

interchange the variables of integrations. This seems to be a very trivial point, but happens to be the main difficulty in the actual calculation of the rearrangement collisions. In fact, this is the main motivation for the formulation of QMP, and ob-

viously we no longer have to evaluate the kernels such as  $K_{12}$ . An improved calculation of the  $e^+H$  pickup collision is in progress using the QMP and incorporating some additional simplifications peculiar to this particular system.<sup>14</sup>

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## Forcing Conservation of Particle Flux in Perturbation-Theory Calculations of Inelastic Scattering

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Two approximations to Seaton's unitarization scheme are described which make it possible to impose the conservation-of-particle-flux requirements on an approximate calculation of inelastic scattering without making calculations of elastic scattering in the two channels which the transition connects. One approximation is based on the black-sphere model of Feshbach and Weisskopf. Another approximation corrects only for back coupling and can be equivalent to a method of Levine. The methods are illustrated by applying them to the Born approximation for the  $1s-2s$  excitation of the hydrogen atom by electron impact.

### I. INTRODUCTION

It is well known that as a consequence of time-reversal invariance and particle-flux conservation for a scattering process, we can assign phases to the wave functions in such a way that the scattering matrix  $S$  is symmetric and unitary, the transition matrix  $T$  is symmetric and satisfies the generalized optical theorem, and the reactance matrix  $R$  is symmetric and real.<sup>1-3</sup> Cross sections and scattering amplitudes calculated by many theoretical approximations to the  $S$  and  $T$  matrices do not satisfy these requirements, even within an artificially limited subset of open channels. Although cross sections can be most directly calculated from  $S$  and  $T$ , it has often been recognized that it is advantageous to make approximations to  $R$  (or to the reaction matrix  $K=2R$ ) rather than directly to  $S$  or  $T$ , because the  $S$  and  $T$  computed from any Hermitian  $R$  (whether approximate or exact) auto-

matically satisfy the conservation and time-reversal requirements.<sup>4</sup> Using these ideas, Seaton proposed a calculational scheme (his method II) in which the conservation and symmetry requirements are fully satisfied even if the conservation laws are violated in the initial approximation.<sup>5</sup> For electron-atom scattering, this scheme has been applied many times.<sup>6-19</sup> It has also been much applied for other quantum-mechanical scattering problems.<sup>20-27</sup> For inelastic scattering, Seaton's method requires approximate calculations not only of the inelastic scattering amplitudes, but also of the elastic scattering amplitudes in at least the initial and final channels. We consider here two similar methods for making the scattering calculation satisfy all the conservation requirements for an inelastic process without calculating the elastic scattering. They are alternatives to Seaton's method which may be considered as approximations of it. They are, however, different ap-

proximations than his and may in some cases be more appropriate. The methods may be applied in approximate treatments of a wide class of quantum-mechanical and other wave-scattering processes; however, in this article we are interested in elucidating the method, not in particular applications.

Computational techniques used recently by Levine<sup>28</sup> and Roberts and Ross<sup>29</sup> are special cases of the general technique discussed here.

## II. THEORY

We consider as an example the scattering of a structureless particle with mass unity and wave number  $k_m$  off a target with spherically symmetric eigenstates  $n=1, 2, \dots$ . For the partial wave with relative orbital angular momentum  $\hbar l$ , the scattering amplitude for scattering angle  $\theta$  and an  $m \rightarrow n$  transition is

$$f_{nm}^l(\theta) = \frac{-1}{2i(k_n k_m)^{1/2}} (2l+1) T_{nm}^l P_l(\cos\theta), \quad (1)$$

where  $T_{nm}^l$  is an element of the  $T$  matrix. The contribution to the integral cross section for the  $m \rightarrow n$  transition is

$$Q_{mn}^l = 2\pi(k_n/k_m) \int_0^\pi |f_{nm}^l(\theta)|^2 \sin\theta d\theta, \quad (2)$$

$$Q_{mn}^l = (\pi/k_m^2)(2l+1) |T_{nm}^l|^2. \quad (3)$$

The reactance and scattering matrices are given by

$$\underline{T} = 2i(\underline{1} - i\underline{R})^{-1}\underline{R}, \quad (4)$$

$$\underline{S} = \underline{1} - \underline{T}, \quad (5)$$

$$\underline{S} = (\underline{1} - i\underline{R})^{-1}(\underline{1} + i\underline{R}). \quad (6)$$

Equation (6) is a general transformation of a Hermitian matrix into a unitary matrix and is known as the Cayley transformation.<sup>30</sup> Beginning with an approximate Hermitian  $R$  matrix  $\underline{R}^a$ , the  $T$  matrix computed from (3) and (4) is automatically symmetric, and satisfies the generalized optical theorem

$$2\text{Re}T_{ii}^l = \sum_j |T_{ij}^l|^2 \quad (7)$$

and the upper bounds imposed by conservation requirements

$$|T_{ij}^l| \leq 1 + \delta_{ij}. \quad (8)$$

Further, the  $S$  matrix computed from (4) and (5), or equivalently from (6), is automatically unitary and symmetric. (The superscript  $l$  identifying the subblock of a matrix to which an element belongs is not always indicated in the rest of the article.)

The direct computation of  $\underline{S}$  or  $\underline{T}$  in a first-order theory (e.g., the Born approximation, the distorted-wave approximation, or any method which does not couple the transition of interest to real

transitions to other channels or to real elastic scattering) is called method I. It is consistent with such a theory to set<sup>5</sup>

$$-2i\underline{R}^a = \underline{T}^I, \quad (9)$$

which is a first-order approximation to (4). Seaton's method II, which has become the usual unitarization scheme, is to calculate  $\underline{T}^{II}$  from this  $\underline{R}^a$  by Eq. (4). Seaton's method II can also be derived using the Lippman-Schwinger equation for the  $T$  matrix by neglecting the principal part of the Green's function and retaining only the contribution from on the energy shell.<sup>24,28,29,31</sup> If the original  $\underline{T}$  is not already symmetric and purely imaginary, it is necessary before applying (9) to symmetrize it

$$\underline{T}^I = \frac{1}{2}(\underline{T} + \underline{T}^T) \quad (9')$$

(where  $\underline{T}^T$  is the transpose of  $\underline{T}$ ), or adjust its phase (see, e.g., Refs 13, 14, and 17)

$$T_{ij}^I = |T_{ij}| i, \quad (9'')$$

or both. Seaton's method III is similar and has been applied a few times,<sup>5,8,9</sup> but will not be further considered here.<sup>32</sup> Ideally,  $\underline{R}^a$  and  $\underline{T}^{II}$  are  $N \times N$  matrices where  $N$  is the number of open channels. In practice, the further approximation is almost always made of treating only  $M \times M$  subblocks of  $\underline{R}^a$  and  $\underline{T}^{II}$  where  $M < N$ . For inelastic scattering, however,  $M$  must be equal to two or larger and the necessary elements of  $\underline{R}^a$  are obtained via (9) from approximate calculations of elastic and inelastic scattering.

We now consider alternative methods of forcing the inelastic cross sections  $Q_{mn}^l (m \neq n)$  to satisfy the conservation laws. Since the unitarization scheme is most important when the transition is strong, a useful model is the black-target model first used for a totally absorbing sphere ("opaque sphere") in nuclear physics<sup>33,34</sup>; there the absorption is into many inelastic channels. This model leads to the elastic cross section being exactly equal to the inelastic cross section (in general, the inelastic cross section may be larger than, equal to, or smaller than the elastic cross section<sup>35</sup>). If we apply this model in a two-channel approximation to the  $m \rightarrow n$  transition, then we want  $Q_{11} = Q_{12} = Q_{21} = Q_{22}$ . If we obtain  $R_{21}^a$  for  $m \neq n$  from Eq. (9), then the desired relation among the cross sections is obtained if  $R_{11}^a = R_{22}^a = R_{21}^a$ . Method IV is to use these approximate reactance matrix elements in the  $2 \times 2$   $m, n$  subblock of (4) to obtain

$$T_{ji}^{IV} = \frac{-2i R_{nm}^a}{1 - 2i R_{nm}^a}, \quad j = n, m; \quad i = n, m \quad (10)$$

$$T_{ji}^{IV} = \frac{T_{nm}^I}{1 + T_{nm}^I}. \quad (10')$$

This is an alternative to Seaton's method II which allows us to correct the inelastic cross sections so as not to violate the conservation theorems without making calculations of the elastic cross sections. Method IV has much the same spirit as the statistical theory<sup>36</sup> when the inelastic coupling is strong (the statistical theory can be defined in a natural way by making averages over the scattering matrix elements corresponding to a range of energies). When the coupling is weak so that  $R_{nm}^a$  is small and the first-order theory is accurate, then method IV is just as accurate (the statistical theory would be inaccurate if applied in such a situation). When the coupling is strong, method IV gives the same kind of results for the inelastic scattering as a 2-channel statistical theory.

Method II for an  $m \rightarrow n$  transition simultaneously includes first-order corrections for back coupling ( $m \rightarrow n \rightarrow m$ ,  $m \rightarrow n \rightarrow m \rightarrow n$ , etc.), successive first-order transitions ( $m \rightarrow p \rightarrow n$ ,  $m \rightarrow m \rightarrow n$ , etc.), and competition ( $m \rightarrow m$ ,  $m \rightarrow n$ ,  $m \rightarrow p$ ). The 2-channel approximation to method II includes back coupling, successive first-order transitions involving the two channels, and a correction for competition between these two channels. Further, in a two-channel approximation, it is the  $2 \times 2$  subblock of  $\underline{S}$  that is unitary and it is the two-channel optical theorem that is satisfied. Method IV is a two-channel approximation which includes a first-order correction for back coupling and approximate corrections (which will usually be too small) for successive first-order transitions involving the two channels and competition between the two channels.

Finally, the inclusion of only back coupling will be called method V. In this method  $R_{nm}^a$  (and  $R_{nn}^a$ ) is determined from Eq. (9) and we set

$$R_{nm}^{a(V)} = R_{nn}^{a(V)} = 0.$$

Then (4) gives

$$T_{nm}^V = \frac{-2iR_{nm}^a}{1 + (R_{nm}^a)^2}, \quad n \neq m \quad (11)$$

$$T_{nn}^V = \frac{T_{nn}^I}{1 + \frac{1}{4}|T_{nn}^I|^2}. \quad (11')$$

Equation (11') is a more general statement of a result obtained previously by Beigman and Vainshtein<sup>37</sup> and obtained by a different derivation by Levine.<sup>28</sup> Levine<sup>28</sup> and Roberts and Ross<sup>29</sup> have applied method V to the problem of atom-rigid rotor scattering.

As a generalization of methods IV and V, the unitarization scheme (9) may be applied to results of weak-coupling theories in approximations including more than two channels by filling in average  $R$  matrix elements or zeros whenever particular  $R_{nm}^a$  values are not available. The results for the transition probability of interest will be essentially

unaffected by such a scheme when the coupling is really weak, but will be improved when the coupling is so strong that violation of the conservation requirements becomes important.

Another generalization is to use the unitarization schemes for the prediction of probabilities in cases where a first approximation is not known. For example, the method of Weare and Thiele<sup>31</sup> (see also Roberts and Johnson<sup>38</sup> and Roberts and Ross<sup>29</sup>) is equivalent to approximating the  $R$  matrix as a tri-diagonal matrix and then using Eqs. (3) and (4) to calculate transition probabilities between states for which  $R_{nm}^a$  is zero. If one further sets the diagonal matrix elements of  $R$  to zero, this becomes a generalization of method V. The use of such a method for a multiple-coupling situation is an example of how these methods might be useful in a weak-coupling situation, whereas in the other cases (methods IV and V and the generalizations of IV) we envision these methods being more useful in strong-coupling situations as discussed above.

These unitarization methods account only for real transitions (transitions on the energy shell), not for virtual transitions. Thus, if increasing the number of channels included in the unitarization scheme does not change the cross sections much, it does not prove that virtual transitions (a polarization effect) to the added states are important. This point has been sometimes misunderstood in the past (see, e.g., Ref. 10).

Although these methods are useful under different circumstances (e.g., method IV and its generalizations might be very useful for the lowest partial waves in molecular collisions since these present a strong-coupling situation<sup>39</sup>), Sec. III gives an example where methods I, II, IV, and V are all applied to one well-studied and fairly well-understood<sup>40</sup> case.

### III. EXAMPLE

As an example of the use of the methods discussed in Sec. II, we now consider their application to the Born approximation for the  $1s \rightarrow 2s$  excitation of the hydrogen atom by electron impact, a well-studied process. In this example we can see separately the effects of coupling of real processes (processes whose initial and final states are both on the energy shell) and the effects of virtual excitations (processes whose initial or final states or both are off the energy shell). The discussion should make clear how the unitarization schemes and various ways of computing the scattering matrix from close-coupling approximations could be interpreted in terms of selective summation of Feynmann diagrams.

Table I gives the integral cross sections (in atomic units)

TABLE I. Integral cross sections  $Q_{12}$  (in  $a_0^2$ ) for  $1s$ - $2s$  excitation of hydrogen by electrons.

Source of $R$ matrix	Born					Close coupling including exchange				
Method to compute S matrix	II	II	IV	V	I	II	II	IV	V	I
$M$ $k_1^2$	4	2	(2)	(2)	1	4	2	(2)	(2)	1
0.81	0.0904 (Ref. 7)	0.0854	0.4855	0.5133	0.5459 <sup>a</sup>					
1.00	0.2227 (Ref. 7)	0.1624	0.6767	0.7224	0.7797 <sup>a</sup>	1.1348 (Ref. 42)	1.1138	8.1340	7.8804	213.4806
1.44	0.3211 (Ref. 7)	0.2279	0.6457	0.6774	0.7168 <sup>a</sup>	0.8201 (Ref. 42)	1.2982	3.4168	4.0811	5.7371
2.25	0.3073 (Ref. 7)	0.2373	0.4923	0.5076	0.5249 <sup>a</sup>	0.4695 (Ref. 42)	0.7534	2.0373	2.3687	5.7542
4.00	0.2317 (Ref. 7)	0.1941	0.3092	0.3145	0.3201 <sup>a</sup>	0.2827 (Ref. 42)	0.2893	1.0714	1.2458	3.4874

<sup>a</sup>First Born approximation.

$$Q_{12} = \sum_l Q_{12}^l \quad (12)$$

for the 11.0–54.4-eV incident energy range as computed by five of the methods. (The reactance matrices for these calculations are taken from the Born-approximation calculations of Lawson *et al.*<sup>41</sup>) The table shows that correcting for back coupling (methods IV and V) only makes a 2–14% reduction of the cross sections. Thus only a small part of the much larger 39–85% reductions found in the  $2 \times 2$  II method is due to back coupling and corrections for conservation of particle flux and unitarity. The larger reductions are thus mainly due to competition. The cross sections from the  $2 \times 2$  II method are much different than those from the  $4 \times 4$  II method. The difference between these two methods is that the latter allows for coupling of real transitions involving the  $2p$  states. Such coupling is therefore very important. Table I also shows the cross sections computed from reactance matrices from the  $1s - 2s - 2p - 2p^*$  close-coupling approximation calculations of Burke *et al.*<sup>42</sup> The close-coupling calculations include not only the complete coupling of these four target states (real and virtual transitions to all orders) but also distortion of the free-electron wave function and exchange. All these effects are neglected in the Born-approximation calculations. The disagreement of the close-coupling results (columns 7–9) with the results I–V (columns 2–6) shows that the effect of coupling virtual processes (polarization) and the effects of distortion and exchange are important. The virtual processes involving excited  $p$  states can be included approximately by using a generalized optical potential such as an induced dipole-polarization potential.<sup>43</sup> The  $4 \times 4$  matrix calculation of the close-coupling S matrix from the  $R$  matrix includes all real and virtual processes among the four states. The  $2 \times 2$  matrix calculation of the close-coupling

S matrix from the  $R$  matrix includes all virtual processes among the four states but only real processes involving the  $1s$  and  $2s$  states. The large difference between these two calculations (columns 7 and 8 of Table I), like the large difference between columns 2 and 3 of Table I, shows that coupling of real processes involving  $2p$  states is important. This coupling of real processes is called the absorptive part of the charge polarization and has been studied less than the virtual dipole effect. It has been studied recently by Mohr,<sup>44</sup> Bonham,<sup>45,46</sup> and Green.<sup>47</sup> The comparisons presented here show the  $2p$  state enters in an important way both as a virtual intermediate and as a real intermediate for the  $1s$ - $2s$  transition. Bonham's study of elastic scattering off the helium atom led to the conclusion that  $p$  states enter in an important way both as virtual intermediates and as real intermediates.<sup>46</sup> The success of the tridiagonal reactance matrix calculations of Weare and Thiele<sup>31</sup> (see also Roberts and Johnson<sup>38</sup>) for  $v = 0$  to  $v = 2$  transitions in collinear atom-vibrator collisions shows that  $v = 1$  states en-

TABLE II. Collision strengths  $\Omega^l(1s-2s)$ .

Method		II	II	IV	V	I
$l$	$M$ $k^2$	4	2	(2)	(2)	1
0	0.81	0.0035	0.0146	0.1171	0.1243	0.1326
	1.00	0.0158	0.0191	0.1637	0.1779	0.1957
	1.44	0.0243	0.0238	0.1547	0.1673	0.1830
	2.25	0.0237	0.0233	0.1167	0.1238	0.1321
	4.00	0.0193	0.0192	0.0722	0.0749	0.0778
2	0.81	0.0106	0.0002	0.0002	0.0002	0.0002
	1.00	0.0282	0.0040	0.0043	0.0043	0.0043
	1.44	0.0124	0.0212	0.0266	0.0267	0.0268
	2.25	0.0317	0.0485	0.0622	0.0666	0.0670
	4.00	0.0644	0.0727	0.0988	0.0998	0.1008

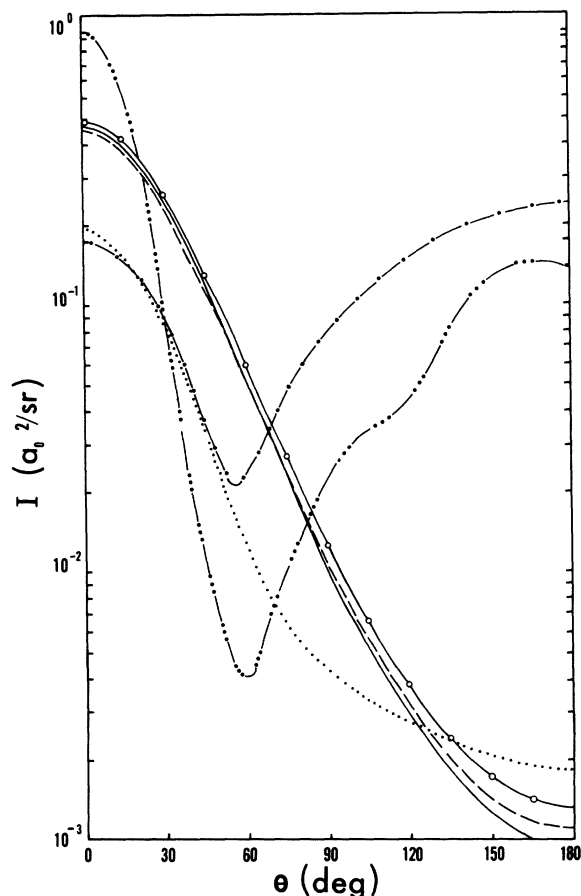


FIG. 1. Differential cross sections vs scattering angle for the 1s-2s excitation of the hydrogen atom by electron impact as calculated for several approximations. The circles indicate Born.I; dots, Born.II; straight line, Born.IV; dashes, Born.V; dash-dot, close coupling with eigenstates  $n \leq 2$  included and S matrix calculated using 1s, 2s submatrix equations ( $2 \times 2$ ); and dash-dot-dot-dot, close coupling with eigenstates  $n \leq 2$  included and usual  $4 \times 4$  calculation of S matrix.

ter essentially only as real intermediates in their cases. Roberts has used this fact to make second-order corrections for atom-vibrator excitation collisions by keeping only contributions from real processes.<sup>48</sup> He got good results. Further, Roberts and Ross [see Eq. (1) of Ref. 29] showed that real transitions dominate in atom-rigid rotor collisions.

Returning to Table I, the large difference between columns 8 and 11 (like the large difference

between columns 3 and 6) shows that real competition effects involving only the 1s and 2s states are also important.

Table II gives the collision strengths

$$\Omega^l(1s, 2s) = (k_1^2/\pi) Q_{12}^l \quad (13)$$

for two partial waves. These results illustrate the well-known fact that the unitarization procedures are most important for the lowest partial waves. They also show that the correction for back coupling becomes small with increasing  $l$  faster than the correction for competition. Figure 1 shows differential cross sections. The Born, unitarized Born, and  $2 \times 2$  matrix calculation in the four-state close-coupling approximation do not show the increased forward scattering caused by interaction with the  $2p$  state. This increased forward scattering is shown by the full close-coupling approximation. This polarization effect requires further study. The difference in large angle scattering between the close-coupling approximation and the unitarized approximations is due to exchange and distortion. The IV and V method results show that back coupling alone makes only a small change in the Born differential cross sections.

#### IV. CONCLUSIONS

Two methods for forcing approximate cross sections for inelastic scattering to satisfy the requirements of conservation of particle flux and time-reversal invariance may be useful in calculations. Generalizations of these methods may also be used to simplify scattering calculations.

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#### APPENDIX

The general solution of a  $2 \times 2$  subblock of (4) is easily obtained. Let  $R_{12} = R_{21}$  and  $U = R_{12}^2 - R_{11}R_{22}$ . Then

$$T_{ii} = \frac{2U - 2iR_{ii}}{1 + U - i(R_{11} + R_{22})}, \quad i = 1, 2$$

$$T_{21} = \frac{-2iR_{21}}{1 + U - i(R_{11} + R_{22})}.$$

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