PHYSICAL REVIEW A VOLUME 22, NUMBER 2 AUGUST 1980

Continuum in the atomic optical model

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(Received 12 December 1979)

The optical potential in principle gives a complete description of the effect of the target continuum on an electron-scattering problem truncated to a discrete set of channels. A momentum-space form for the optical potential has been derived and computed for the continuum in various approximations for the case of hydrogen. The total ionization cross section is excellently reproduced in the weak-coupling approximation above 100 eV by the most detailed model, and is tolerable as low as 50 eV.

I. INTRODUCTION

Current theories of atomic reactions initiated by electrons[1] may be described in terms of the Feshbach[2] projection operator formalism. The space of reaction channels is divided into two complementary subspaces by means of projection operators P and Q. P space consists of a finite set of discrete channels, including the entrance channel in which the target is in its ground state. The remaining channels, including the continuum, comprise Q space.

In practice a discrete set of coupled equations can be treated numerically by the close-coupling method. P space is defined to be the set of channels treated in this way. Computational methods differ in their treatment of the channels in Q space, most difficulty being caused by the continuum.

The pseudostate method[1] represents Q space by a finite set of discrete pseudostates at excitation energies higher than those associated with P space. In the close-coupling calculation, it is found that the description of scattering involving channels whose energies are much lower than those of the pseudostates is a considerable improvement over the situation where only a physical P space is used. The reason is that flux which physically goes into Q space is absorbed in the calculation by the pseudostates. The drawback of the method is that it cannot adequately represent scattering at energies near those of the pseudostates where, for example, pseudoresonances and pseudothresholds occur.

The optical potential method[1] is formally an exact treatment of scattering involving only the P-space channels. The projected Schrödinger equation for Q space is formally solved and its solution included with the potentials coupling the P-space channels i and j to give an optical potential matrix $V_{ij}^{(Q)}$.

The optical potential has most often been calculated only for elastic scattering. In this case P space consists only of the entrance channel $i=0$. The optical potential consists of a first-order static-exchange potential and a complex polarization term describing real and virtual excitations of Q space.

The data that must be described by the ground-state optical potential $V_{00}^{(Q)}$ are elastic differential cross sections and spin polarizations and the total reaction cross section $\sigma_R^{(Q)}$, i.e., the total cross section for excitation into Q space.

The simplest *ab initio* optical potential is obtained by making the closure approximation for the target states.[3] It is necessary to approximate Q-space eigenvalues by a closure energy which is treated as a parameter. It is not a free parameter, since it may be chosen so that the long-range real polarization potential approximates the dipole form, which can be calculated.

The purpose of the present work is to consider the continuum in much more detail. In order to go further than the closure approximation, it is necessary to make a specific model for the structure of the target states. We understand the structure in terms of an independent-particle-model representation based on target Hartree-Fock orbitals. Final states may be described in terms of configuration interaction which splits the states given by the single-particle excitation model. The $(e,2e)$ reaction[4] has shown that the splittings are usually confined to a range less than 10 eV from the corresponding Hartree-Fock single-particle values, for continuum excitations of reasonably high energy. Therefore, all the excitation strength is given by the independent-particle model in such cases, and we are justified in using it for considerations of the total ionization cross section. This is what we will be concerned with in the present work.

In the independent-particle model, excitations are given by a three-body problem involving the incident electron, one target electron, and an inert core. The principles of the reaction are therefore illustrated by considering the case of a hydrogen-atom target. We will confine our discussion to hydrogen.

In the case of hydrogen, the validity of the weak-coupling approximation has been demonstrated by McCarthy and McDowell.[5] In this approximation the total reaction cross section obtained from a one-channel calculation with an optical potential $V_{00}^{(Q)}$ is equal to the cross section for exciting states in Q space. We are interested in investigating the continuum part of the optical potential and therefore choose Q to be the space of ionized target states. The measurable quantity that we calculate is the total ionization cross section $\sigma_R^{(Q)} = \sigma_I$.

The present work uses a formulation and computational technique that is entirely new in the field. The optical potential is formulated in momentum space. It takes the form of an integral over all possible final states in Q space of an integrand, which is essentially the product of two three-body excitation amplitudes, each with the same final state in Q space. It is of course impossible to calculate three-body amplitudes with Coulomb forces exactly. The approximation used for the three-body amplitude characterizes the optical potential.

The momentum-space formulation has the great computational advantage that the three-body amplitudes are smooth functions of the momentum coordinates and can be written completely in terms of elementary functions. We can thus use multidimensional integration and avoid partial-wave expansions in the evaluation of the potential. The method can be generalized to target systems larger than hydrogen with not too much greater numerical effort, and of course is equally effective at very high energy.

The object of this work is to find an approximation to the optical potential which involves the minimum numerical effort and which reproduces the experimental values of the total ionization cross section with reasonable accuracy. We take success in this as an indication that our treatment of the continuum is correct. Once a correct treatment of the continuum has been achieved, the continuum contribution to the potential may be added to the potential used in standard methods of calculating elastic and inelastic scattering.

Since the potential is calculated in momentum space, calculation of the total reaction cross section is done by solving the Lippmann-Schwinger integral equation in partial-wave form. We show that the reaction cross section in an approximation with incident plane waves is proportional to the diagonal optical potential in momentum space. This gives us an approximation which is accurate for high partial waves and enables the partial-wave expansion to be cut off at a manageably small number.

Comparisons are made with a calculation of the optical potential for ionization by Alton, Garrett, Reeves, and Turner,[6] who used a coordinate-space method in the approximation of a plane-wave propagator.

In Sec. II we formulate the optical potentials. In Sec. III we relate the present calculation of the total ionization cross section to the more conventional method of integrating kinematically complete differential cross sections over phase space. The equivalent local approximation for the optical potential is discussed in Sec. IV. This is used to reduce the magnitude of the computation. In Secs. V and VI we discuss different approximations for the ionization amplitude and their effects on the total ionization cross section. Section VII gives examples of the imaginary potential in coordinate space. In order to enable the reader to follow the methods, some computational details are given in the Appendix.

II. THE OPTICAL MODEL

We consider the optical model for a hydrogen-atom target, which is typical of the three-body system that is considered when making the independent-particle model for a larger target. Hydrogen has the computational advantage that some relevant functions are known in closed form. We use the momentum representation and atomic units throughout our discussion, and neglect the kinetic energy of the heavy nucleus.

The Hamiltonian for the electron-hydrogen system is

$$H = K_1 + K_2 + v_1 + v_2 + v_3 , \tag{1}$$

where K and v stand for kinetic energy and potential operators, respectively. Since we are not interested in three-body rearrangements, it is simpler not to use the cyclic notation usual in the three-body problem. The potentials v_1 and v_2 act in the two-body subsystems defined by electrons 1 and 2 and the nucleus. The interelectron Coulomb potential is v_3. We first consider operators governing the scattering. One does not consider antisymmetry at this stage. Antisymmetry is introduced by using properly normalized antisymmetric state vectors in matrix elements of the symmetric operators.[7]

The reaction channels j are labeled by the hydrogen-atom functions $\phi_j(\vec{p})$:

$$(\epsilon_j - K_2 - v_2)\phi_j = 0 . \tag{2}$$

We think of electron 2 as the initially bound target electron, although the operator formalism must be made symmetric in the labels 1 and 2. For convenience of notation, we sometimes use discrete notation j for continuum target states $\chi^{(-)}(\vec{k}_2)$. Integrations over k_2 are then denoted by $\sum_j$.

The definition of the optical potential $V_{ij}^{(Q)}(\vec{q}',\vec{q})$ for transitions within P space is understood in terms of an operator notation. The three-body Schrödinger equation is written as

$$E-K=v\,, \tag{3}$$

where we make the approximation that the nucleus is infinitely massive:

$$K=K_1+K_2\,, \tag{4}$$

$$v=v_1+v_2+v_3\,. \tag{5}$$

The operators operate on the three-body wave function $|\Psi\rangle$. By using the projection operators

$$P=\sum_{i\in P}|\phi_i\rangle\langle\phi_i|\,, \tag{6}$$

$$Q=1-P\,, \tag{7}$$

we separate the total Schrödinger equation (3) into two projected equations

$$P(E-K-v)P=PvQ\,, \tag{8}$$

$$Q(E-K-v)Q=QvP\,. \tag{9}$$

Solving (9) and substituting in (8) we have

$$P(E-K-V^{(Q)})P=0\,, \tag{10}$$

where

$$V^{(Q)}=v+vQ[1/Q(E^{(+)}-K-v)Q]Qv\,. \tag{11}$$

The potential v_2 does not connect P and Q spaces. We therefore have

$$PvQ=P(v_1+v_3)Q\,. \tag{12}$$

It is necessary to discuss the full three-body Green's function of (11) in more detail. First we make a spectral representation[8] and use the property $Q^2=Q$:

$$\frac{1}{Q(E^{(+)}-K-v)Q}=Q\sum_n|\Psi_n^{(-)}\rangle\frac{1}{E^{(+)}-E_n}\langle\Psi_n^{(-)}|Q\,. \tag{13}$$

The spectral index n is a discrete notation for the continuum. It defines the asymptotic partition of the three-body system into bound or ionized states and specifies the quantum numbers and momenta within each partition.

We make the approximation that the Green's function is diagonal in Q space. The minimum requirement for this is that v_3 be diagonal in Q space, as it is, for example, if the state vectors of Q space are plane waves.

The optical potential is now written explicitly as an operator in three-body space (defined by the momentum coordinates of particles 1 and 2):

$$V^{(Q)}=v_1+v_3+\sum_n\sum_{m\in Q}(v_1+v_3)|\phi_m\rangle\langle\phi_m|\Psi_n^{(-)}\rangle(E^{(+)}-E_n)^{-1}\langle\Psi_n^{(-)}|\phi_m\rangle\langle\phi_m|(v_1+v_3)\,. \tag{14}$$

The problem of scattering involving only transitions within P space is reduced to the solution of the P-space equation (10), which may be expanded in the usual discrete close-coupling expansion using channels restricted to P space. For incident energy E_0 and momentum K we have

$$(E^{(+)}-K_1)f_i(\vec{K},\vec{q})=\int d^3q'\sum_j v_{ij}^{(Q)}(\vec{q}',\vec{q})f_j(\vec{K},\vec{q}')\,,\qquad i,j\in P\,. \tag{15}$$

The momentum-space representation $V_{ij}^{(Q)}$ for the potential connecting channels i and j in P space is

$$V_{ij}^{(Q)}(\vec{q}',\vec{q})=\langle\vec{q}',\phi_i|V^{(Q)}|\phi_j,\vec{q}\rangle\,,\quad i,j\in P\,. \tag{16}$$

Equations (14) and (16) display the dependence of the momentum representation of the optical potential on the amplitude F_{ki} for the excitation of the three-body channel k ($\equiv mn$), starting from the three-body channel $|\phi_i,\vec{q}\rangle$:

$$F_{ki}=\langle\Psi_n^{(-)}|\phi_m\rangle\langle\phi_m|v_1+v_3|\phi_i,\vec{q}\rangle\,. \tag{17}$$

We may think of the partial overlap $\langle\phi_m|\Psi_n^{(-)}\rangle$ as a distorted wave in the space of electron 1 and write

$$\langle\phi_m|\Psi_n^{(-)}\rangle\equiv|\chi_k^{(-)}\rangle\,. \tag{18}$$

If v_3 is completely excluded from the Green's function (11), then $\chi_k^{(-)}$ is simply an eigenstate of K_1+v_1 with ingoing-spherical-wave boundary conditions. However, the retention of the part of v_3 diagonal in Q space allows us to make screening arguments for approximations used later.

Singlet and triplet contributions to the optical potential with neglect of spin-orbit coupling are introduced first by adding the term corresponding to (14) for the optical potential with particle labels 1 and 2 reversed so as to obtain the symmetric optical potential operator $V_{\text{sym}}^{(0)}$. Writing particle 1 on the right of a three-body state vector, we calculate singlet and triplet potentials, respectively, by using the matrix elements

$$V^{(Q)}_{ijS/T}(\vec{q}\,',\vec{q}) = \tfrac{1}{2}(\langle \vec{q}\,', \phi_i | \pm \langle \phi_i, \vec{q}\,' |) V^{(Q)}_{\mathrm{sym}}(| \phi_j, \vec{q}\rangle \pm | \vec{q}, \phi_j\rangle) . \quad (19)$$

We continue to use the unsymmetric form in order to simplify the discussion. The operations described by (19) are represented by the antisymmetrization operator A.

III. THE WEAK-COUPLING APPROXIMATION

The weak-coupling approximation neglects off-diagonal optical potentials in the entrance-channel equation of the set (15). This decouples the entrance-channel equation from the remainder. We write it as

$$(E^{(+)} - K_1) f_0(\vec{K},\vec{q}) = \int d^3q' V^{(Q)}_{00}(\vec{q}\,',\vec{q}) f_0(\vec{K},\vec{q}\,') . \quad (20)$$

From this equation we can calculate complex phase shifts $\delta^{(Q)}_l$ and a reaction cross section for Q space:

$$\sigma^{(Q)}_R = (\pi/K^2) \sum_l (2l+1)[1 - |\exp(2i\delta^{(Q)}_l)|^2] . \quad (21)$$

The total nonelastic cross section for P and Q spaces is

$$\sigma_R = \sigma^{(Q)}_R + \sum_{i \in P} \sigma^{(i)}_R , \quad (22)$$

where $\sigma^{(i)}_R$ is the cross section for exciting the discrete channel i.

The central role in the weak-coupling approximation is played by the entrance-channel equation (20). We separate the ground-state optical potential into first- and second-order terms

$$V^{(Q)}_{00} = V_1 + V_2 ,$$

$$V_1(\vec{q}\,',\vec{q}) = A\langle \vec{q}\,', \phi_0 | v_1 + v_3 | \phi_0, \vec{q}\rangle , \quad (23)$$

$$V_2(\vec{q}\,',\vec{q}) = A \sum_k F^*_{0k}(\vec{q}\,')[1/(E^{(+)} - E_k)] F_{k0}(\vec{q}) , \quad k \in Q ,$$

where we have used the transition amplitudes F_{k0} defined by (19).

Using the distorted-wave notation (18), the second-order potential becomes

$$V_2(\vec{q}\,',\vec{q}) = A \sum_k \langle \vec{q}\,', \phi_0 | v_1 + v_3 | \phi_k, \chi^{(-)}_k\rangle [1/(E^{(+)} - E_k)] \langle \chi^{(-)}_k, \phi_k | v_1 + v_3 | \phi_0, \vec{q}\rangle , \quad k \in Q . \quad (24)$$

The first-order potential is the static-exchange potential. The second-order term V_2 is conveniently separated into Hermitian and anti-Hermitian parts:

$$V_2 = -U - iW , \quad (25)$$

where U and W contain the real and imaginary parts of the Green's function, respectively. The Hermitian property of W, for example, is expressed by

$$W(\vec{q}\,',\vec{q}) = W^*(\vec{q},\vec{q}\,') . \quad (26)$$

U is the real polarization term involving virtual (off-energy-shell) excitations into Q space. W is the absorptive term involving on-shell excitations. In fact, the projection operator for discrete states is real, so that U and W are both seen to be real by subtraction from the closure sum.

Absorption from the entrance channel is understood in terms of the divergence of the probability flux $j(\vec{r})$. This is a coordinate-space concept. We discuss it in terms of the coordinate-space analog of the entrance-channel equation (20):

$$(\nabla^2 + K^2) f_0(\vec{K},\vec{r}) = 2 \int d^3r' [U(\vec{r}\,',\vec{r}) + iW(\vec{r}\,',\vec{r})] \times f_0(\vec{K},\vec{r}\,') . \quad (27)$$

The total reaction cross section $\sigma^{(Q)}_R$ is the integral over all space of the divergence of the flux, divided by the incident flux K.

$$\sigma^{(Q)}_R = K^{-1} \int d^3r \vec{\nabla} (2i)^{-1} [f^*_0(\vec{K},\vec{r}) \vec{\nabla} f_0(\vec{K},\vec{r}) - f_0(\vec{K},\vec{r}) \vec{\nabla} f^*_0(\vec{K},\vec{r})] . \quad (28)$$

Substituting from (27) and using the Hermitian property (26), we find

$$\sigma^{(Q)}_R = (2/K)(2\pi)^3 \langle f_0(\vec{K}) | W | f_0(\vec{K})\rangle . \quad (29)$$

Equation (29) is combined with the anti-Hermitian part of the weak-coupling optical potential (24) to give an approximate sum rule, valid in the weak-coupling limit. The sum rule is similar to one derived by Coulter[9] under somewhat more restricted approximations:

$$\sigma^{(Q)}_R = \sum_k \sigma^{(k)}_R , \quad k \in Q \quad (30)$$

where the partial reaction cross section $\sigma^{(k)}_R$ for channel $k \in Q$ is given by

$$\sigma^{(k)}_R = K^{-1}(2\pi)^4 A \langle f_0(\vec{K}), \phi_0 | v_1 + v_3 | \phi_k, \chi^{(-)}_k\rangle \times \langle \chi^{(-)}_k, \phi_k | v_1 + v_3 | \phi_0, f_0(\vec{K})\rangle , \quad E_k = E . \quad (31)$$

Note that with the discrete channel notation k, $\sigma^{(k)}_R$ is a differential cross section in the kinematic variables of 1 and 2 electrons in the cases of bound and ionized target states, respectively.

The amplitudes in (31) are the distorted-wave Born approximation to the amplitudes for excitation of channel k. In fact, $\sigma_R^{(k)}$ is the distorted-wave Born approximation to the cross section for exciting the channel k.

The importance of the sum rule is that cross sections for excitation of parts of Q space are given by the reaction cross section calculated from the entrance-channel equation using an optical potential with the projection operator corresponding to the same part of Q space.

The sum rule has been tested by McCarthy and McDowell,[5] who used a phenomenological imaginary potential chosen to give the experimental value of the total reaction cross section in a close-coupling calculation where P space consisted of the n channels of lowest excitation energy. The close-coupling value of $\sigma_R^{(Q)}$ agreed with the weak-coupling value within about 5% at energies ranging from 30 to 200 eV for $n=3$.

IV. THE EQUIVALENT LOCAL APPROXIMATION

The potential V_2 and the exchange term of V_1 are nonlocal. Computationally this complicates the elastic scattering problem in coordinate space, because the Schrödinger equation becomes an integrodifferential equation. For this reason, there have been several attempts to approximate nonlocal potentials in atomic scattering by an equivalent local potential, and thus reduce the Schrödinger equation to the standard differential equation. For example, the equivalent local potential of Furness and McCarthy[10] is obtained by replacing the gradient operator in a Taylor expansion of $f_0(\vec{K},\vec{r}\,')$ about $\vec{r}$ by the self-consistent local value of the momentum. It gives very satisfactory results for the exchange term of V_1. We call this the self-consistent-local (SCL) approximation and generalize the concept to describe the potential V_2, in addition.

Since our approach and calculations are based on the momentum representation, we first derive the representation of the equivalent local potential in momentum space. In operator notation the equivalent local potential[10] has the form

$$V_{\text{local}}(\vec{r}) = (2\pi)^3 \langle \vec{K}\,|\,\vec{r}\rangle \langle \vec{r}\,|\,V\,|\,\vec{K}\rangle\,, \tag{32}$$

where V on the right-hand side is the exact nonlocal potential and the matrix element is taken in a conjugate representation of coordinate and momentum space. Regarded as an operator, we have for V_{local}

$$\langle \vec{r}\,|\,V_{\text{local}}\,|\,\vec{r}\,'\rangle = V_{\text{local}}(\vec{r})\,\delta(\vec{r}\,'-\vec{r})\,, \tag{33}$$

and on taking the Fourier transform, the momentum-space representation of the equivalent local potential becomes

$$\langle \vec{q}\,'\,|\,V_{\text{local}}\,|\,\vec{q}\rangle = \langle \vec{q}-\vec{q}\,'+\vec{K}\,|\,V\,|\,\vec{K}\rangle\,. \tag{34}$$

It is clear from (34) that the potential is a function of $\vec{q}-\vec{q}\,'$, so we write the momentum-space matrix element as $V_{\text{local}}(\vec{q}-\vec{q}\,')$.

Since the exact potential $\langle \vec{q}\,'\,|\,V\,|\,\vec{q}\rangle$ depends only on $\vec{q}\,'$, $\vec{q}$, and $\vec{q}\,'\cdot\vec{q}$, apart from the energy dependence of $K=(2E_0)^{1/2}$, V_{local} is a function only of P and u, where

$$\begin{aligned} \vec{P} &= \vec{q}-\vec{q}\,'\,,\\ u &= \vec{P}\cdot\vec{K}/PK\,. \end{aligned} \tag{35}$$

Thus we may expand V_{local} in a multipole expansion in u:

$$V_{\text{local}}(\vec{P}) = \sum_{\lambda} V^{(\lambda)}(P)\,P_{\lambda}(u)\,. \tag{36}$$

The equivalent local potential (34), defined for a general potential, lacks one important property of the optical potential, namely the symmetry under interchange of $\vec{q}$ and $\vec{q}\,'$. If we impose this additional constraint, odd multipoles vanish:

$$V^{(\lambda)}(P) = \begin{cases} \frac{1}{2}\displaystyle\int_{-1}^{1} du\,(2\lambda+1)\,V_{\text{local}}(\vec{P})\,P_{\lambda}(u)\,, & \lambda \text{ even}\\ 0\,, & \lambda \text{ odd}\,. \end{cases} \tag{37}$$

The term $V^{(0)}(P)$ is local and central and one would hope that it would be by far the major contribution to V_{local}. The approximation $V_{\text{local}}=V^{(0)}$ can be tested for the static-exchange potential by comparing the singlet and triplet phase shifts for hydrogen using this approximation with the exact phase shifts calculated by Vanderpoorten.[11] This comparison is made in Table I together with the SCL phase shifts for $E=50$ and 100 eV.

We are encouraged by these results to use the approximation $V_2^{(0)}$ for the second-order potential V_2. The contribution of the higher even multipoles in the expansion (36) was tested by adding $V_2^{(2)}$ to $V_2^{(0)}$ and solving the Lippmann-Schwinger equation for the resulting momentum-space potential. This was done at 40 eV using the Born approximation for F_{k0} in the case where Q projects onto the continuum. Addition of the quadrupole term had a negligible effect. The effect will be smaller at higher energies.

The purpose of using the equivalent local potential is to reduce the magnitude of the numerical computation. This becomes particularly important in the case of $\langle \vec{q}\,'\,|\,V_2\,|\,\vec{q}\rangle$, whose calculation is quite time consuming. The saving in the case of the solution of the Lippmann-Schwinger equation is in the number of matrix elements of V_2 that must be calculated. For the exact nonlocal potential, the solution requires a knowledge of $\langle \vec{q}'|V|\vec{q}\rangle$ for arbitrary q, $|\vec{q}-\vec{q}'|$, and u. The equivalent local central potential $V^{(0)}$ is completely specified as a function of the single variable $P=|\vec{q}-\vec{q}'|$ at a given incident energy. This is true also for the higher multipoles (37).

V. CALCULATION OF IONIZATION CROSS SECTIONS

As our first application of the optical model, we consider Q space to be the space I of ionized channels. The optical potential V_2, making the equivalent local and weak-coupling approximations, is

$$V_2(P)=\tfrac{1}{2}\int_{-1}^{1}du\int d^3q''\int d^3p''A\langle \vec{K}+\vec{P},\phi_0|v_3|\chi^{(-)}(\vec{p}'')\chi^{(-)}(\vec{q}'')\rangle \frac{1}{E^{(+)}-\frac{1}{2}(q''^2+p''^2)}\langle \chi^{(-)}(\vec{q}'')\chi^{(-)}(\vec{p}'')|v_3|\phi_0,\vec{K}\rangle . \tag{38}$$

We have dropped the terms in v_1 from the ionization amplitudes. They correspond to heavy-particle knockout, which is a minor effect.[12]

Compared with the direct part of V_1, the real part of V_2 is insignificant for the calculation of the ionization cross section σ_I. We have therefore computed only the imaginary part $W(P)$ of (38). Since the exchange term of V_1 makes less than 1% difference to σ_I, it too is omitted.

We are able to find analytic approximations (discussed in Sec. VI) for the amplitudes. The calculation of W thus involves a six-dimensional integral, which is computed directly using the Monte Carlo integration method of Lepage.[13] The technical details are discussed in the Appendix. For $P<2$, we normally require the standard error estimate to be less than 1% of the potential value. For higher P we allow up to 3%.

The total ionization cross section σ_I has been calculated in two basic approximations involving the optical potential $W(P)$. The simplest is the incident plane-wave approximation which comes from approximating the entrance-channel distorted wave $f_0(\vec{K})$ in (29) by a plane wave:

$$\sigma_I^B=(2/K)(2\pi)^3W(0). \tag{39}$$

The use of the full optical potential in the approximation V_1-iW, where V_1 is the static real potential and $-W$ is the imaginary part of $V_2(P)$ given by (38), is equivalent to using the full entrance-channel function $f_0(\vec{K})$ in (29). The total ionization cross section is computed by (21) using phase shifts derived from the solution of the Lippmann-Schwinger equation for the partial wave l. For large enough l the partial-wave contribution to the reaction cross section is negligibly different from the unitarized Born approximation, given by neglecting the real part of the free-particle Green's function. In turn for some larger $l=l_{\max}$, the unitarized Born approximation is sufficiently close to the partial-wave contribution to (39) [denoted by $\sigma_I(l)$], to enable one to compute the contribution of all higher partial waves by means of the identity

$$\begin{aligned}\sigma_I(l>l_{\max})&=\sum_{l>l_{\max}}(2l+1)\sigma_I^B(l)\\&=\sigma_I^B-\sum_{0\le l\le l_{\max}}(2l+1)\sigma_I^B(l).\end{aligned} \tag{39'}$$

TABLE I. The first-order approximation for electron-hydrogen phase shifts. The exact (EX) and self-consistent local (SCL) values were obtained by Vanderpoorten (Ref. 11). The column headed $V_1^{(0)}$ gives the results of the spherical approximation in momentum space.

Case	l	EX	SCL	$V_1^{(0)}$
100 eV singlet	0	0.532	0.539	0.51
	1	0.187	0.193	0.179
	2	0.0796	0.0809	0.077
	3	0.0364	0.0365	0.036
100 eV triplet	0	0.667	0.662	0.69
	1	0.302	0.297	0.31
	2	0.145	0.144	0.149
	3	0.0712	0.0711	0.072
50 eV singlet	0	0.541	0.547	0.44
	1	0.0953	0.109	0.077
	2	0.0275	0.0277	0.021
	3	0.00898	0.00797	0.0087
50 eV triplet	0	0.854	0.838	0.95
	1	0.334	0.321	0.37
	2	0.124	0.123	0.135
	3	0.04663	0.0474	0.048

The ionization cross section for hydrogen has previously been computed by Alton *et al.*[6] using an optical potential calculated from the free-particle propagator with no exchange contribution and by Coulter and Garrett[14] who added first-order exchange to this approximation. The results of Alton *et al.* are given in the column headed AGRT in Table II.

VI. DIFFERENT APPROXIMATIONS FOR THE IONIZATION CROSS SECTION

The approximations used in the present calculation are characterized by the approximations used for the ionization amplitudes in (38). They are restricted to approximations in which one of the distorted waves in the projector is represented by a plane wave. There is no difficulty in principle in using more detailed distorted waves, but computing time is reduced considerably since the plane wave in momentum space is a delta function. The other

TABLE II. The ionization cross section for hydrogen in units πa_0^2. The column headed Born contains the Born approximation. The next four columns are the results of optical-model calculations with different projectors described in the text. Experimental data in the last column are centered on the data of Fite and Brackmann (Ref. 15) with error estimates provided by Teubner (Ref. 16).

E(eV)	Born	DB	AGRT	SB	OBO	Expt.
20	0.61	0.62	0.56	0.45		0.33 ± 0.08
40	1.21	1.18	1.15	0.97	0.88	0.68 ± 0.17
60	1.10	1.07	1.04	0.96	0.88	0.75 ± 0.18
80	0.96	0.94	0.87	0.86	0.80	0.72 ± 0.17
100	0.85	0.83	0.72	0.77	0.72	0.68 ± 0.16
150	0.64	0.62	0.56	0.60	0.57	0.57 ± 0.13
200	0.52	0.51	0.48	0.49	0.46	0.49 ± 0.11
300	0.37	0.37		0.37	0.34	0.37 ± 0.08
500	0.25	0.25		0.25	0.23	0.24 ± 0.04

distorted wave is represented by a Coulomb wave with unit charge. All approximations make use of analytic expression for the Coulomb transform of the hydrogen-atom ground state:

$$\int d^3p\langle \chi^{(-)}(\vec{k})|\vec{q}+\vec{p}\rangle\langle\vec{p}|\phi_0\rangle$$

$$=\pi^{-1/2}\int d^3r e^{-\eta r}e^{-i\vec{q}\cdot\vec{r}}\chi^{(+)}(\vec{k},\vec{r})$$

$$=\pi 2^{3/2}\langle\vec{q}|\chi^{(+)}(\vec{k}),\eta\rangle\,,\qquad \eta=1 \tag{40}$$

where

$$\langle\vec{q}|\chi^{(+)}(\vec{k}),\eta\rangle=-\pi^{-2}\Gamma(1-i\nu)e^{\pi\nu/2}$$
$$\times\left(\frac{-\nu(k+i\eta)}{A}+\frac{\eta(-1+i\nu)}{B}\right)\frac{1}{B}\left(\frac{A}{B}\right)^{-i\nu},$$

$$A=q^2-(k+i\eta)^2\,,$$
$$B=|\vec{q}-\vec{k}|^2+\eta^2\,,$$
$$\nu=1/k\,. \tag{41}$$

A. Direct Born (DB)

In this approximation $\chi^{(-)}(\vec{q}'')$ is a plane wave, $\chi^{(-)}(\vec{p}'')$ is a Coulomb wave for charge 1. Exchange terms in (38) are omitted. This approximation is not expected to give a very realistic reaction cross section, but it is interesting from the point of view of obtaining an independent check of our numerical analysis.

The DB value of the optical potential W at $P=0$ is

$$W(0)=\pi\int d^3q''\int d^3p''\langle\vec{K},\phi_0|v_3|\chi^{(-)}(\vec{p}''),\vec{q}''\rangle$$
$$\times\delta[E-\tfrac{1}{2}(p''^2+q''^2)]$$
$$\times\langle\vec{q}'',\chi^{(-)}(\vec{p}'')|v_3|\phi_0,\vec{K}\rangle\,, \tag{42}$$

which is the usual Born approximation for σ_I. Our calculation of σ_I in the Born approximation agrees with the parabolic-coordinate calculation of Omidvar and Sullivan[17] within less than 1% at all energies from 20 to 200 eV. The results are given in the column of Table II headed Born.

The results for σ_I using the DB optical model phase shifts are shown in the column of Table II headed DB. Even at low energies they are quite close to the incident-plane-wave approximation (Born), indicating that the plane-wave approximation for the wave function of an electron incident on a hydrogen atom is quite good in distorted-wave approximations for reactions.

For energies less than 100 eV, the DB ionization cross section is not very close to the experimental values. This indicates either that the distorted-wave (weak-coupling) approximation is not good for the ionization amplitudes, or that the direct Born approximation is insufficient to represent the antisymmetrized final state.

A similar conclusion can be drawn from the results of Alton *et al.* who have solved the full integro-differential Schrödinger equation. Considering the different method of solution and our use of an equivalent local potential, the results are in reasonable agreement, although their cross sections are slightly lower with the largest difference occurring for energies above 80 eV. It seems possible that this discrepancy may be due to the inclusion of too few partial waves in their calculation at higher energies.

B. Symmetric Born (SB)

The simplest way of taking second-order exchange into account is a semiclassical method in which the faster of the two outgoing electrons is represented in (38) by a plane wave, but the on-shell energy integration for the imaginary potential is cut off at $E/2$. The incident-plane-wave approximation (39) for this model gives much better results than the Born approximation for lower energies.[18]

The full SB optical model is a considerable improvement over DB below 200 eV.

C. Orthogonalized Born-Oppenheimer (OBO)

This is the most complete model that can be made within the distorted-wave approximation taking into account the computational restriction that a plane wave must be used for one of the distorted waves in the projector of (38).

The full Coulomb wave is used for the slower of the two electrons. The faster of the two electrons is represented by a plane wave orthogonalized to the ground state of hydrogen. This partially fulfills the requirement that P space and Q space must be orthogonal. Antisymmetry is approximately taken into account within the plane-wave restriction by using the peaking approximation of Ochkur.[19]

The approximation contains elements of the screening effect mentioned in the discussion of Eq. (18). The presence of the potential v_3 considerably reduces the effect of the nuclear charge on the wave function of the faster electron. The direct amplitude D in the OBO approximation is

$$\begin{aligned} D(\vec{q}\,',\vec{p}\,'',\vec{q}\,'') &= \int d^3p'\, v_3(|\vec{q}\,'-\vec{q}\,''|)[\langle\phi_0|\vec{p}\,'\rangle\langle\vec{p}\,'+\vec{q}\,'-\vec{q}\,''|\chi^{(-)}(\vec{p}\,'')\rangle],\; q''p'' \\ &= \int d^3p' \int d^3q_1 \int d^3p_1 \langle\phi_0|\vec{p}\,'\rangle v_3(|\vec{q}\,'-\vec{q}_1|)\delta(\vec{p}_1-\vec{q}\,'-\vec{p}\,'+\vec{q}_1) \\ &\quad\times[\langle\vec{p}_1|\vec{p}\,''\rangle\langle\vec{q}_1|\chi^{(-)}(\vec{q}\,'')-\langle\vec{p}_1|\phi_0\rangle\langle\phi_0|\vec{p}\,''\rangle\langle\vec{q}_1|\chi^{(-)}(\vec{q}\,'')\rangle],\quad q''\leqslant p''. \end{aligned} \tag{43}$$

The Ochkur peaking approximation is used to reduce the $\vec{p}\,'$ integration to the form (40) for $q''\leqslant p''$. In the argument of v_3 we replace $\vec{q}_1$ by $\vec{q}\,''$, to obtain

$$\begin{aligned} D(\vec{q}\,',\vec{p}\,'',\vec{q}\,'') &= v_3(|\vec{q}\,'-\vec{q}\,''|)\int d^3p'\Big[\langle\phi_0|\vec{p}\,'\rangle\langle\vec{p}\,'+\vec{q}\,'-\vec{p}\,''|\chi^{(-)}(\vec{q}\,'')\rangle \\ &\quad-\langle\phi_0|\vec{p}\,''\rangle\Big(\int d^3p_1\langle\phi_0|\vec{p}\,'\rangle\langle\vec{p}\,'+\vec{q}\,'-\vec{p}_1|\chi^{(-)}(\vec{q}\,'')\rangle\langle\vec{p}_1|\phi_0\rangle\Big)\Big],\quad q''\leqslant p''. \end{aligned} \tag{44}$$

Repeated application of (40) and (41) gives an analytic expression for the integral in the orthogonality-defect term:

$$\int d^3p' \int d^3p_1\langle\phi_0|\vec{p}\,'\rangle\langle\vec{p}\,'+\vec{q}\,'-\vec{p}_1|\chi^{(-)}(\vec{q}\,'')\rangle\langle\vec{p}_1|\phi_0\rangle = (2\pi)^{1/2}\pi^2 8\langle\vec{q}\,'|\chi^{(+)}(\vec{q}\,''),2\rangle. \tag{45}$$

The exchange amplitude $E(\vec{q}\,',\vec{p}\,'',\vec{q}\,'')$ is given by interchanging $\vec{p}\,'',\vec{q}\,''$ in the direct amplitude. In the calculation we ignored the relatively small contribution to the real potential V_1 from first-order exchange and combined the singlet and triplet second-order terms to obtain for the imaginary potential

$$\begin{aligned} W(\vec{q}\,',\vec{q}) = \pi\int d^3q''\int d^3p''[&D(\vec{q}\,',\vec{p}\,'',\vec{q}\,'')^*D(\vec{q},\vec{p}\,'',\vec{q}\,'') \\ &-\tfrac{1}{2}D(\vec{q}\,',\vec{p}\,'',\vec{q}\,'')^*D(\vec{q},\vec{q}\,'',\vec{p}\,'')] \\ &\times\delta[E-\tfrac{1}{2}(q''^2+p''^2)]. \end{aligned} \tag{46}$$

The ionization cross section calculated from the OBO optical model is given in the corresponding column of Table II. It agrees well with experiment above 100 eV and is tolerable for energies as low as 50 eV, below which it is possible to estimate σ_I by the pseudostate method.[20]

It is interesting to compare direct and exchange contributions to σ_I. Since the effect of incident-wave distortion is small, they have been calculated for the OBO optical model in approximation (39). The comparison is shown in Table III. The direct to exchange ratios are within a few percent of the values measured by Alguard *et al.*[21]

VII. CHARACTERISTICS OF THE CONTINUUM IMAGINARY POTENTIAL

The imaginary potential $W(P)$ for the electron-hydrogen continuum is an extremely smooth function of the momentum coordinate P, whose shape varies little as E is varied. Its magnitude is greatest at about 80 eV. At higher energies, where all the calculated models essentially give the same value for σ_I, the shape is essentially independent of the model.

The chief usefulness of $W(P)$ is in coupled-channels calculations of electron-hydrogen reactions

TABLE III. Direct and exchange contributions to σ_I in the OBO optical model using Eq. (39), units πa_0^2.

E(eV)	40	60	80	100	150	200	300	400
Dir	1.19	1.14	1.00	0.87	0.64	0.53	0.37	0.27
Exch	0.57	0.50	0.37	0.27	0.16	0.10	0.05	0.03

starting with the ground state, where it is added to the ground-state potential to give a representation of the continuum. In principle it is necessary to calculate the potentials $V_{ij}^{(I)}$ of (16) for all channels i,j in the calculation, but since the second-order part is considerably smaller than the first-order part, it has a negligible effect in all but the 0,0 case. This has been confirmed numerically by McCarthy and McDowell,[5] who used a phenomenological imaginary potential chosen to give the correct total reaction cross section.

In coupled-channels calculations the coordinate-space representation is normally used. We have therefore transformed the OBO approximation for $W(P)$ to coordinate space and given values in Table IV suitable for interpolation for different energy and r values. Figure 1 shows the total coordinate-space imaginary potentials for 100 and 200 eV. Their shape is very close to $\exp(-r)$, which is proportional to the square root of the density, not to the density as has been assumed in phenomenological form factors.[5,10]

Figure 2 shows the effect of exchange in the 100 eV imaginary OBO second-order potential. The singlet potential is dominant up to a distance of about 1.5 a.u. At larger distances the triplet potential is of larger magnitude and longer range. The singlet and triplet potentials are relevant to close-coupling calculations of electron scattering from hydrogen.

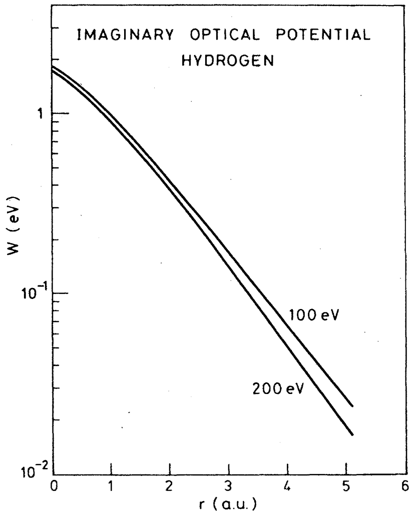

FIG. 1. The imaginary optical potential in coordinate space for 100 and 200 eV.

VIII. CONCLUSIONS

We have derived an expression [(14, (16)] for the optical potential matrix $V_{ij}^{(Q)}$ relevant to a truncation of the electron scattering problem to a discrete set P of channels. If sufficient channels are taken (in practice this means about 6 for hydrogen), the cross section for reactions to channels outside the discrete set is essentially the total ionization cross section, and we can take Q to be the ionization space I.

Since the second-order part of the optical potential is small compared to the first-order part, it is sufficient to neglect second-order parts in all but $V_{00}^{(I)}$ if we are calculating cross sections for reactions starting with the target ground state.

We have derived a local approximation $-W(P)$ in momentum space to the imaginary part of $V_{00}^{(I)}$, which for hydrogen has been calculated in various approximations. The orthogonalized Born-Oppenheimer approximation reproduces experimental total ionization cross sections very well for $E > 100$ eV, and tolerably for E as low as 50 eV. This is regarded as an excellent test of the potential.

For use in a coupled-channels calculation of electron-hydrogen reactions, it is not difficult to calculate the second-order real potential (continuum contribution to the polarization potential) and to separate the potentials into singlet and triplet parts. This has not been done for ionization cross sections since it makes little difference.

The extremely satisfactory state of affairs for electron-hydrogen scattering at intermediate energies has been brought about by the use of a completely new method. The momentum-space formu-

TABLE IV. Imaginary optical potential in coordinate space (OBO) (eV).

E(eV) \ r	0.02	0.14	0.62	1.26	2.22	3.18	4.14	5.1
40	1.69	1.61	1.23	0.72	0.29	0.117	0.048	0.021
60	1.81	1.72	1.33	0.79	0.35	0.142	0.056	0.025
80	1.92	1.82	1.39	0.81	0.36	0.141	0.061	0.025
100	1.92	1.82	1.37	0.81	0.35	0.140	0.061	0.024
150	1.84	1.74	1.29	0.76	0.33	0.126	0.047	0.0194
200	1.71	1.62	1.20	0.72	0.30	0.117	0.043	0.0168

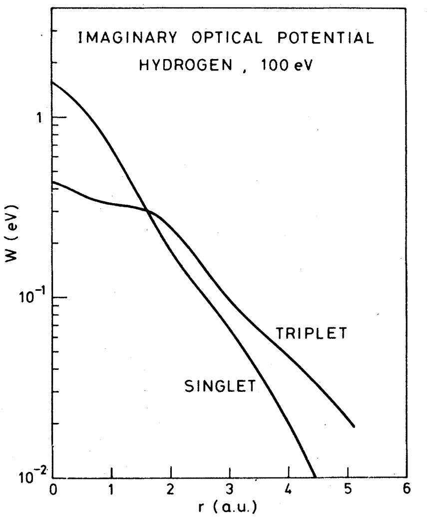

FIG. 2. The singlet and triplet imaginary optical potentials in coordinate space for 100 eV.

lation of the optical potential allows integration by the multidimensional Monte Carlo method, in which the use of Cartesian coordinates eliminates difficulties caused, for example, by two-center integrals and enables partial-wave expansions to be eliminated in the integration. The method is equally effective for targets larger than hydrogen, although the analytic integrations possible for hydrogen become rather clumsy in the general case. It is probably necessary to perform these integrations numerically. This is not a serious difficulty for the Monte Carlo method, where increased dimensionality does not cause a disastrous increase in computing time.

The most attractive possibility for nonhydrogenic targets is suggested by considering the shape of W for hydrogen. It is a very smooth function in both coordinate and momentum space with a weak dependence on the incident energy. This suggests that it may be possible to find a simple translationally invariant second-order potential, analogous to the first-order interelectron Coulomb potential, which can be folded into the density to obtain the optical potential for the continuum in the case of larger target systems. The universality of such an operator would depend on the fact, established here, that non-Coulomb distortion in the projection operator for ionization is a minor effect.

ACKNOWLEDGMENTS

We would like to acknowledge very helpful discussions with Dr. I. R. Afnan, Professor B. H. Bransden, Professor C. J. Joachain, and Dr. P. J. O. Teubner. We thank Mr. R. W. Martin for considerable help with computing and Dr. G. P. Lepage for the use of his Monte Carlo integration program VEGAS. One of us (A. T. S.) is grateful to the Australian Institute for Nuclear Science and Engineering for a research fellowship. This work was also supported by the Australian Research Grants Committee.

APPENDIX: NUMERICAL METHODS

In order to illustrate our numerical procedure, we consider the optical potential $V_2^{(0)}(P)$ for the direct Born model of Sec. VI A. Using Eqs. (38), (40), and (41) we have

$$V_2^{(0)}(P)=4\pi^2\int_{-1}^{1}du\int d^3q''\int d^3p''\langle\vec{\mathrm{K}}+\vec{\mathrm{P}}-\vec{\mathrm{q}}''|\chi^{(+)}(\vec{\mathrm{p}}''),1\rangle^{*}v_3(\vec{\mathrm{K}}+\vec{\mathrm{P}}-\vec{\mathrm{q}}'')[E^{(+)}-\tfrac{1}{2}(q''^2+p''^2)]^{-1}$$
$$\times\langle\vec{\mathrm{K}}-\vec{\mathrm{q}}''|\chi^{(+)}(\vec{\mathrm{p}}''),1\rangle\, v_3(\vec{\mathrm{K}}-\vec{\mathrm{q}}''),\qquad\text{(A1)}$$

where $|\vec{\mathrm{K}}|=(2E_0)^{1/2}$ and $v_3(\vec{\mathrm{Q}})$, the momentum-space representation of the e-e interaction, is given by

$$v_3(\vec{\mathrm{Q}})=1/2\pi^2Q^2\,.\qquad\text{(A2)}$$

The spherical symmetry inherent in the integrand suggests the use of spherical polar coordinates to evaluate the integral. In an obvious notation we write

$$V_2^{(0)}(P)=4\pi^2\int_{-1}^{1}du\int d\Omega_{q''}\int d\Omega_{p''}\int_0^\infty dq''\int_0^\infty dp''F(P,\hat{u},\hat{q}'',\hat{p}'',q'',p'')[E^{(+)}-\tfrac{1}{2}(q''^2+p''^2)]^{-1},$$

and on introducing the transformation

$$q''=r\sin\alpha\,,$$
$$p''=r\cos\alpha\,,\quad 0\leqslant\alpha\leqslant\pi/2\,,\quad r>0\,,\qquad\text{(A3)}$$

decompose the Green's function into its principal value and imaginary parts to give

$$V_2^{(0)}(P)=4\pi^2\int_{-1}^{1}du\int d\Omega_{q''}\int d\Omega_{p''}\int_0^{\pi/2}d\alpha\left(P\int_0^{\infty}r\,dr\,\frac{F(P,u,\hat{q}'',\hat{p}'',q'',p'')}{(E-\frac{1}{2}r^2)}-i\pi F(P,u,\hat{q}'',\hat{p}'',q_E'',p_E'')\right),\quad\text{(A4)}$$

where

$$\begin{aligned}q_E''&=r_E\sin\alpha\,,\\ p_E''&=r_E\cos\alpha\,,\\ r_E&=(2E)^{1/2}\,.\end{aligned}\quad\text{(A5)}$$

The function F has in general real and imaginary components, but the general requirements of Hermiticity [Eqs. (24) and (26)] for the two components of V, coupled with the local approximation, lead to the prescription that one needs only to compute the integral for the real part of F.

For the computations carried out in the present paper we have concentrated on the calculation of the imaginary part of the second-order potential. Calculation of the real part requires modification of the form given in (A4), since use of Monte Carlo multidimensional integration precludes treatment of the principal-value integral by direct integration. However by making use of the identity

$$P\int_0^{\infty}\frac{dr}{E-\frac{1}{2}r^2}=0\,,\quad\text{(A6)}$$

we can subtract out the singularity, which leads to an equivalent nonsingular representation of the real part of $V_2^{(0)}$ suitable for computation by Monte Carlo techniques:

$$\mathrm{Re}\,V_2^{(0)}(P)=4\pi^2\int_{-1}^{1}du\int d\Omega_{q''}\int d\Omega_{p''}\int_0^{\pi/2}d\alpha$$

$$\times\int_0^{\infty}dr\,\frac{rp''^2q''^2F(P,u,\hat{q}'',\hat{p}'',q'',p'')-r_Ep_E''^2q_E''^2F(p,u,\hat{q}'',\hat{p}'',q_E'',p_E'')}{E-\frac{1}{2}r^2}\,.\quad\text{(A7)}$$

The Monte Carlo integration program we used is based on an adaptive algorithm due to Lepage.[13] The integral is evaluated for a number of iterations and the adaptive feature optimizes the weighting of the integration points over successive iterations. For the numerical calculation of the imaginary second-order potential we found that about six iterations of the order of 12 000 calls to the integrand per iteration were sufficient to evaluate the six-dimensional integral to within 1 or 2 percent. The accuracy obtained depended marginally on the energy but did vary with the value of P. Attainment of the required accuracy proved most difficult in the region $1.5 < P < 2.5$ a.u. The resultant potential had a smooth dependence on P, enabling one to calculate it for a few points and to obtain all other values by interpolation. In practice the potential had become negligibly small by $P = 7$ a.u,

A technique that we found helpful in reducing the time required to calculate the potential for successive P values was to use the weighting of the integrand points from the last iteration for the previous value. This proved to be very close to the optimum choice for the computation of the potential at the next value, thus reducing the number of iterations needed to obtain the desired accuracy.

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