	1.3056	1.5782	1.1642	1.2557	1.2414	1.2475
$K_{22}(10)$	−4.1034	−4.5650	−5.5358	−4.1783	−4.3479	−4.4093	−4.3163
$K_{11}(15)$	0.2928	0.2125	0.1101	0.2253	0.1956	0.2014	0.1988
$K_{12}(15)$	1.4821	1.1963	1.6210	1.1673	1.2522	1.2365	1.2410
$K_{21}(15)$	1.0957	1.1963	1.5462	1.1673	1.2472	1.2365	1.2411
$K_{22}(15)$	−5.1025	−4.1766	−5.4116	−4.1131	−4.3407	−4.3033	−4.3122
$K_{11}(20)$							0.1986
$K_{12}(20)$							1.2417
$K_{21}(20)$							1.2417
$K_{22}(20)$							−4.3144

Table V contains the computed values of the matrix elements $K_{cd}(N)$ for several basis sizes N. The wave number k_1 is fixed by $k_1^2=1.21$ a.u. In addition, we show the results of Abdallah and Truhlar.[31] These calculations have been carried out by using the Kohn method,[2] the minimum norm method,[51] and a modified least-squares method[22–31] which are denoted by KA, MNA, and VLSA, respectively ($A=0,1$). Here $A=0$ refers to the zero-order results, and $A=1$ indicates the first-order results which have been calculated by using the Kohn variational expression.[31] (The results of the Rubinow method are omitted.) In Table VI we present similar results at $k_1^2=2.25$ a.u.

Of course, the multichannel LVM-ST and the VLS methods are closely related. The essential difference is the choice of the test-function space. The VLS methods[22–31] include the oscillatory functions of nonvanishing asymptotic amplitudes [see Eq. (3.4)] into the space of the test functions $\chi_h^{(b)}$. Therefore, both the zero-order and the first-order VLS calculations involve free-free matrix elements too. On the other hand, the test-function space of the multichannel LVM-ST is spanned by a set of square-integrable (Hilbert-space) basis functions $\chi_h^{(b)}$. Consequently, our method involves only bound-bound and bound-free matrix elements $\langle\chi_h^{(b)}|\hat{D}^{(bc)}|\varphi_i^{(c)}\rangle$. This property of the functional (3.10) is attractive from a theoretical point of view.

The contents of Tables V and VI show a remarkable convergence of the zero-order K-matrix elements calculated by the multichannel LVM-ST. Note that our zero-order matrix elements $K_{12}(20)$ and $K_{21}(20)$ are the same up to four or five digits. Thus, we are motivated to define the approximations of the symmetric reactance matrix $\bar{K}$ by the simple equation (3.18). No anomalies have been encountered in our calculations.

Let us mention that Abdallah and Truhlar[31] employ an exponential basis set in the subspace of the square-integrable basis functions. The good convergence of our results may be (partly) connected with the use of Slater-type basis functions as given by Eqs. (3.5), (3.8), and (3.24).

V. COMMENTS

The results of this paper indicate that the multichannel LVM-ST offers an efficient theoretical tool to solve scattering problems. Of course, the general theoretical framework of the calculation must be carefully selected. Some principal difficulties of the naive close-coupling procedure may be avoided by using powerful alternative expansions. (For reviews and references, see, e.g., Refs. 13–15.)

The calculations of the present work have been carried out by using the standard form of the operator $\hat{D}^{(bc)}$ as given by Eq. (2.5). One may consider other choices $\hat{D}^{(bc)}\to\hat{D}^{(bc)}_{\rm TVM}$ which correspond to various kinds of traditional variational methods (TVM) along the lines discussed in Ref. 17, p. 158. All these operators $\hat{D}^{(bc)}_{\rm TVM}$ can be inserted in the error functional which is defined by Eq. (3.10). By carrying out the variation, we obtain the system of inhomogeneous linear equations corresponding to the choice of the operator $\hat{D}^{(bc)}_{\rm TVM}$ [see Eqs. (3.13)–(3.16)]. The calculation of the matrix elements $\langle\chi_h^{(b)}|\hat{D}^{(bc)}_{\rm TVM}|\varphi_i^{(c)}\rangle$ can be greatly simplified by using convenient square-integrable (Hilbert-space) test functions $\chi_h^{(b)}$.

In summary, we suggest the variational method of Sec. III with a judicious choice of the operator $\hat{D}^{(bc)}_{\rm TVM}$. The results must satisfy the requirements (i), (ii), and (iii) which are imposed in the last part of Sec. I. To demonstrate the utility of our method, we calculated the solutions of some simple scattering problems. In these cases, impressive results have been obtained by using the standard form of the operator $\hat{D}^{(bc)}$ as given by Eqs. (2.5)–(2.9).

ACKNOWLEDGMENTS

We are deeply indebted to Professor E. O. Alt, Professor J. Pipek, and Professor E. W. Schmid for helpful discussions. One of us (K. L.) would like to express his gratitude to Professor B. Vasvári for the warm hospitality at the Institute of Physics, Technical University, Budapest, Hungary.

[1]L. Hulthén, K. Fysiogr. Saellsk. Lund Foerh. **14**, 257 (1944).
[2]W. Kohn, Phys. Rev. **74**, 1763 (1948).
[3]J. Schwinger, Phys. Rev. **72**, 742 (1947); **78**, 135 (1950).
[4]C. Schwartz, Ann. Phys. (N.Y.) **16**, 36 (1961); C. Schwartz, Phys. Rev. **124**, 1468 (1961).
[5]R. K. Nesbet, Phys. Rev. **175**, 134 (1968); R. K. Nesbet and J. D. Lyons, Phys. Rev. A **4**, 1812 (1971).
[6]B. L. Moiseiwitsch, *Variational Principles* (Wiley, New York, 1966).
[7]F. E. Harris and H. H. Michels, Methods Comput. Phys. **10**, 143 (1971).
[8]D. G. Truhlar, J. Abdallah, and R. L. Smith, Adv. Chem. Phys. **25**, 211 (1974).
[9]R. K. Nesbet, Adv. Quantum Chem. **9**, 215 (1975).
[10]R. K. Nesbet, Adv. At. Mol. Phys. **13**, 315 (1977).
[11]D. G. Truhlar, *Semiempirical Methods of Electronic Structure Calculation* (Plenum, New York, 1977), part B.
[12]B. L. Moiseiwitsch, Rep. Prog. Phys. **40**, 843 (1977).
[13]J. Callaway, Phys. Rep. **45**, 89 (1978).
[14]J. Callaway, Adv. Phys. **29**, 771 (1980).
[15]R. K. Nesbet, *Variational Methods in Electron-Atom Scattering Theory* (Plenum, New York, 1980).
[16]M. A. Abdel-Raouf, Phys. Rep. **84**, 163 (1982).
[17]M. A. Abdel-Raouf, Phys. Rep. **108**, 1 (1984).
[18]K. Ladányi, Nuovo Cimento A **70**, 405 (1970).
[19]K. Ladányi, Nuovo Cimento A **61**, 173 (1969).
[20]K. Ladányi and T. Szondy, Nuovo Cimento B **5**, 70 (1971).
[21]K. Ladányi, V. Lengyel, and T. Szondy, Theor. Chim. Acta **21**, 176 (1971).
[22]E. W. Schmid and K. H. Hoffmann, Nucl. Phys. A **175**, 443 (1971).
[23]E. W. Schmid and J. Schwager, Nucl. Phys. A **180**, 434 (1972).
[24]J. N. Bardsley, E. Gerjuoy, and C. V. Sukumar, Phys. Rev. A **6**, 1813 (1972).
[25]E. W. Schmid, Acta Phys. Austriaca Suppl. **9**, 44 (1972).
[26]F. H. Read and J. R. Soto-Montiel, J. Phys. B **6**, L15 (1973).
[27]E. W. Schmid, Nuovo Cimento A **18**, 771 (1973).
[28]J. Schwager and E. W. Schmid, Nucl. Phys. A **205**, 168 (1973).
[29]J. Schwager, Nuovo Cimento A **18**, 783 (1973).
[30]I. Wladawsky, J. Chem. Phys. **58**, 1826 (1973).
[31]J. Abdallah and D. G. Truhlar, J. Chem. Phys. **60**, 4670 (1974).
[32]E. J. Kanellopoulos and Th. V. Kanellopoulos, J. Phys. A **8**, 637 (1975).
[33]B. Gazdy, J. Phys. A **9**, L39 (1976).
[34]B. Gazdy, Phys. Lett. A **64**, 193 (1977).
[35]D. A. Levin, T. N. Rescigno, and V. McKoy, Phys. Rev. A **16**, 157 (1977).
[36]M. A. Abdel-Raouf and D. Belschner, J. Phys. B **11**, 3677 (1978).
[37]M. A. Abdel-Raouf, J. Phys. B **12**, 3349 (1979).
[38]M. A. Abdel-Raouf, Acta Phys. Hung. **48**, 31 (1980).
[39]M. A. Abdel-Raouf, Can. J. Phys. **60**, 577 (1982).
[40]A. L. Merts and L. Collins, J. Phys. B **18**, L29 (1985).
[41]B. Gazdy and K. Ladányi, J. Chem. Phys. **80**, 4333 (1984).
[42]G. A. Erskine and H. S. W. Massey, Proc. R. Soc. Ser. **A212**, 521 (1952).
[43]B. L. Moiseiwitsch, J. Phys. B **16**, 4015 (1983).
[44]R. K. Nesbet and R. S. Oberoi, Phys. Rev. A **6**, 1855 (1972).
[45]T. Szondy, Acta Phys. Hung. **17**, 303 (1964).
[46]É Szondy and T. Szondy, Acta Phys. Hung. **20**, 253 (1966).
[47]M. G. Hegyi, M. Mezei, and T. Szondy, Theor. Chim. Acta **15**, 283 (1969); **21**, 168 (1971); **21**, 176 (1971).
[48]T. L. John, Proc. Phys. Soc. London **76**, 532 (1960).
[49]J. Horáček and T. Sasakawa, Phys. Rev. A **30**, 2274 (1984).
[50]K. Smith, W. F. Miller, and A. J. P. Mumford, Proc. Phys. Soc. London **76**, 559 (1960).
[51]F. E. Harris and H. H. Michels, Phys. Rev. Lett. **22**, 1036 (1969).