Iterative approach to the Schwinger variational principle for electron-molecule collisions

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We present an iterative approach which uses the Schwinger variational principle to solve the Lippmann-Schwinger equation for electron-molecule scattering. This method combines the use of discrete basis functions to describe the effects of the noncentral molecular potential with an iterative procedure which provides systematic convergence of the scattering solutions. Results for electron-H_2 scattering in the static-exchange approximation show that the method converges rapidly and gives very accurate results.

I. INTRODUCTION

The Schwinger variational principle for the T matrix has been found to be very useful in obtaining accurate solutions for electron-molecule scattering. This method was introduced as a discrete-basis-function approach to scattering[1] and has evolved as a general numerical technique.[2] The Schwinger variational principle has been successfully applied to the scattering of low-energy electrons by He, He^+, H_2, H_2^+, N_2^+, and LiH (Refs. 1–7). In the present paper we apply an iterative approach to the Schwinger variational principle[8–10] to obtain scattering solutions to the electron-molecule collision problem. The method uses trial scattering wave functions which contain both discrete basis functions and numerical wave functions which explicitly satisfy the scattering boundary conditions. The discrete basis functions effectively describe the scattering wave function in the region near the nuclei where electron-exchange and partial-wave coupling are strong. The numerical wave functions are obtained from the Lippmann-Schwinger equation using a procedure which does not require solving coupled integro-differential equations. This is a powerful method for electron-molecule scattering combining the advantages of using discrete basis functions with an iterative procedure which allows convergence to an exact solution for the potential chosen to describe the interaction.

We apply the iterative Schwinger method to electron-H_2 scattering in the static-exchange approximation. The results of these applications show that the method is very effective and converges rapidly. Although the formal theory is given in terms of the T matrix and wave functions which satisfy outgoing-wave boundary conditions, for numerical convenience we actually perform all calculations using the K matrix and wave functions which satisfy standing-wave boundary conditions.

II. THEORY

The iterative Schwinger method starts with the solution of the Lippmann-Schwinger equation for the T matrix

$$T = U + UG_0^{(+)}T \tag{1}$$

using a separable approximation to the exact potential. The form of the separable potential used here is

$$\langle \vec{r}|U^{SO}|\vec{r}'\rangle = \sum_{\alpha_i,\alpha_j \in R} \langle \vec{r}|U|\alpha_i\rangle (U^{-1})_{ij} \langle \alpha_j|U|\vec{r}'\rangle, \tag{2}$$

where R is an initial set of expansion functions and $U = 2V$. With this separable potential the solution of the Lippmann-Schwinger equation Eq. (1) is given by

$$\langle \vec{r}|T^{SO}|\vec{r}'\rangle = \sum_{\alpha_i,\alpha_j \in R} \langle \vec{r}|U|\alpha_i\rangle [(D^{(+)})^{-1}]_{ij} \langle \alpha_j|U|\vec{r}'\rangle, \tag{3}$$

where

$$D_{ij}^{(+)} = \langle \alpha_i|U - UG_0^{(+)}U|\alpha_j\rangle . \tag{4}$$

As has been pointed out by several authors,[11–13] this form of the T matrix is equivalent to that obtained from the Schwinger variational expression

$$T_{ll'm} = \langle \phi_{klm}|T|\phi_{kl'm}\rangle = \frac{\langle \phi_{klm}|U|\psi_{kl'm}^{(+)t}\rangle \langle \psi_{klm}^{(-)t}|U|\phi_{kl'm}\rangle}{\langle \psi_{klm}^{(-)t}|U - UG_0^{(+)}U|\psi_{kl'm}^{(+)t}\rangle}, \tag{5}$$

where the partial-wave trial functions are linear combinations of the expansion functions

$$\psi_{klm}^{(\pm)t}(\vec{r}) = \sum_{\alpha_i \in R} C_{klm,i}^{(+)} \alpha_i(\vec{r}) . \tag{6}$$

The form of the T matrix given in Eq. (3) or equivalently Eq. (5), has been used by the present authors to obtain scattering results in several systems.[1–5] The errors that exist in this Schwinger variational T matrix are due to the difference

between the exact potential U and the approximate separable potential U^{s0} given in Eq. (2). It is possible to eliminate these errors due to the difference potential by an iterative procedure.

Our iterative procedure begins by constructing the scattering wave functions which correspond to the Schwinger T matrix given in Eq. (3). There are no coupled equations to solve to obtain these wave functions since the corresponding T matrix is exactly known. The scattering solutions are computed using the partial-wave expansion of the wave function

$$\Psi_{\vec{k}}^{(+)}(\vec{r}) = \left(\frac{2}{\pi}\right)^{1/2} \sum_{lm} i^l \psi_{klm}^{(+)}(\vec{r}) Y_{lm}^*(\hat{k}) . \tag{7}$$

For a linear target molecule, $\psi_{klm}^{(+)}$ may in turn be expanded in a partial-wave series by

$$\psi_{klm}^{(+)}(\vec{r}) = \sum_{l'} \psi_{ll'm}^{(+)}(k,r) Y_{l'm}(\hat{r}) . \tag{8}$$

The Lippmann-Schwinger equation for the wave function is

$$\psi_{klm}^{(+)s0}(\vec{r}) = \phi_{klm}(\vec{r}) + \langle \vec{r} | G_0^{(+)} U^{s0} | \psi_{klm}^{(+)s0} \rangle , \tag{9}$$

where $\phi_{klm}(\vec{r})$ are the free-particle solutions

$$\phi_{klm}(\vec{r}) = j_l(kr) Y_{lm}(\hat{r}) . \tag{10}$$

By using the identity

$$\langle \vec{r} | U^{s0} | \psi_{klm}^{(+)s0} \rangle = \langle \vec{r} | T^{s0} | \phi_{klm} \rangle , \tag{11}$$

we obtain an expression for the wave function in terms of the T matrix

$$\psi_{klm}^{(+)s0}(\vec{r}) = \phi_{klm}(\vec{r}) + \langle \vec{r} | G_0^{(+)} T^{s0} | \phi_{klm} \rangle . \tag{12}$$

This equation for $\psi_{klm}^{(+)s0}$ is now uncoupled, and the partial-wave functions are given by

$$\psi_{ll'm}^{(+)s0}(k,r) = j_l(kr)\delta_{ll'} - \sum_{\alpha_i, \alpha_j \in R} k \langle j_{l'}(kr_<) h_{l'}^{(+)}(kr_>) Y_{l'm}(\hat{r}) | U | \alpha_i \rangle [(D^{(+)})^{-1}]_{ij} \langle \alpha_j | U | j_l(kr) Y_{lm}(\hat{r}) \rangle . \tag{13}$$

The asymptotic form of the partial-wave solutions are then

$$\psi_{ll'm}^{(+)s0}(k,r) \sim j_l(kr)\delta_{ll'} - k \langle \phi_{kl'm} | T^{s0} | \phi_{klm} \rangle h_{l'}^{(+)}(kr) . \tag{14}$$

The radial function $\psi_{ll'm}^{(+)}$ is readily obtained from Eq. (13) by numerical integration.

The iterative procedure proceeds by augmenting the expansion set R of Eq. (2) by the set of functions $S_0 = \{\psi_{kl_1m}^{s0}, \psi_{kl_2m}^{s0}, \ldots, \psi_{kl_pm}^{s0}\}$ which consists of the scattering solutions corresponding to the T matrix given in Eq. (3). Using this augmented set of functions, the first iteration is completed by calculating a new T matrix given by

$$\langle \vec{r} | T^{s1} | \vec{r}' \rangle = \sum_{\chi_i, \chi_j \in R \cup S_0} \langle \vec{r} | U | \chi_i \rangle [(D^{(+)})^{-1}]_{ij} \langle \chi_j | U | \vec{r}' \rangle . \tag{15}$$

Note that the expansion functions contained in the set $R \cup S_0$ include both the initial set of expansion functions $R = \{\alpha_i\}$ and the continuum solutions given by Eq. (12).

A second iteration is begun by constructing the set of solutions $S_1 = \{\psi_{kl_1m}^{s1}, \ldots, \psi_{kl_pm}^{s1}\}$ which are associated with the matrix T^{s1} given by Eq. (15). The set S_1 combined with the initial trial function set R yields a new T matrix T^{s2}. In general, T^{sn}, ψ_{klm}^{sn}, and the set of functions S_n are given by

$$\langle \vec{r} | T^{sn} | \vec{r}' \rangle = \sum_{\chi_i \chi_j \in R \cup S_{n-1}} \langle \vec{r} | U | \chi_i \rangle [(D^{(+)})^{-1}]_{ij} \langle \chi_j | U | \vec{r}' \rangle \tag{16}$$

and

$$S_n = \{\psi_{kl_1m}^{sn}, \ldots, \psi_{kl_pm}^{sn}\} , \tag{17}$$

where

$$\psi_{kl_im}^{(+)sn}(\vec{r}) = \phi_{kl_im}(\vec{r}) + \langle \vec{r} | G_0^{(+)} T^{sn} | \phi_{kl_im} \rangle . \tag{18}$$

This iterative scheme is repeated until the wave functions converge.

If the wave functions do converge such that

$$\psi_{klm}^{(+)s_{n+1}}(\vec{r}) = \psi_{klm}^{(+)sn}(\vec{r}) , \tag{19}$$

and if we have

$$\langle \psi_{kl_im}^{(-)sn} | U - U G_0^{(+)} U | \psi_{kl_jm}^{(+)sn} \rangle = \langle \phi_{kl_im} | U | \psi_{kl_jm}^{(+)sn} \rangle \tag{20}$$

for $1 \leq i \leq p$ and $1 \leq j \leq p$, and

$$\langle \psi_{kl_im}^{(-)sn} | U - U G_0^{(+)} U | \alpha_j \rangle = \langle \phi_{kl_im} | U | \alpha_j \rangle \tag{21}$$

for $1 \leq i \leq p$ and $\alpha_j \in R$, then it follows that the functions $\psi_{klm}^{(+)sn}$ satisfy the Lippmann-Schwinger equation for the exact potential U. This can be demonstrated by substituting Eq. (16) into Eq. (18) to yield

$$\psi_{klm}^{(+)s_{n+1}}(\vec{r}) = \phi_{klm}(\vec{r}) + \sum_{\chi_i, \chi_j \in R \cup S_n} \langle \vec{r} | G_0^{(+)} U | \chi_i \rangle \times [(D^{(+)})^{-1}]_{ij} \langle \chi_j | U | \phi_{klm} \rangle . \tag{22}$$

Then using the relationships given in Eq. (20) and Eq. (21), Eq. (22) reduces to

$$\psi^{(+)s_{n+1}}_{klm}(\vec{r}) = \phi_{klm}(\vec{r}) + \langle \vec{r}|G_0^{(+)}U|\psi^{(+)s_n}_{klm}\rangle . \tag{23}$$

Thus if Eq. (19) is also satisfied, Eq. (23) reduces to

$$\psi^{(+)s_n}_{klm}(\vec{r}) = \phi_{klm}(\vec{r}) + \langle \vec{r}|G_0^{(+)}U|\psi^{(+)s_n}_{klm}\rangle , \tag{24}$$

which is just the Lippmann-Schwinger equation for the exact potential U.

It is of interest to note that Eq. (20) and Eq. (21) are identically satisfied if $\psi^{s_n}_{klm}$ is the exact solution. This suggests that the degree of convergence of an approximate wave function can be judged by how well the relations given in Eq. (20) and Eq. (21) are satisfied. Also note that each side of Eq. (20) is a nonvariational approximation to the partial-wave T matrix where $\psi^{s_n}_{klm}$ is an approximate trial function. Thus the convergence of the wave function can also be judged by how well the two sides of Eq. (20) compare with the variationally stable partial-wave T matrix given by

$$T^{s_n}_{ll'm} = \langle \phi_{klm}|T^{s_n}|\phi_{kl'm}\rangle = \sum_{\chi_i,\chi_j \in R\cup S_{n-1}} \langle \phi_{klm}|U|\chi_i\rangle \times [(D^{(+)})^{-1}]_{ij}\langle \chi_j|U|\phi_{kl'm}\rangle . \tag{25}$$

One of our original motivations for using the approximate solutions $\psi^{s_0}_{klm}$ in a new separable expansion as a way of calculating an improved wave function was an observation of Ernst *et al.*[14] They noted that if one had the exact solution to the Lippmann-Schwinger equation, then the potential given by a one-term separable approximation of the form in Eq. (2), where instead of the set R one uses the exact solutions, would give the exact on-shell and half off-shell T matrix. Thus it can be expected that the use of an approximate wave function satisfying the scattering boundary conditions in the separable expansion of Eq. (2) would give improved estimates of the T matrix from which an improved trial wave function could be calculated.

A more precise understanding of the nature of the convergence of the iterative procedure outlined above is obtained by dividing Eq. (16) into two parts giving[15]

$$\langle \vec{r}|T^{s_n}|\vec{r}'\rangle = \langle \vec{r}|T^{s_0}|\vec{r}'\rangle + \sum_{1\le i\le p,\,1\le j\le p} \langle \vec{r}|(1+T^{s_0}G_0^{(+)})\Delta U|\psi^{(+)s_n-1}_{kl_im}\rangle [(E^{(+)})^{-1}]_{ij}\langle \psi^{(-)s_n-1}_{kl_jm}|\Delta U(G_0^{(+)}T^{s_0}+1)|\vec{r}'\rangle , \tag{26}$$

where

$$E^{(+)}_{ij} = \langle \psi^{(-)s_n-1}_{kl_im}|\Delta U - \Delta U G_s^{(+)}\Delta U|\psi^{(+)s_n-1}_{kl_jm}\rangle \tag{27}$$

and with

$$\Delta U = U - U^{s_0} . \tag{28}$$

Equation (26) clearly shows the different contributions from the two sets of functions R and S_{n-1}. The Green's function $G_s^{(+)}$ in Eq. (27) is the Green's function for the separable potential U^{s_0} and satisfies the Lippmann-Schwinger equation

$$G_s^{(+)} = G_0^{(+)} + G_0^{(+)}U^{s_0}G_s^{(+)} . \tag{29}$$

Thus $G_s^{(+)}$ is given by

$$\langle \vec{r}|G_s^{(+)}|\vec{r}'\rangle = \langle \vec{r}|G_0^{(+)}|\vec{r}'\rangle + \sum_{\alpha_i,\alpha_j\in R} \langle \vec{r}|G_0^{(+)}U|\alpha_i\rangle \times [(D^{(+)})^{-1}]_{ij}\langle \alpha_j|UG_0^{(+)}|\vec{r}'\rangle . \tag{30}$$

The expression for the partial-wave T matrix elements obtained from Eq. (26) is then

TABLE I. Convergence of the Schwinger variational K matrix starting from plane waves for $^2\Sigma_g$ symmetry in H_2 with $k = 0.5$ a.u. Values in parentheses indicate powers of ten, $a(b) = a\times 10^b$.

(l,l')	$n=0$	$K^{s_n}_{ll'm0}$ 1	2	3	4
(0,0)	0	−2.931	−1.701	−1.552	−1.548
(0,2)	0	0.128(−1)	0.133(−1)	0.134(−1)	0.134(−1)
(2,2)	0	0.163(−1)	0.163(−1)	0.163(−1)	0.163(−1)

TABLE II. Convergence of nonvariational approximations to the K matrix starting from plane waves for $^2\Sigma_g$ symmetry in H_2 with $k=0.5$ a.u. Values in parentheses indicate powers of ten, $a(b)=a\times10^b$.

	$\langle\phi_{kl0}\vert U\vert\psi^{s_n}_{kl',0}\rangle$				
(l,l')	$n=0$	1	2	3	4
(0,0)	3.055	−2.931	−1.331	−1.603	−1.515
(0,2)	0.521(−1)	0.128(−1)	0.180(−1)	0.127(−1)	0.139(−1)
(2,0)	0.521(−1)	0.128(−1)	0.135(−1)	0.135(−1)	0.134(−1)
(2,2)	0.165(−1)	0.163(−1)	0.163(−1)	0.163(−1)	0.163(−1)
	$\langle\psi^{s_n}_{kl0}\vert U-UG_0^{(P)}U\vert\psi^{s_n}_{kl',0}\rangle$				
(l,l')	$n=0$	1	2	3	4
(0,0)	−2.921	−5.045	−1.139	−1.659	−1.483
(0,2)	0.129(−1)	0.120(−1)	0.180(−1)	0.128(−1)	0.138(−1)
(2,2)	0.163(−1)	0.162(−1)	0.163(−1)	0.163(−1)	0.163(−1)

$$T^{s_n}_{ll'm}=T^{s_0}_{ll'm}+\sum_{1\le i\le p,\,1\le j\le p}\langle\psi^{(-)s_0}_{klm}\vert\Delta U\vert\psi^{(+)s_{n-1}}_{kl_im}\rangle\times[(E^{(+)})^{-1}]_{ij}\langle\psi^{(-)s_{n-1}}_{kl_jm}\vert\Delta U\vert\psi^{(+)s_0}_{kl'm}\rangle\,. \tag{31}$$

Thus, after the first iteration, first- and second-order errors in the difference potential ΔU have been eliminated from $T^{s_1}_{ll'm}$ since with $n=1$, Eq. (31) should give at least as good a correction to $T^{s_0}_{ll'm}$ as a distorted-wave second Born approximation would.[16] Further iterations will give still higher-order corrections.

III. RESULTS

We have used the iterative method described above to study electron-H_2 scattering in the static-exchange approximation. The target self-consistent-field (SCF) wave function is constructed from a (5s2z) Cartesian Gaussian basis set as given by Watson *et al.*[4] The Hartree-Fock energy for H_2 in this basis set is −1.1330 a.u. and the quadrupole moment is 0.452 a.u.

The results of a study of the convergence behavior of the iterative Schwinger method are given in Tables I–IV. The results presented in Tables I and II are obtained by starting the iterative procedure with $\psi^{s_0}_{klm}$ just equal to the free particle states ϕ_{klm}. This starting point corresponds to $U^{s_0}=0$. It can be seen in Table I that the varia-

TABLE III. Convergence of the Schwinger variational K matrix starting from one discrete scattering function for $^2\Sigma_g$ symmetry in H_2 with $k=0.5$ a.u. Values in parentheses indicate powers of ten, $a(b)=a\times10^b$.

	$K^{s_n}_{ll',0}$		
(l,l')	$n=0$	1	2
(0,0)	−2.045	−1.552	−1.548
(0,2)	−0.276(−1)	0.133(−1)	0.134(−1)
(2,2)	−0.372(−3)	0.163(−1)	0.163(−1)

TABLE IV. Convergence of nonvariational approximations to the K matrix and of matrix elements involving the discrete function starting from one discrete scattering function for $^2\Sigma_g$ symmetry in H_2 with $k=0.5$ a.u. Values in parentheses indicate powers of ten, $a(b)=a\times10^b$.

	$\langle\phi_{kl0}\vert U\vert\psi^{s_n}_{kl',0}\rangle$		
(l,l')	$n=0$	1	2
(0,0)	−1.602	−1.567	−1.549
(0,2)	0.179(−1)	0.131(−1)	0.134(−1)
(2,0)	−0.107(−1)	0.136(−1)	0.135(−1)
(2,2)	0.161(−1)	0.163(−1)	0.163(−1)
	$\langle\psi^{s_n}_{kl0}\vert U-UG_0^{(P)}U\vert\psi^{s_n}_{kl',0}\rangle$		
(l,l')	$n=0$	1	2
(0,0)	−1.642	−1.586	−1.550
(0,2)	0.667(−2)	0.132(−1)	0.135(−1)
(2,2)	0.155(−1)	0.162(−1)	0.163(−1)
	$\langle\phi_{kl0}\vert U\vert\alpha\rangle$[a]		
l			
0		6.180	
2		0.834(−1)	
	$\langle\psi^{s_n}_{kl0}\vert U-UG_0^{(P)}U\vert\alpha\rangle$[a]		
l	$n=0$	1	2
0	6.190	6.224	6.180
2	0.170	0.824(−1)	0.830(−1)

[a]See Eq. (21).

TABLE V. Iterated Schwinger variational K-matrix elements for $^2\Sigma$ symmetry in H_2. Values in parentheses indicate powers of ten, $a(b) = a \times 10^b$.

	$^2\Sigma_g^+$		$^2\Sigma_u^+$	
k	K^s_{000}	K^{CRM}_{000}	K^s_{110}	K^{CRM}_{110}
0.1	−0.217	−0.217 [a]	0.123(−1) [b]	0.127(−1) [a]
0.3	−0.722	−0.722	0.113	0.119
0.5	−1.55	−1.55	0.411	0.421
1.0	8.04	8.05	1.34	1.34
	K^s_{020}	K^{CRM}_{020}	K^s_{130}	K^{CRM}_{130}
0.1	0.406(−2)	0.39(−2)	0.105(−2) [b]	0.15(−2)
0.3	0.978(−2)	0.11(−1)	0.335(−2)	0.34(−2)
0.5	0.134(−1)	0.15(−1)	0.703(−2)	0.71(−2)
1.0	0.122	0.11	0.304(−1)	0.29(−1)
	K^s_{220}	K^{CRM}_{220}	K^s_{330}	K^{CRM}_{330}
0.1	0.165(−2)	0.21(−2)	0.971(−3) [b]	0.73(−3)
0.3	0.687(−2)	0.74(−2)	0.290(−2)	0.31(−2)
0.5	0.163(−1)	0.18(−1)	0.520(−2)	0.56(−2)
1.0	0.914(−1)	0.93(−1)	0.190(−1)	0.20(−1)

[a] All numbers in this column are from Ref. 17 [Collins, Robb, and Morrison (CRM)].

[b] A grid extending to 125 a.u. is used to obtain this K-matrix element.

tional Schwinger K matrix converges to three places in four iterations. However, Table II shows that the nonvariational estimates of the partial-wave K matrices from the left- and right-hand sides of Eq. (20) converge more slowly. In this calculation, these nonvariational K matrices require another four iterations before they converge to three places. Table III gives the variational Schwinger K matrix for an iterative calculation where U^{s0} is a one-term separable approximation to U, constructed using a single s Cartesian Gaussian of exponent 0.5 centered on the nuclei. With this starting point, the iterative procedure converges in two iterations. Also note that the nonvariationally stable matrix elements given in Table IV, which are associated with Eq. (20) and Eq. (21), are well converged by the second iteration also.

In Tables V and VI we present K-matrix elements at several energies for both $^2\Sigma$ and $^2\Pi$ symmetries. We also compare the present results with those of Collins *et al.*[17] The separable potentials U^{s0} used in these calculations are four-term approximations. The potentials are constructed from Cartesian Gaussian functions centered at the nuclei. The Cartesian Gaussian functions have exponents of 0.3 and 1.0 and are of s and z types for the $^2\Sigma$ symmetries and x and xz types for the $^2\Pi$ symmetries. All variational K matrices converge to three places by the first iteration. This extremely rapid convergence is expected since the difference potential ΔU should be small.

All integrals were calculated using single-center expansions as is described elsewhere.[3,18] The integrations are performed on a grid extending to

TABLE VI. Iterated Schwinger variational K-matrix elements for $^2\Pi$ symmetry in H_2. Values in parentheses indicate powers of ten, $a(b) = a \times 10^b$.

	$^2\Pi_u$		$^2\Pi_g$	
k	K^s_{111}	K^{CRM}_{111}	K^s_{221}	K^{CRM}_{221}
0.1	−0.296(−2)	−0.306(−2) [a]	0.106(−2) [b]	0.103(−2) [a]
0.3	0.195(−1)	0.218(−1)	0.368(−2)	0.400(−2)
0.5	0.102	0.108	0.103(−1)	0.114(−1)
1.0	0.334	0.335	0.692(−1)	0.713(−1)
	K^s_{131}	K^{CRM}_{131}	K^s_{241}	K^{CRM}_{241}
0.1	0.110(−2)	0.12(−2)	0.493(−3) [b]	0.63(−3)
0.3	0.267(−2)	0.28(−2)	0.148(−2)	0.15(−2)
0.5	0.483(−2)	0.50(−2)	0.235(−2)	0.24(−2)
1.0	0.142(−1)	0.14(−1)	0.564(−2)	0.58(−2)
	K^s_{331}	K^{CRM}_{331}	K^s_{441}	K^{CRM}_{441}
0.1	0.286(−3)	0.55(−3)	0.465(−3) [b]	0.18(−3)
0.3	0.217(−2)	0.23(−2)	0.139(−2)	0.15(−2)
0.5	0.392(−2)	0.42(−2)	0.245(−2)	0.26(−2)
1.0	0.157(−1)	0.17(−1)	0.611(−2)	0.67(−2)

[a] All numbers in this column are from Ref. 17.

[b] A grid extending to 125 a.u. is used to obtain this K-matrix element.

40 a.u., except as noted in Tables V and VI where a grid extending to 125 a.u. is used to accurately compute some integrals at low energy.

As can be seen, the K matrix elements are in good agreement with those of Collins *et al.*[17] The small discrepancies which exist are probably due to differences in the potentials used.

IV. CONCLUSIONS

The iterative Schwinger variational method presented here is a powerful method for computing electron-molecule scattering solutions. With a sufficient number of iterations, this method gives accurate scattering results which are independent of the initial discrete basis set used. However, it is important to note that even though the variationally stable T matrix may converge in a particular calculation, it is necessary to check that the conditions given in Eqs. (19), (20), and (21) are satisfied to be assured that the T matrix has converged to the correct solution.

The Schwinger method does not require the solution of integrodifferential equations. All equations are decoupled integral equations which are solved by straightforward integration procedures. With a reasonable choice of the initial separable potential U^{s}_{0}, this iteration method converges in only a few iterations. Applications to larger molecular systems are underway.

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