Ab Initio Method for Calculating Total Cross Sections

A. K. Bhatia,[1] B. I. Schneider,[2] and A. Temkin[1]
[1]*Goddard Space Flight Center, Code 680, NASA, Greenbelt, Maryland 20771*
[2]*Physics Division, National Science Foundation, Washington, D.C. 20550*
(Received 13 October 1992)

A method for calculating total cross sections without formally including nonelastic channels is presented. The idea is to use a one channel T-matrix variational principle with a complex correlation function. The derived T matrix is therefore not unitary: Elastic scattering is calculated from $|T|^2$, but total scattering is derived from the imaginary part of T using the optical theorem. The method is applied to the spherically symmetric model of electron-hydrogen scattering. No spurious structure arises; results for σ_{el} and σ_{total} are in excellent agreement with calculations of Callaway and Oza. The method has wide potential applicability.

PACS numbers: 34.80.Bm, 34.80.Dp, 36.10.Dr

Although it is well known phenomenologically how to modify the scattering formalism so as to calculate total cross sections including only the elastic channel explicitly [1], it has been a much more difficult task to do this in an *ab initio* yet practical way. One approach along these lines, developed by Rescigno and Reinhardt [2], constructs the Fredholm determinant using an L^2 basis set; results for model problems were very satisfactory. The method, which involves a rather elaborate analytic continuation analysis, was extended to the static (i.e., no exchange) approximation for electron-hydrogen scattering [3].

Kindred methods have been applied to real problems including positron-hydrogen scattering [4], and electron-hydrogen and lithium scattering [5], with very good results. However, these methods and calculations have been confined to the lower energy (inelastic and ionization) regime, in contrast to our method, which is here directed at purely the ionization region going up to much higher energies. Also, as will be seen, our method is very simple in principle and widely applicable.

Other methods for deducing specific and total cross sections have been applied to a model of (S wave) e-H scattering introduced by one of us [6], which is rich enough to include resonances and inelasticity [7]. We have recently generalized the model (for use as part of a new, proposed dispersion relation for e-atom scattering) [8] by writing it as a full Schrödinger equation (Ry units throughout):

$$[-\nabla_1^2-\nabla_2^2-2/r_<-E]\Psi_{na}^{(0)}(r_1,r_2)=0\,. \tag{1}$$

The model interaction, $2/r_<$ (where $r_<$ is the lesser of r_1,r_2), is derived from the full interaction, $-2/r_1-2/r_2+2/r_{12}$, by retaining only the spherically symmetric term in the expansion of $2/r_{12}$. We have called this the spherically symmetric model [8]; to reduce (1) to its explicit, partial wave form, one expands the most general form of solution in this model containing the ground state,

$$\Psi_{na}^{(0)}=(r_1r_2)^{-1}\sum_L[\psi_L^{(1)}(r_1,r_2)Y_{L0}(\hat{r}_1)Y_{00}(\hat{r}_2)+\psi_L^{(2)}(r_1,r_2)Y_{00}(\hat{r}_1)Y_{L0}(\hat{r}_2)]\,, \tag{2}$$

and inserts it into Eq. (1) to derive ($i=1,2$)

$$\left[-\frac{\partial^2}{\partial r_1^2}-\frac{\partial^2}{\partial r_2^2}+\frac{L(L+1)}{r_i^2}-\frac{2}{r_<}-E\right]\Psi_L^{(i)}(r_1,r_2)=0\,, \tag{3}$$

with appropriate boundary conditions for $\psi_L^{(1)}$ and $\psi_L^{(2)}$: for $r_1\geq r_2$ (with + for singlet and − for triplet)

$$\psi_L^{(2)}(r_1,r_2)=\pm\psi_L^{(1)}(r_2,r_1)\,,$$

$$\lim_{r_1\to\infty}\psi_L^{(i)}(r_1,r_2)=\left[\frac{\sin(kr_1-\pi L/2)}{k}+T_Le^{ikr_1}\right]\phi_{10}(r_2)\delta_{i1}\,.$$

The model even in its S-wave form has proven to be nontrivial: We expanded the solution in terms of exact separable solutions and minimized the deviation from the exact boundary conditions along $r_1=r_2$ [6,7]; but severe round-off problems are encountered when too many such terms are included. Subsequently, Poet [9] overcame these problems by perturbing the higher separable terms in such a way as to keep the round-off errors under control. His remarkably accurate results are in agreement with those we had previously obtained; in addition, he calculated cross sections at such a fine energy grid as to obtain the resonant structure that arises for $k^2<1$. Of prime importance, both sets of results showed significant deviations from close coupling [10] and pseudostate results [11], the major differences occurring as a result of spurious pseudothreshold effects in the latter. Later calculations [12,13] continue to show this phenomenon, although suitably averaging over artificial resonances yields reasonably accurate cross sections as Callaway and Oza [14] have more recently confirmed, by numerically integrating Eq. (3) (for $L=0$).

Most recently Bray and Stelbovics [15], using a many term close coupling expansion in a T-matrix integral equation formalism, obtained *smooth* results when the number of states was large enough. Although it is not clear from their paper, the method did include positive energy pseudostates, which were found to be necessary to reproduce the correct magnitudes of the various cross sections [16]. We would have expected pseudoresonant structure to have shown up near pseudoresonant thresholds, but none has been seen in the converged calculations [15,16]. The results are, nevertheless, very impressive.

The method which we shall put forward in this Letter is quite different. We shall utilize a one channel Kohn T-matrix variational principle as developed by Schneider, Rescigno, McCurdy, and Lengsfield [17], but using a *complex* correlation function Φ_L. For electron-hydrogen scattering this means using a wave function of the form (with + for singlet and − for triplet)

$$\Psi_L = \left[\frac{u_L(r_1)}{r_1} Y_L(\hat{r}_1)\phi_{10}(r_2)Y_{00}(\hat{r}_2) \pm (1 \leftrightarrow 2) \right] \pm \Phi_L^{(\pm)} . \tag{4}$$

Specifically we here take the correlation function to be of the form

$$\Phi_L^{(\pm)} = e^{-(\gamma_1 r_1 + \gamma_2 r_2)} Y_{L0}(\hat{r}_1) Y_{00}(\hat{r}_2) \times \sum_{n,m}^{N} C_{nm} r_1^n r_2^m \pm (\mathbf{r}_1 \leftrightarrow \mathbf{r}_2) , \tag{5}$$

where the γ_i are complex: $\gamma_i = \gamma_i^{(R)} + i\gamma_i^{(I)}$. (For convergence of all integrals $\gamma_i^{(R)} > 0$.)

The Kohn T-matrix variational principle [13] corresponds to $\delta(I_L - i^L T_L) = 0$, where the functional I_L is

$$I_L \equiv \langle \tilde{\Psi}_L | H - E | \Psi_L \rangle . \tag{6}$$

$\tilde{\Psi}_L$ is constructed from Ψ_L [cf. Eq. (5)] by complex conjugating only the spherical harmonics, not the γ_i nor the C_{mn}. Thus T_L, which is obtained from the asymptotic behavior of $u_L(r)$,

$$\lim_{r \to \infty} u_L(r) = \frac{1}{k} \sin(kr - \pi L/2) + T_L e^{ikr} , \tag{7}$$

will not be real, nor will it be unitary ($\sigma_{el} \neq \sigma_T$), where

$$\sigma_{el}^{(L)} = 4\pi(2L+1)|T_L|^2, \quad \sigma_T^{(L)} = (4\pi/k)\mathrm{Im}(T_L) . \tag{8}$$

The nonunitarity is, we maintain, an advantage, because (and this is the thesis of our argument) if the long-range part of Ψ_L is dominated by the elastic channel (meaning elastic scattering is, by far, the largest individual cross section in the energy range with which we shall be concerned), then all remaining channels correspond to absorption, and they have their dominant effect in the interior part of the wave function. The complex correlation function has the capability of mocking up the oscillatory behavior of both electrons to reasonably large radial distances, if (in this calculation the complex exponents of) the correlation function is suitably chosen.

The proof of this pudding is obviously in the eating, and we have tested it on the spherically symmetric model [6–8] described above. We use an optical potential formalism, whereby u_L of Eq. (1) satisfies

$$\left[-\frac{d^2}{dr^2} + \frac{L(L+1)}{r^2} + V_d \pm V_{ex} + \mathcal{V}_{op} - k^2 \right] u_L = 0 , \tag{9}$$

where V_d and V_{ex} are static and exchange terms, and the optical potential is expanded in the usual way:

$$\mathcal{V}_{op} u_L^{(r)} = r \sum_{s}^{N} \frac{\langle Y_{L0}^* Y_{00}^* (H-E) Q \Phi_s \rangle \langle Q \tilde{\Phi}_s (H-E) P \Psi_L \rangle}{E - \mathcal{E}_s} . \tag{10}$$

The eigenspectra, Φ_s and $\mathcal{E}_s$, come out of a QHQ calculation, about which we need only say that, given the form Φ_L above, $\mathcal{E}_s$ and hence $\mathcal{V}_{op}$ are complex.

One technical item of note is that the P (and Q) operators that are called for in the program that is used (see below) are not the usual ones ($P = P_1 + P_2 - P_1 P_2$) but rather

$$P = P_1 + P_2 - 2P_1 P_2 , \tag{11}$$

where the projectors have their usual meaning: $P_i = \phi_{10}(r_i)\rangle\langle\phi_{10}(r_i)$. One can easily show that this operator, and the corresponding $Q = 1 - P$, are also idempotent and have the necessary asymptotic properties. What this Q does do is to give one added eigenfunction to the QHQ problem, simulating the $(1s)^2$ state of H^- (at $\mathcal{E}_{s=1} \simeq -0.78$ Ry). This term must be included in the optical potential, but it causes no resonance because the numerator also goes to zero at the same E. Moreover, this form of P turns out to be a special case of the projection operators already used in a many-electron Kohn formalism of Schneider, Rescigno, McCurdy, and Lengsfield [17,18].

In the present calculation, the Φ_s and $\mathcal{E}_s$ are determined as an ordinary QHQ problem [19], using the above Q operator and the program minimally generalized to handle complex Φ. The u_L are parametrized and the parameters plus the T matrix are determined from the conventional variational equations using a previous program [17,18], also suitably modified to handle a complex optical potential. Linear constants are determined by the usual Kohn equations: $\partial I_L/\partial C_{mn} = 0$, $\partial I_L/\partial T_L = i^L$.

Results will, of course, depend on the nonlinear parameters. It is not yet clear at this initial stage of the methodology to what extent absolute stationarity with respect to them can be achieved and would be meaningful. Nevertheless, criteria for a reasonable choice are clear: They must be such as to yield all $\mathcal{E}_s$ with a negative imaginary part (corresponding to absorption from the elastic channel), and, for any given set of γ_i, results should converge

TABLE I. Results for ^1S cross sections in the spherically symmetric model. Cross sections, in a_0^2, do not include statistical factor. Upper entry corresponds to σ_{el}; lower entry to σ_T. Nonlinear parameters are $-\gamma_1 = -\gamma_2 = -0.6 + i(0.1)$.

k^2 (Ry) \ N	20	25	30	36	Callaway & Oza[a]
1.0	4.13	4.10	4.17	4.10	4.12
	4.78	4.72	4.80	4.75	4.76
1.1	3.62	3.57	3.54	3.60	3.53
	4.25	4.27	4.21	4.26	4.39
1.21	3.10	3.10	3.11	3.10	3.07
	3.84	3.76	3.82	3.79	3.77
1.44	2.43	2.40	2.45	2.44	2.42
	3.09	3.15	3.13	3.13	3.13
1.7	1.99	1.97	1.95	2.02	1.97
	2.67	2.61	2.63	2.67	2.63
2.0	1.60	1.66	1.66	1.64	1.65
	2.18	2.28	2.23	2.25	2.24
2.25	1.47	1.40	1.47	1.46	1.43
	1.96	1.96	2.02	1.99	1.99
2.50	1.37	1.27	1.27	1.33	1.29
	1.82	1.74	1.80	1.82	1.78
3.00	1.10	1.13	1.06	1.06	1.09
	1.55	1.50	1.44	1.49	1.50
4.00	0.73	0.77	0.85	0.83	0.82
	1.01	1.10	1.13	1.08	1.09

[a]Reference [14].

in a practical sense as N [the number of linear parameters in Φ; cf. Eqs. (5) and (10)] is increased. Most important cross sections must be such that $\sigma_T \geq \sigma_{el}$.

Table I contains results for the ^1S partial wave. It is gratifying that a single set of $\gamma_1 = \gamma_2$ does satisfy the above criteria. Other reasonable sets have been tried, and—providing problems of linear dependence do not arise—they yield similar results. Most significantly, the results compare very favorably with Callaway and Oza [14]. We have also examined results on a fine mesh in k^2 and we find no spurious resonances (nor should there be any) in the ionization domain.

In conclusion, it is evident that the method should be applicable and useful in a practical way for whole variety of many-electron target systems. In addition, the method can clearly be generalized to include any (group of) discrete states explicitly, the remaining ones being then implicitly included as above, with the Q operator augmented appropriately. And finally, one can readily apply the method to positron scattering, where (if one is interested in total cross sections) it avoids the necessity of including the very difficult positronium formation channels altogether [4].

The work of two of us (A.T. and A.K.B.) has been done under the aegis of NASA RTOP No. 170-38-51.

[1] Cf., for example, J. M. Blatt and V. W. Weisskopf, *Theoretical Nuclear Physics* (Wiley, New York, 1952), Chap. VIII.
[2] T. N. Rescigno and W. P. Reinhardt, Phys. Rev. A **8**, 2828 (1973).
[3] E. J. Heller, T. N. Rescigno, and W. P. Reinhardt, Phys. Rev. A **8**, 2946 (1973).
[4] J. R. Winick and W. P. Reinhardt, Phys. Rev. A **18**, 910 (1978); **18**, 925 (1978).
[5] T. N. Rescigno and C. W. McCurdy, Chem. Phys. Lett. **140**, 232 (1987).
[6] A. Temkin, Phys. Rev. **126**, 130 (1962).
[7] H. L. Kyle and A. Temkin, Phys. Rev. **134**, A600 (1964).
[8] A. Temkin and A. K. Bhatia, *Abstracts of the Sixteenth International Conference on the Physics of Electronic and Atomic Collisions, New York, 1989,* edited by A.

Dalgarno *et al.* (XVI ICPEAC Program Committee, New York, 1989), p. 144; *Abstracts of the Seventeenth International Conference on the Physics of Electronic and Atomic Collisions, Brisbane, 1991,* edited by I. E. McCarthy, W. R. MacGillivray, and M. C. Standage (Griffith University, Australia, 1991), p. 97.

[9] R. Poet, J. Phys. B **11**, 3081 (1978).

[10] R. Marriott, Proc. Phys. Soc. London **72**, 121 (1958).

[11] P. G. Burke and J. F. Mitchell, J. Phys. B **6**, 320 (1973).

[12] D. H. Oza and J. Callaway, Phys. Rev. A **27**, 2840 (1983).

[13] B. H. Bransden, R. Hewitt, and M. Plummer, J. Phys. B **23**, 2645 (1988).

[14] J. Callaway and D. H. Oza, Phys. Rev. A **29**, 2416 (1984).

[15] I. Bray and A. T. Stelbovics, Phys. Rev. Lett. **69**, 53 (1992).

[16] I. Bray (private communication).

[17] B. I. Schneider, T. N. Rescigno, C. W. McCurdy, and B. H. Lengsfield, in *Aspects of Electron-Molecule Scattering and Photoionization,* edited by A. Herzenberg (AIP Conf. Proc. No. 204 (AIP, New York, 1990), p. 83.

[18] B. I. Schneider and T. N. Rescigno, Phys. Rev. A **37**, 3749 (1988).

[19] A. K. Bhatia and A. Temkin, Phys. Rev. A **11**, 2018 (1975).