Coupled equations for medium-energy scattering. II. Electron and positron scattering from atomic hydrogen

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The effective-channel approach to medium-energy scattering has been formulated previously by constructing a set of coupled equations for the elastic-scattering and average inelastic-scattering channels, with the evaluation of the average fluctuation potential and the average excitation energy to be carried out by a variational procedure. The formalism is applied here to the electron and positron scattering from atomic hydrogen in the energy range 50–500 eV. The various quantities which parametrize the effective channel are explicitly calculated. An approximate solution of the coupled equations is then obtained using a set of Green's functions in the semiclassical approximation. Contributions to the elastic-scattering amplitude which arise from the static interaction and the coupling to the average inelastic-scattering channel are isolated for the purpose of ready comparison with previous calculations. The present calculation contains in effect no free adjustable parameters when the information from the total-cross-section data is incorporated into the theory through the use of the optical theorem.

I. INTRODUCTION

Scattering of electrons and positrons from composite target atoms at low energies has been the subject of intense investigations both experimentally and theoretically for the past several years, and we have now a variety of theoretical approaches which can be used to treat the effect of distortions of the target and also the exchange and rearrangement processes at these low energies. When the scattering energy is very high, e.g., above 500 eV, the first Born approximation or its slight variations seems to work reasonably well in predicting the elastic scattering, inelastic excitations, and ionization cross sections.

The theoretical situation in the medium-energy range, 50–500 eV, is less favorable, however, mainly because the effect of distortions of the target system during the collision is still substantial and yet there are very many open channels now which may be strongly coupled to the elastic channel. These make the various theoretical methods, which are applicable either at low energies or at high energies, less effective in the medium-energy region.

In the first paper[1] of this series of reports, we have discussed in detail an approach to medium-energy scattering which incorporates some of the salient ingredients of the theoretical methods developed for the other energy regions. It involves a construction of the average inelastic channel to simulate the coupling of the elastic channel to all the open and closed inelastic channels. The various parameter functions which characterize this effective channel have to be specified, and we have given in I a detailed discussion of different ways to evaluate these quantities.

Once the relevant coupled equations are specified, then the scattering amplitude is obtained by solving these equations with appropriate boundary conditions. As a fairly large number of partial waves contribute at these energies, with severe cancellations at large angles, it is desirable to solve the equations without the expansion of the scattering functions in spherical harmonics. We have described in I a simple procedure which is based on the Green's-function technique[2] in the semiclassical approximation, and the angle-averaging procedure to simplify the amplitude integrals.[3]

The theory outline in I is here applied to the scattering of electrons and positrons from atomic hydrogen. Much work has been done in the past on these systems using different techniques, such as the close-coupling,[4] Glauber approximation,[5] and eikonal distorted waves.[6] The approach we follow here is similar to that formulated by Feshbach *et al.*[7] and applied by Joachain and Mittleman[8] to the electron-helium scattering, but with the obvious improvement in that all parameter functions in the theory are explicitly calculated. Therefore, we obtain our result essentially free of any adjustable parameters, just as in the first Born approximation and in the Glauber approximation.[9]

II. THEORY

Construction of a set of coupled equations for the elastic and effective inelastic channels has

been discussed in the paper I, and we briefly summarize here those parts of the result which are relevant to the present calculation. The inelastic components of the total scattering function is represented collectively by $Q\Psi$, where

$$Q = 1 - P$$

and P is the projection operator for the target hydrogen in its ground state and thus for the elastic channel. It is defined by

$$P = |\psi_0(\vec{r})\rangle \langle \psi_0^*(\vec{r}\,')| .$$

Since we are going to neglect the exchange effect in most of the discussion, the e^+H and e^-H systems can be treated with very minor changes. Therefore, the formalism will be written out explicitly for the e^+H system for definiteness. The necessary modifications associated with the e^-H system will be indicated later. The effect of exchanges will be estimated also at a later stage. The amplitude calculation includes this effect explicitly.

The Hamiltonian for the system e^+H is then given by

$$H = T_{\vec{R}}(\vec{R}) + H_T(\vec{r}) + V(\vec{r}, \vec{R}), \tag{2.1}$$

where $\vec{R}$ and $\vec{r}$ denote the positron and electron coordinates, respectively. The target states are generated by H_T, as

$$H_T(\vec{r})\psi_n(\vec{r}) = E_n \psi_n(\vec{r}). \tag{2.2}$$

The coupled equations are derived in I from the ansatz on the total scattering function Ψ in the form

$$\Psi(\vec{r}, \vec{R}) \approx \psi_0(\vec{r}) u_0(\vec{R}) + \varphi_t(\vec{r}, \vec{R})\omega(\vec{R}), \tag{2.3}$$

where φ_t is chosen to be orthogonal to the elastic channel so that it represents the distortion of the target during the collision and thus the coupling to all the inelastic channels. The functions u_0 and ω are to be determined by solving the resulting coupled equations when (2.3) is substituted into the scattering equation and the $\vec{r}$ dependence is averaged over.

The choice of φ_t is therefore critical in obtaining a reliable estimate of the inelastic-channel contributions, and we chose the form

$$\varphi_t(\vec{r}, \vec{R}) = W_2^{-1/2}(\vec{R})[V^a(\vec{r}, \vec{R}) - \langle V^a \rangle]\psi_0(\vec{r}), \tag{2.4}$$

with

$$\int |\varphi_t(\vec{r}, \vec{R})|^2 d\vec{r} = 1. \tag{2.5}$$

In (2.4), we have chosen a slightly modified form of the potential V^a defined as

$$V = + \frac{e^2}{R} - \frac{e^2}{|\vec{r} - \vec{R}|} - \frac{e^2}{R + a} - \frac{e^2}{|\vec{r} - \vec{R}| + a} \equiv V^a(\vec{r}, \vec{R}), \tag{2.6}$$

such that some of the integrals involving V^2 and V^3 are less singular. The $W_2^{-1/2}$ factor is included in (2.4) to have φ_t properly normalized at each fixed value of $\vec{R}$. That is, from (2.5), we have

$$W_2(\vec{R}) = (\psi_0, [V^a]^2\psi_0)_{\vec{r}} - (\psi_0, V^a\psi_0)^2_{\vec{r}} \equiv \langle [V^a]^2 \rangle - \langle V^a \rangle^2 . \tag{2.7}$$

The choice (2.4) for φ_t is of course not *unique*, and we have introduced in fact one single parameter a in V^a to avoid possible difficulty with the various integrations. Furthermore, we have discussed in great detail in Ref. 1, other possible ansatz one can make to simulate the inelastic channels at medium energies. However, as the first attempt in studying the effectiveness of the formalism, we will concentrate on the choice (2.3).

A. Coupled equations

Substitution of (2.3) into the scattering equations and integrating out the $\vec{r}$ variable, we obtain[1]

$$(T_{\vec{R}} + V_{00} - E_0')u_0(\vec{R}) = - V_{0\varphi}(\vec{R})\omega(\vec{R}), \tag{2.8a}$$

$$(T_{\vec{R}} + V_{\varphi\varphi} + J_{\varphi\varphi} + \bar{E}_\varphi - E)\omega(\vec{R}) = - V_{\varphi 0} u_0(\vec{R}), \tag{2.8b}$$

where

$$V_{00}(\vec{R}) = (\psi_0, V\psi_0)_{\vec{r}}, \qquad E_0' = E - E_0, \tag{2.9}$$

and

$$V_{0\varphi} = (\psi_0, V\varphi_t)_{\vec{r}} = V^*_{\varphi 0}, \quad V_{\varphi\varphi} = (\varphi_t, V\varphi_t)_{\vec{r}}, \quad J_{\varphi\varphi} = (\varphi_t, T_{\vec{R}}\varphi_t)_{\vec{r}}, \quad \bar{E}_\varphi(\vec{R}) = (\varphi_t, H_T\varphi_T)_{\vec{r}} . \tag{2.10}$$

If we further define the quantity

$$W_3(\vec{R}) = (\psi_0, V^a V V^a \psi_0)_{\vec{r}} - 2(\psi_0, V^a\psi_0)_{\vec{r}}(\psi_0, V V^a\psi_0)_{\vec{r}} + (\psi_0, V^a\psi_0)^2_{\vec{r}}(\psi_0, V\psi_0)_{\vec{r}}, \tag{2.11}$$

then, some of the quantities in (2.10) may be rewritten in the form

$$V_{0\varphi} = V_{\varphi 0} = W_2^{1/2} \equiv V_c, \qquad V_{\varphi\varphi} = W_3/W_2, \tag{2.12}$$

and

$$\bar{E}_\varphi = Y(\vec{R})/W_2 \to \bar{E}_F, \text{ as } R \to \infty, \tag{2.13}$$

where

$$Y(\vec{R}) = (\psi_0, V^a H_T V^a \psi_0)_{\vec{r}} - E_0(\psi_0, V^a\psi_0)^2_{\vec{r}}. \tag{2.14}$$

For convenience, we define the average potential in the Q channel by

$$\bar{V}(\vec{R}) \equiv \frac{W_3 + Y}{W_2} - \bar{E}_F \equiv \bar{V}_Y + \bar{Y}, \tag{2.15}$$

where $\bar{E}_F$ is our average excitation energy. As was shown previously,[10] W_2 and W_3 are directly related to the two- and three-particle correlation functions. In the following, we will neglect the term $J_{\varphi\varphi}$, i.e., for simplicity we set

$$J_{\varphi\varphi} \approx 0. \tag{2.16}$$

With this approximation (2.16), the set (2.8) is exactly the form we have derived in Ref. 10 using a variational procedure on the operator QHQ. Thus, the equation we will consider in the present paper is

$$[T_{\vec{R}} + V_{00}(\vec{R}) - E_0'] u_0(\vec{R}) = - V_c(\vec{R}) \omega(\vec{R}), \tag{2.17a}$$

$$[T_{\vec{R}} + \bar{V}(\vec{R}) - E_F'] \omega(\vec{R}) = - V_c(\vec{R}) u_0(\vec{R}), \tag{2.17b}$$

where we set

$$E = \bar{E}_F + E_F' .$$

Instead of (2.15), we could also define $\bar{V}$ to be that derived from V, as

$$\bar{V} \approx \bar{V}_V = V_{\varphi\varphi} . \tag{2.15a}$$

The effect of the choice (2.15a) rather than (2.15) will also be studied numerically.

B. Scattering amplitude

The elastic amplitude may be calculated once the solutions u_0 and ω are obtained from (2.17). Formally,

$$u_0 = u_0^P + g_0^P V_c \omega, \tag{2.18}$$

$$\omega = g_\varphi V_c u_0, \tag{2.19}$$

where

$$(T_{\vec{R}} + V_{00} - E_0') u_0^P = 0,$$

and

$$\begin{aligned} g_0^P &= (E_0' + i\epsilon - T_{\vec{R}} - V_{00})^{-1}, \\ g_\varphi &= (E_F' + i\epsilon - T_{\vec{R}} - \bar{V})^{-1}. \end{aligned} \tag{2.20}$$

For convenience, the elastic scattering amplitude f_{el} is written as

$$f_{el} \equiv - \frac{1}{2\pi} \mathcal{T}_{el}, \tag{2.21}$$

and thus

$$\sigma(E, \Theta) = |f_{el}|^2 = |\mathcal{T}_{el}|^2 / 4\pi^2 . \tag{2.22}$$

Then, $\mathcal{T}_{el}$ is given by u_0 and ω as

$$\begin{aligned} \mathcal{T}_{el} &= (u_f^{(0)}, V_{00} u_0^P) + (u_f^{(0)}, V_{00} g_0^P V_c \omega) + (u_f^{(0)}, V_c \omega) \\ &\approx (u_f^{(0)}, V_{00} u_0^P) + (u_f^{(0)}, V_c g_\varphi V_c u_i^{(0)}) \\ &\equiv \mathcal{T}_{el}^P + \mathcal{T}_{el}^Q . \end{aligned} \tag{2.23}$$

In (2.23) we used

$$u_i^{(0)} = e^{i\vec{K}_i \cdot \vec{R}},$$

$$u_f^{(0)} = e^{i\vec{K}_f \cdot \vec{R}},$$

where $\vec{K}_i$ and $\vec{K}_f$ are the initial and final momenta of the projectile, respectively, and we have neglected all terms which involve more than one g_0^P or g_φ. This is purely an approximation at this stage in order to simplify the evaluation of $\mathcal{T}_{el}$ by not iterating. However, this is a very reasonable one in view of the high-energy projectiles which are involved here.

The separation of $\mathcal{T}_{el}$ into two parts, as has been done in (2.23), makes it very convenient in assessing the importance of the effect of the Q space which contains *all* the inelastic channels (including the exchange, pickup, and ionization channels). We may further separate out the Born term from $\mathcal{T}_{el}^P$, as

$$\begin{aligned} \mathcal{T}_{el}^P &= (u_f^{(0)}, V_{00} u_i^{(0)}) + (u_f^{(0)}, V_{00} g_0^P V_{00} u_i^{(0)}) \\ &\equiv \mathcal{T}_{el}^B + \mathcal{T}_{el}^{CP} . \end{aligned} \tag{2.24}$$

For the evaluation of $\mathcal{T}_{el}^{CP}$ and $\mathcal{T}_{el}^Q$, which involve g_0^P and g_φ, respectively, we have adopted the semiclassical form[2]

$$g_0^P(\vec{R}, \vec{R}') \approx - e^{i\kappa^P(t)s} / 2\pi s \equiv g_{0,sc}^P , \tag{2.25}$$

where

$$\kappa^P(t) = [2E_0' - 2V_{00}(t)]^{1/2}, \tag{2.26}$$

$$\vec{s} = \vec{R} - \vec{R}', \quad \vec{t} = \tfrac{1}{2}(\vec{R} + \vec{R}'); \tag{2.27}$$

and similarly,

$$g_\varphi(\vec{R}, \vec{R}') \approx - e^{i\kappa^Q(t)s} / 2\pi s \equiv g_{\varphi,sc} , \tag{2.28}$$

with

$$\kappa^Q(t) = [2E_F' - 2\bar{V}(t)]^{1/2} . \tag{2.29}$$

Thus, we have explicitly,

$$f_{el} \approx f_{el}^B + f_{el}^{CP} + f_{el}^Q , \tag{2.30}$$

where

$$f_{el}^B = - \frac{1}{q} \int_0^\infty R\, dR\, V_{00}(R) \sin qR, \tag{2.31}$$

and

$$\begin{aligned} f_{el}^{CP} = \frac{1}{4\pi^2} \int\int d\vec{s}\, d\vec{t}\, V_{00}(\vec{t} + \tfrac{1}{2}\vec{s}) V_{00}(\vec{t} - \tfrac{1}{2}\vec{s}) \\ \times e^{i\vec{q}\cdot\vec{t} - i\vec{K}_a \cdot \vec{s}} e^{i\kappa^P(t)s} / s, \end{aligned} \tag{2.32}$$

$$\begin{aligned} f_{el}^Q = \frac{1}{4\pi^2} \iint d\vec{s}\, d\vec{t}\, V_c(\vec{t} + \tfrac{1}{2}\vec{s}) V_c(\vec{t} - \tfrac{1}{2}\vec{s}) \\ \times e^{i\vec{q}\cdot\vec{t} - i\vec{K}_a \cdot \vec{s}} e^{i\kappa^Q(t)s} / s. \end{aligned} \tag{2.33}$$

In (2.31)–(2.33), we have used

$$\vec{q} = \vec{K}_i - \vec{K}_f, \quad \vec{K}_a = \tfrac{1}{2}(\vec{K}_i + \vec{K}_f). \tag{2.34}$$

The forms (2.32) and (2.33) involve integrations over six variables. As discussed in I, they can be considerably simplified, however, by introducing the *angle-averaging approximation*.[3] It involves the following replacements in the factors $V_{00}(\vec{t}+\frac{1}{2}\vec{s})$ $V_{00}(\vec{t}-\frac{1}{2}\vec{s})$ and $V_c(\vec{t}+\frac{1}{2}\vec{s})V_c(\vec{t}-\frac{1}{2}\vec{s})$;

$$\vec{t}\cdot\vec{s}\to \alpha ts, \tag{2.35}$$

with

$$\alpha = 1/\sqrt{3} = (\cos^2\theta)_{av}^{1/2}, \tag{2.36a}$$

where θ is the angle between $\vec{s}$ and $\vec{t}$, or

$$\alpha = (1/\sqrt{3})(1-q/2K). \tag{2.36b}$$

Note that we are still retaining the θ dependence in the exponential factors in (2.32) and (2.33). The approximation (2.35) reduces the integrals to that involving only two variables, scalar t and s. The validity of (2.35) has been tested[3] in the case of potential scattering and the result seems to be reliable for a variety of forms of the potential. (We have also examined in Ref. 3 the angle approximation of Chen and Watson,[11] and obtained substantial improvement in the large-angle behavior of the amplitude.) The differential cross sections in the various approximations are given by

$$\sigma_B = |f_{el}^B|^2, \tag{2.37a}$$

$$\sigma_P = |f_{el}^P|^2 = |f_{el}^B + f_{el}^{CP}|^2, \tag{2.37b}$$

$$\sigma = |f_{el}|^2, \tag{2.37c}$$

as they appear in the tables.

C. e^-H system and the exchange effect

We have given in (2.12)–(2.15) the potentials $\overline{V}$, $\overline{V}_c$, and $\overline{V}_V$ for the e^+H system. Insofar as the direct-channel contribution is concerned, we obtain the corresponding quantities for the e^-H system as

$$V_c^- = V_c^+ = V_c, \quad V_{00}^- = V_{00}^+, \tag{2.38}$$

$$\overline{V}^- = \overline{V} + \overline{V}_V^-, \tag{2.39}$$

where

$$\overline{Y}^- = Y/W_2 - \overline{E}_F = \overline{Y}^+ = \overline{Y} \tag{2.40}$$

and

$$\overline{V}_v^- = -\overline{V}_V^+ = -V_{\varphi\varphi}. \tag{2.41}$$

In (2.38)–(2.41), the superscript + and – are for the e^+H and e^-H systems, respectively. Note that $\overline{V}^-$ of (2.39) differs from $\overline{V}^+$ by more than a sign change, although (2.41) is, in fact $\overline{V}^- = \overline{V}^+ - 2\overline{V}_V^+$. By construction, the coupling potential V_c is unchanged as we change the charge of the projectile particle. (Its effect appears as V_c^2.)

In order to estimate the exchange effect in the e^-H problem, we have to generalize the ansatz (2.3) on the wave function to a form,

$$\Psi_\epsilon \approx [\psi_0(\vec{r}_1)u_{0\epsilon}(\vec{r}_2) + \epsilon\psi_0(\vec{r}_2)u_{0\epsilon}(\vec{r}_1)] + [\varphi(\vec{r}_1,\vec{r}_2)\omega_\epsilon(\vec{r}_2) + \epsilon\varphi(\vec{r}_2,\vec{r}_1)\omega_\epsilon(\vec{r}_1)], \tag{2.42}$$

with $\epsilon = \pm 1$ for the singlet and triplet spin states, and φ is still given by (2.4), where $\vec{R}\to\vec{r}_2$, $\vec{r}\to\vec{r}_1$ or vice versa. Substitution of (2.42) to the scattering equation and integrating out one of the variables, we obtain

$$[T_{\vec{2}} + V_{00}(\vec{2}) - E_0']u_{0\epsilon}(\vec{2}) = -\epsilon\psi_0(\vec{2})\int \psi_0(\vec{1})(2E_0 + V_{12} - E)u_{0\epsilon}(\vec{1})d\vec{1} - \left[\int \psi_0(\vec{1})[H-E]\varphi(\vec{1},\vec{2})d\vec{1}\right]\omega_\epsilon(\vec{2}) - \epsilon\int \psi_0(\vec{1})[H-E]\varphi(\vec{2},\vec{1})\omega_\epsilon(\vec{1})d\vec{1} \tag{2.43}$$

and

$$[T_{\vec{2}} + (\varphi,(V_2+V_{12})\varphi)_{\vec{1}} + (\varphi,(T_{\vec{2}}\varphi))_{\vec{1}} + (\varphi,(T_{\vec{1}}+V_1)\varphi)_{\vec{1}} - E]\omega_\epsilon(\vec{2}) = -\int \varphi(\vec{1},\vec{2})V_{12}\psi_0(\vec{1})d\vec{1}\,u_{0\epsilon}(\vec{2}) - \epsilon\int \varphi(\vec{1},\vec{2})(H-E)u_{0\epsilon}(\vec{1})d\vec{1}\cdot\psi_0(\vec{2}) - \epsilon\int \varphi(\vec{1},\vec{2})(H-E)\varphi(\vec{2},\vec{1})\omega_\epsilon(\vec{1})d\vec{1}. \tag{2.44}$$

The subscripts $\epsilon = \pm$ denote the singlet or triplet spin states. The scattering amplitude can be calculated from $u_{0\epsilon}$ and ω_ϵ. However, we evaluate in this paper an approximate amplitude in the form

$$\mathcal{T}_{el\epsilon}^- \cong \mathcal{T}_{el}^{D-} + \epsilon(u_{f0}^{(0)}, V_{00}^- g^{P-}\psi_0\chi_0) + \epsilon(u_{f0}^{(0)}, V_c\bar{g}^-\psi_0\chi_c) = \mathcal{T}_{el}^{D-} + \epsilon\,\mathcal{T}_{el}^{xP} + \epsilon\,\mathcal{T}_{el}^{xQ}, \tag{2.45}$$

where

$$\chi_0(\vec{2}) = \int \psi_0(\vec{1})(2E_0 + V_{12} - E)u_{0i}^{(0)}(\vec{1})d\vec{1},$$

$$\chi_c(\vec{2}) = \int \varphi(\vec{1},\vec{2})(H-E)u_{0i}^{(0)}(\vec{1})d\vec{1}.$$

As we find from the actual calculation that the

effect of the φ channel is rather small, especially at large angles, we will neglect the effective-channel exchange contribution, i.e., $\mathcal{T}_{el}^{xQ} \approx 0$. It is rather simple to evaluate χ_0, which is given approximately by

$$\chi_0(\vec{\xi}) \approx -4(4\pi)^{1/2}\left(\frac{E_0'+1}{(1+K^2)^2} + \frac{e^{-r_2}}{K^2}\, e^{i\vec{K}_f\cdot\vec{r}_2}\right). \qquad (2.46)$$

The form (2.46) provides an immediate evaluation of the integral following exactly the same routine that is used to evaluate the integrals for $\mathcal{T}_{el}^{-D}$ for the direct contribution.

D. Optical theorem and the total cross section

As we emphasized in (2.6), the present calculation depends on one single parameter a. However, this parameter may be fixed conveniently by incorporating the information on the total cross section. From the optical theorem

$$\sigma_t = (4\pi/K)\,\mathrm{Im} f_{el} \quad (\Theta = 0). \qquad (2.47)$$

We can thus adjust the parameter a such that the calculated forward elastic amplitude has an imaginary part which is consistent with the experimental total cross sections. It could even be that a can be made to be energy dependent. In fact, the choice of a is very critical in getting the correct magnitude of $\mathrm{Im} f_{el}$ $(\Theta = 0)$.

The total cross section σ_t can also be estimated from the wave function Ψ we have constructed. That is,

$$\sigma_t = \sigma_{el} + \sigma_{inel},$$

where the inelastic scattering cross section is given by

$$\sigma_{inel} = \frac{1}{4\pi^2}\,|\mathcal{T}_{inel}|^2$$

$$= \frac{1}{4\pi^2}\sum_{n\neq 0}(\Psi, V\psi_n u_{fn}^{(0)})(\psi_n u_{fn}^{(0)}, V\Psi)$$

$$= \frac{1}{4\pi^2}[(\Psi, V^2\Psi) - (\Psi, V\psi_0 u_{f0}^{(0)})(u_{f0}^{(0)}\psi_0, V\Psi)],$$

or

$$\sigma_{inel} = \frac{1}{4\pi^2}(\Psi, V^2\Psi) - \sigma_{el}. \qquad (2.48)$$

Since we have the function Ψ once u_0 and ω are obtained as a solution to the equation (2.17), we can readily estimate the term

$$\sigma_t \approx (1/4\pi^2)(\Psi, V^2\Psi). \qquad (2.49)$$

This will then provide further constraint on the parameter a which appears in the function φ, and also on the shapes of $\bar{V}$ and V_c.

The problem of exchange effect and the use of the optical theorem we have discussed above were not treated in detail in I, and we have spelled them out explicitly to clarify the approximations involved in the calculation which is reported in Sec. III.

III. RESULT OF THE CALCULATION

A. Average potentials and average energies

The formalism summarized in Sec. II requires an explicit evaluation of the potential parameters $\bar{V}$, V_c, and the average energy $\bar{E}_F$. As noted in (2.6), the parameter a is introduced in the trial function φ_t to avoid the singular behavior of the

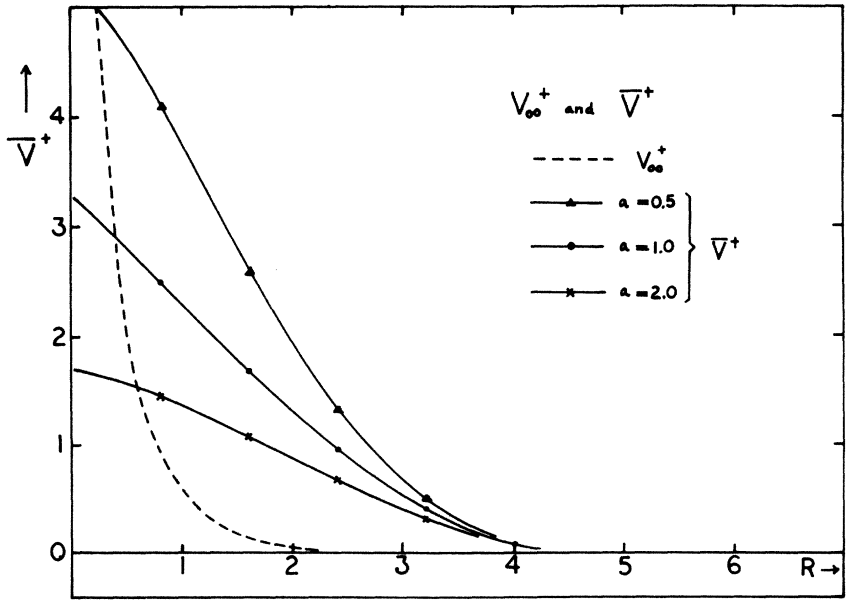

FIG. 1. Static potential V_{00}^+ for the elastic-scattering channel and the average potential $\bar{V}^+$ for the effective inelastic-scattering channel for the system e^+H. The variation of $\bar{V}^+$ as a function of a is studied for the values $a = 0.5a_0$, $1.0a_0$, and $2.0a_0$. The potentials are given in Rydberg units. $\bar{V}^+$ has a much longer range than V_{00}^+.

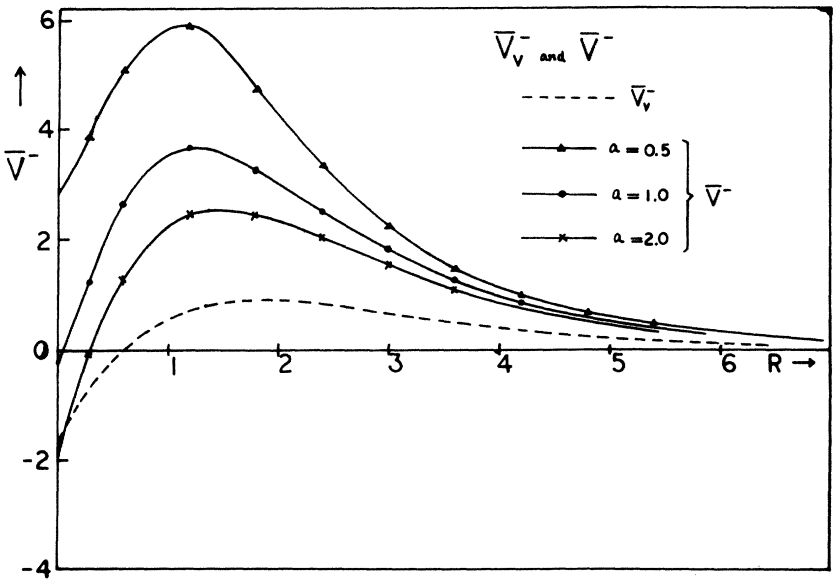

FIG. 2. Average potential $\overline{V}^-$ for the effective channel for the e^-H system. The variation of $\overline{V}^-$ as a function of the parameter a is studied, with $a = 0.5a_0$, $1.0a_0$, and $2.0a_0$. The static potential $V_{00}^- = -V_{00}^+$, and the potential $\overline{V}_{\overline{V}}^-$ which results from $V_{\varphi\varphi}$ alone, without $\overline{V}$, is also presented. Both $\overline{V}_{\overline{V}}^-$ and $\overline{V}^-$ have longer ranges than V_{00}^-.

integrals for W_3. The details of the algebra is given in the Appendix.

First of all, the average energy $\overline{E}_F$ came out to be very small for the values $a = 0.5$, 1.0, and 2.0 in the atomic units ($a_0 = 1$), and within our numerical accuracy,

$$\overline{E}_F \approx 0.1 \pm 0.3 \text{ Ry}, \tag{3.1}$$

which we will use in all our calculations. The error in (3.1) comes mainly from the slow convergence to the limit in (2.13) as $R \to \infty$. This is related to the form of φ_t we have used. On the other hand, with $a = 1.0$ and $\Theta = 0$,

$$\overline{E}_F \approx \int R^2 Y\, dR \Big/ \int R^2 W_2\, dR \approx 0.5 \pm 0.2 \text{ Ry}.$$

The average potential for the e^+H system is defined by (2.15), which we have conveniently fitted by a function of the form

$$\overline{V}^+ \approx 24a^{-1}e^{-1.25R}\,\frac{(0.4 + R^2)}{(3 + R^2)} \tag{3.2}$$

in the Ry units. Note that $\overline{V}^+$ is nearly inversely proportional to a. The form of $\overline{V}^+$ for three different values of a

$$a = 0.5a_0,\ 1.0a_0, \text{ and } 2.0a_0 \tag{3.3}$$

are given in Fig. 1. We emphasize that the fitting

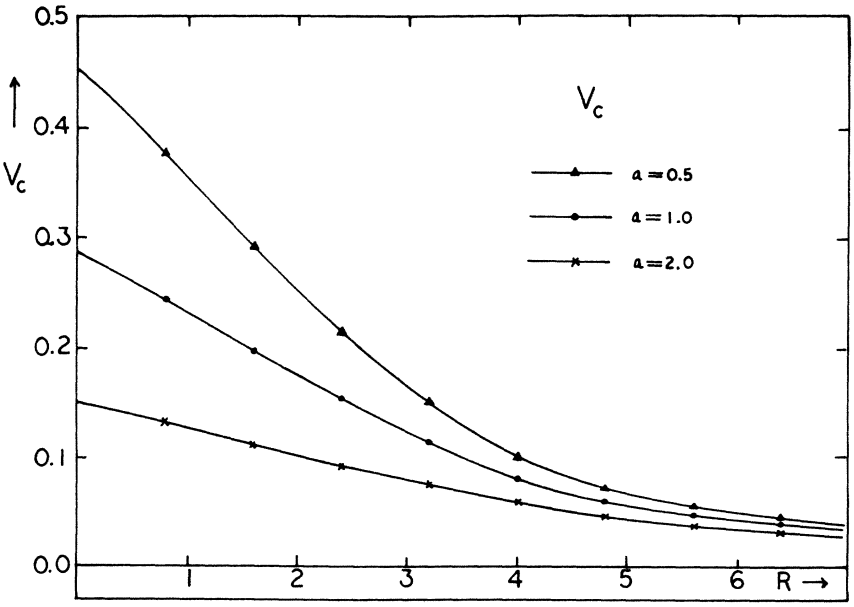

FIG. 3. Coupling potentail between the elastic and effective inelastic channels is given for different set of parameter values. V_c is the same both for e^-H and e^+H systems, and is roughly a factor of 10 smaller than $\overline{V}$. A slightly modified V_c' is used to test the sensitivity of the amplitude on V_c. V_c has longer tails than V_{00} or $\overline{V}$.

TABLE I. Variation of the differential cross section σ^- for the e^-H system as a function of the parameter a is studied, at $E_0'=200$ eV ($Ka_0=3.835$) and in the angular range $0°<\Theta<120°$. The exchange effect is not included here. σ_B denotes the Born cross section, σ_P includes the multiple-scattering effect due to V_{00} only. The cross sections are given in the πa_0^2 units.

Θ (deg)	qa_0	σ_B	σ_P	σ^- ($a=0.5$)	σ^- ($a=1.0$)	σ^- ($a=2.0$)
0	0.000	0.318	0.325	1.816	0.566	0.375
30	1.985	0.0457	0.0473	0.0461	0.0470	0.0472
60	3.835	0.0054	0.0056	0.0063	0.0055	0.0056
90	5.423	0.0014	0.0015	0.0015	0.0015	0.0015
120	6.642	0.0007	0.0007	0.0007	0.0007	0.0007

of the various potentials we have calculated is done purely to facilitate the handling of these quantities as they are given in numerical forms, and thus does not introduce new parameters. The figure also contains the static potential for the positron-hydrogen system given by

$$V_{00}^+ = 2e^{-2R}(1+1/R) = -V_{00}^- . \tag{3.4}$$

Note the extremely long range exhibited by $\bar{V}^+$ compared with V_{00}^+. This is more or less as expected, because $\bar{V}^+$ is the average interaction between the incoming positron and the target in its various excited states, which produce a more extended configuration.

So far, the parameter a is left arbitrary, although we expect that its value should be near $1a_0$. This parameter can, however, be determined by the value of the total cross section obtained by the optical theorem (2.47) and the experimental value at the particular energy, if it is available. As noted in Sec. IIC, the average potential $\bar{V}^-$ for the e^-H system came out to be quite different in shape from $\bar{V}^+$, because the change in the over-all sign in the potential V changes the sign of $\bar{V}_V^+$ but not $\bar{V}$. Thus, we have a simple fit for $\bar{V}^-$ as

$$\bar{V}^- = \bar{V}^+ - 2\bar{V}_V^+, \tag{3.5}$$

where

$$\bar{V}_V^+ \approx 1.8a^{-1}e^{-0.8R}(1-1.7R) \tag{3.6}$$

with

$$\bar{V}_V^+ = -\bar{V}_V^- , \tag{3.7}$$

and $\bar{V}^+$ is given by (3.2). $\bar{V}^-$ for different values of a are shown in Fig. 2.

Again $\bar{V}^-$ shows a long tail compared with V_{00}^-, and in addition shows an interesting structure near the origin. $\bar{V}^-$ is also dependent on a^{-1}.

Finally, the coupling potential V_c in the coupled equations (2.17) is evaluated and fitted simply as

$$V_c \approx 32a^{-1}e^{-0.3R}(100+R^2)^{-1}, \tag{3.8}$$

in the Ry units. Of course, from the definition (2.12) for V_c, we have

$$V_c^+ = V_c^- = V_c . \tag{3.9}$$

The actual form for V_c is plotted in Fig. 3 for different values of a. It is apparent that V_c has an extremely long tail compared with $\bar{V}$ and V_{00}, but otherwise is fairly small in magnitude and has very simple structure. This immediately suggests that V_c will not play an important role in the large-angle region.

B. Determination of the parameter a

As we have seen in the figures, $\bar{V}$ and V_c vary considerably as functions of a. Insofar as the original formulation of the effective-channel theory, as given in Ref. 1 and being applied here, no parameters are to be adjusted during the amplitude calculation. However, the singular nature of the original V makes it necessary to introduce the parameter a in φ_t. This parameter may be determined by matching the calculated total cross section to the known experimental values.

Thus, we have calculated the differential cross sections for the different values of a, at $E_0'=200$ eV. The result is presented in Table I. The large-angle behavior of σ is hardly affected by the change in a, but the forward cross section is extremely sensitive to the choice of a. The main reason for this is that the Born amplitude dominates at large angles.

The above feature is exactly what is needed to

TABLE II. Total cross section for the e^-H scattering with exchanges is estimated at $E_0'=50, 100, 200$, and 500 eV by the optical theorem. This is denoted $\sigma_t^{-\,\mathrm{opt}}$. The experimental values $\sigma_t^{-\,\mathrm{expt}}$ is obtained by combining the elastic, $n=2$ excitation, and estimated excitations to $n>2$ states. Therefore, $\sigma_t^{-\,\mathrm{expt}}$ may not be very reliable, but it is sufficient to indicate that the parameter a may be determined from $\sigma_t^{-\,\mathrm{expt}}$, if accurate values are available. The parameter a may be approximately $0.8a_0$, but we fix a to be $a=1.0a_0$ throughout the calculation. We also note that a could be mildly E_0' dependent.

E_0' (eV)	$\sigma_t^{-\,\mathrm{opt}}$	$\sigma_t^{-\,\mathrm{expt}}$	$\sigma_t^{n=2\,\mathrm{exc}(-)}$	$\sigma_t^{n\geq 3\,\mathrm{exc}(-)}$
50	1.6	1.5	0.90	.15
100	0.90	1.1	0.72	.08
200	0.54	0.75	0.50	.06
500	0.25	0.35	0.22	.03

TABLE III. Elastic-scattering amplitudes for the e^-H system at $E_0' = 200$ eV. σ_B is the Born amplitude, σ_P the static amplitude with V_{00} only, without exchange, and σ_D the amplitude with the Q-space effects included but without the exchange term. (D is for direct.) σ_+ and σ_- are the cross sections in the units πa_0^2 for the singlet and triplet, respectively, ($a = 1.0a_0$).

Θ (deg)	Ref_B	Ref_P	Ref_D	Ref_+	Ref_-	Imf_P	Imf_D	Imf_+	Imf_-	σ_D	σ_+	σ_-
0	1.000	1.001	1.231	1.232	1.231	0.132	0.513	0.513	0.512	0.566	0.567	0.565
30	0.379	0.373	0.371	0.373	0.368	0.098	0.102	0.108	0.096	0.0470	0.0480	0.0461
60	0.130	0.121	0.120	0.120	0.119	0.055	0.055	0.063	0.046	0.0055	0.0059	0.0052
90	0.067	0.061	0.061	0.060	0.062	0.034	0.034	0.034	0.034	0.0015	0.0015	0.0016
120	0.045	0.041	0.041	0.040	0.041	0.025	0.025	0.025	0.026	0.0007	0.0007	0.0008

determine a from σ_t as obtained by the optical theorem involving Imf at $\Theta = 0$.

In Table II, we estimated the experimental total cross sections at various scattering energies E_0' from the total excitation cross section and the total elastic cross section. The numbers for σ_t^{expt} in Table II may not be very reliable, but $a = 0.8$ perhaps would have been a better choice to reproduce the data. But, as we are not interested in the accuracy of the cross section so much, but in the applicability of the formalism itself, we have taken the value $a = 1.0a_0$ for all our subsequent calculations, i.e.,

$$a \approx 1.0a_0. \tag{3.10}$$

C. Exchange effect

As we have discussed in Sec. IIC, the exchange effect is included only in the elastic component only, i.e., we have neglected the $\mathcal{T}_{el}^{xQ}$ term in (2.45). In view of the fact that the Born amplitude dominates the cross section away from the forward direction, this is a reasonable approximation. However, for small angles, $\mathcal{T}_{el}^{xQ}$ may not be negligible, just as $\mathcal{T}_{el}^{Q}$ is appreciable there.

Table III shows the details of the effect of the exchange. The subscripts + and − denote the singlet and triplet states. The result here is consistent with the conclusion of Takeda and Watson[12] that the exchange effect is negligible at high energies.

Table IV contains the elastic differential cross sections calculated in the Born approximation (σ_B), in the static approximation (σ_P) with multiple scattering effect coming from the V_{00}^- part, and the cross section (σ_D) which includes the effect of distortions but not the exchange effect.[13] The spin-averaged cross section σ_{av} includes the exchange effect only in the elastic-channel part, as discussed in Sec. IIC. We have evaluated the cross sections using the amplitude expression in the form (2.45) with $\mathcal{T}_{el}^{xQ} \approx 0$, and the angle-averaging procedure was adopted. Of course, (2.30) and (2.45) indicate that all the multiple-scattering terms involving V_{00}^- and $\bar{V}^-$ are incorporated here, but the effect of V_c is included only to second order.

Evidently, throughout the energy range $50 \lesssim E_0' \lesssim 500$ eV under consideration, the first Born amplitude dominates the scattering at all angles $\Theta \gtrsim 30°$. Furthermore, the iteration of the V_{00}^- makes a significant contribution to the cross section at all angles, specially for $E_0' \lesssim 200$ eV. Referring back to Table IV, we also see that the imaginary part of the amplitude f_P shows a substantial change from the Born result, Im$f_B = 0$.

The form of the amplitude (2.30) is especially

TABLE IV. Differential elastic-scattering cross sections for the e^-H system at the scattering energies E_0' = 50, 100, 200, and 500 eV. B is the Born and P is the static multiple scattering without the exchange; D is the direct scattering with the Q-space effect but without the exchange; σ_{av} is the spin-averaged cross section. σ's are given in the units πa_0^2 ($a = 1.0a_0$). Finer adjustment of the parameter a to the total-cross-section data was not made.

E_0' (eV)	Θ (deg)	σ_B^-	σ_P^-	σ_D^-	σ_{av}^-
50	0	0.318	0.343	0.846	0.886
	30	0.166	0.183	0.159	0.179
	60	0.0500	0.0569	0.0603	0.0743
	90	0.0181	0.0212	0.0273	0.0292
	120	0.0090	0.0108	0.0136	0.0132
100	0	0.318	0.331	0.702	0.707
	30	0.0996	0.1054	0.1024	0.1055
	60	0.0181	0.0196	0.0202	0.0220
	90	0.0054	0.0059	0.0055	0.0055
	120	0.0025	0.0028	0.0028	0.0027
200	0	0.318	0.325	0.566	0.567
	30	0.0457	0.0473	0.0470	0.0475
	60	0.0054	0.0056	0.0055	0.0057
	90	0.0014	0.0015	0.0015	0.0015
	120	0.0007	0.0007	0.0007	0.0007
500	0	0.318	0.321	0.444	0.444
	30	0.0110	0.0113	0.0112	0.0112
	60	0.0009	0.0010	0.0010	0.0010
	90	0.0002	0.0003	0.0003	0.0003
	120	0.0001	0.0001	0.0001	0.0001

convenient in estimating the contribution of the inelastic channels on the elastic amplitude. The change from σ_P to σ_D is drastic at small Θ, the scattering angle, although for $E_0' \gtrsim 100$ eV, both σ_P and σ_D approach the Born values at large Θ. The change in σ_D from σ_P is mainly brought about by the huge increase in the imaginary part of the amplitude, $\mathrm{Im}f_D$. This is seen in Table III. This sheds some light on the contents of the Glauber approximation in which the amplitude is calculated by writing the scattering function Ψ in the form

$$\Psi \approx e^{i\vec{K}_i\cdot\vec{R}}\,\psi_0(\vec{r})\exp\left(-\frac{i}{K}\int_{-\infty}^{z} V(\vec{r},\vec{R}')\,dZ'\right) \quad (3.11)$$

with

$$\vec{R}' = \vec{b} + \vec{Z}'.$$

The V- dependent factor in Ψ of (3.11) is understood to simulate the multiple-scattering effect which comes from the V_{00}^- as in T_{el}^P and also the distortion effect of the inelastic channels. Thus, it is not at all clear whether the resulting amplitude in this approximation incorporates enough contributions from the Q channel (inelastic). The present calculation clearly shows that, except at small angles and $E_0' \lesssim 50$ eV, the potential $V(\vec{r},\vec{R})$ in (3.11) can be replaced by a simpler expression $V_{00}^-(\vec{R})$ without affecting the cross section very much. This substitution reduces the original three-body problem into a simple potential scattering.

Insofar as the present approach is concerned, it is extremely fortunate that f_D and σ_D, which include the Q-space channel effect, are very sensitive to the parameter a. In fact, $\mathrm{Im}f_D(0)$, or more precisely $\mathrm{Im}f_{av}$ with the exchange effect included, can be used to precisely determine the parameter. (As the total cross sections are not available in any absolute scale, we made an estimate of the magnitude from the elastic and excitation cross sections which are dominated by the $n=1\to n=2$ transitions in the $l=1$ states. (See Table II.) It seems that a is close to 1 Bohr radius ($a \approx 0.8a_0$). We also note that a may be mildly energy dependent. We ignore this fine detail and adjustment.

The change in the cross section due to the exchange effect is small but significant at small Θ and $E_0' \approx 50$ eV, but its effect rapidly decreases as we go to larger angles or to higher energies. Originally, it was hoped that the exchange effect,

TABLE V. Elastic-scattering differential cross sections for the e^+H system at $E_0' = 50$, 100, 200, and 500 eV. B represents Born; P represents static; σ^+ includes the Q-space effect ($a = 1.0a_0$) Cross sections are given in the πa_0^2 units.

E_0' (eV)	Θ (deg)	σ_B^+	σ_P^+	σ^+
50	0	0.318	0.257	0.522
	30	0.166	0.129	0.0926
	60	0.0500	0.0353	0.0325
	90	0.0181	0.0118	0.0093
	120	0.0091	0.0055	0.0032
100	0	0.318	0.292	0.410
	30	0.100	0.0892	0.0800
	60	0.0181	0.0161	0.0156
	90	0.0054	0.0049	0.0049
	120	0.0025	0.0023	0.0023
200	0	0.318	0.287	0.355
	30	0.0460	0.0379	0.0370
	60	0.0054	0.0040	0.0040
	90	0.0015	0.0011	0.0011
	120	0.0007	0.0006	0.0006
500	0	0.318	0.304	0.328
	30	0.0110	0.0105	0.0105
	60	0.0010	0.0009	0.0009
	90	0.0003	0.0003	0.0003
	120	0.0001	0.0001	0.0001

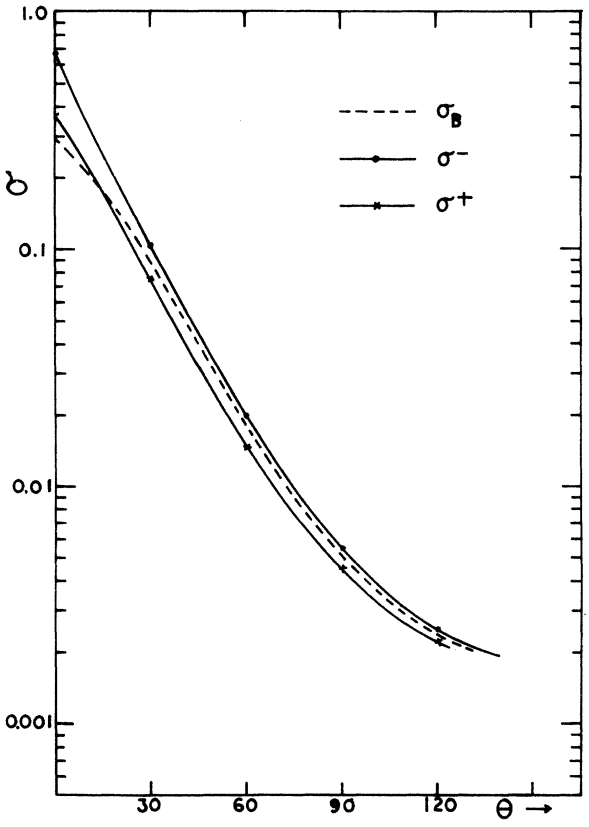

FIG. 4. δ^+ and δ_{av}^- for the positron and electron scattering are compared at $E_0' = 100$ eV. The Born cross sections are the same, $\delta_B^+ = \delta_B^-$, and is given by the dashed curve. Solid curve represents δ_{av}^-; dash-dot curve represents δ^+. The cross sections are given in the units πa_0^2, and the scattering angles Θ in degrees.

which was not included in the earlier Glauber-type calculations, may be responsible for the apparent discrepancy in the cross-section data at 200 eV and at angles $\Theta \gtrsim 60°$. Obviously, σ_{av} does not resolve this when the theoretical and experimental cross sections are normalized at $\Theta = 60°$. We have tried to change the various potentials, $\bar{V}^-$, V_c, and also the exchange term, to bring about the necessary change in $\sigma_{av}(\Theta)$ to make it agree with the experimental points. Within the reasonable range for the parameters which were varied, we were unable to bring the theoretical cross sections up to the experimental points.

D. Positron-hydrogen scattering

As the formalism given in Sec. II is readily applicable both to the e^-H and e^+H systems with very minor changes, we have also calculated the positron scattering from hydrogen. The general feature of σ_B^+, σ_P^+, and σ^+ is roughly the same as in the e^-H case, but the difference between σ_{av}^- and σ^+ is very large at small Θ for all values of E_0'. They tend to come together at large angles and high energies, as more or less expected from the dominance of the Born amplitude in this region. σ^+ and σ_{av}^- are compared in Fig. 4.

E. Approximations in the effective channel

We recall that the complicated Q space is treated in this calculation as one effective channel and $\bar{V}^-$ and V_c are estimated by a single trial function φ_t. Furthermore, the effects of $J_{\varphi\varphi}$ term in (2.10) and the exchange process coming from φ_t as contained in T_{el}^{xQ} of (2.45) were neglected. In the evaluation of the amplitude, we have also neglected all the higher-order contributions which involve V_c more than the second order.

In order to estimate these approximations, we have calculated the cross sections for the e^-H system at $E_0' = 200$ eV with $\bar{V}^- \approx \bar{V}_v^-$, i.e., the effect of $\bar{V}$ in (2.40) is neglected. The potential $\bar{V}_v^-$ is shown in Fig. 2, and the result is given in Table VI.

Evidently, $\bar{V}$ seems to have a very small effect on the cross section at all angles. This is more or less expected for the $e^\pm$H system, as the Born term dominates, but is a disappointment in the sense that we will learn very little from such an elastic scattering experiment about the dynamic structure of the target system, except the simple static density effect. To learn about the structure especially for more complex but interesting target systems, we may have to study inelastic processes.

Finally, there is always the question of whether the angle-averaging procedure adopted here to simplify the amplitude integrations is valid at large angles. We have studied this question in a previous report[3] and found that, for potentials which have relatively smooth behavior, the approximation is rather good. As we made the same approximation in g_0^P and g_φ, we examined this question by modifying the parameter α in (2.35) to the form (2.36b) instead of (2.36a), which was used throughout the calculation. The result is also included in Table VI for comparison. This indicates, although not absolutely conclusively, that the approximation is reasonable, within the accuracy we are interested in.

IV. CONCLUSION

We have applied the effective-channel approach to the medium-energy scattering of composite systems to the simple e^+H and e^-H system. The coupled equations for the elastic and effective inelastic channels are solved approximately, and various contributions to the elastic amplitude were separately analyzed. The theory as applied here contains effectively no adjustable parameter, as the only constant a in φ_t is presumably fixed by the total-cross-section data, as discussed in Sec. III. Although the calculation has been carried out with reasonable accuracy in the resulting cross sections, our main purpose has been to examine whether the approach outlined in Ref. 1 is indeed applicable to systems more complicated than the hydrogen. Some of the main findings from the present study are the following:

(1) The calculation shows that, as many of the earlier calculations have concluded, the Born amplitude dominates the cross section at angles, away from the forward direction, and at energies higher than 100 eV.

(2) The multiple-scattering contribution coming from the static interaction V_{00} is sufficient to predict the real part of the amplitude at all angles, but the imaginary part is not reliable at $\Theta \approx 0$.

(3) The imaginary part of the amplitude in the

TABLE VI. The effect of replacing $\bar{V}^-$ by $\bar{V}_V^-$ is studied for the e^-H system at 200 eV. The resulting cross section is denoted by σ_{AW}^-. σ_A^{-1} is obtained when the angle-averaging parameter α is set as $\alpha = 1\sqrt{3}(1 - q/2K)$, rather than $\alpha = 1\sqrt{3}$ which is used throughout the calculation ($a = 1.0\,a_0$).

Θ (deg)	σ_{av}^-	σ_{AW}^-	σ_A^{-1}
0	0.567	0.553	0.567
30	0.0475	0.0471	0.0475
60	0.0057	0.0058	0.0058
90	0.0015	0.0015	0.0015
120	0.0007	0.0007	0.0007

near forward direction is completely *dominated* by the contribution from the inelastic channel. As $\mathrm{Im}f(\Theta=0)$ is directly related to the total cross section, this result is what we expected. At least one parameter in the description of the inelastic channel can be fixed therefore from the total-cross-section data.

(4) The parameter a in φ_t is expected from physical grounds to be of the order of $1a_0$. However, the total-cross-section data indicates that it could be somewhat smaller. We may interpret this as an effect of the high-energy scattering, because the projectile with high energy may more readily penetrate inside the target, so that the region which is "insensitive" to the scattering may be much smaller than the density distribution in the ground state. This information will be useful in the future parametrization for more complex systems. However, for the present purpose, it was not thought to be meaningful to make a finer adjustment of this parameter, and we have taken $a=1.0a_0$ throughout the calculation.

(5) The average energy $\bar{E}_F$ for the hydrogen is approximately zero (or very small positive number) and we have set $\bar{E}_F$ 0.1 ± 0.3 Ry.

(6) The average potential $\bar{V}$ and the coupling potential V_c both have a very *long range* compared to the V_{00} potential. Again, this is as expected, because the effective channel simulates the target in the excited (Q space) states which spread out more in the configuration space. In fact, $\bar{V}$ may even have a tail which may decay at large R like some inverse power law, since the Q space includes both excited bound states as well as continuum states.

Therefore, we have shown that the coupled-equations approach to medium-energy scattering, as formulated in Ref. 1, can be rather simply applied to composite-system scattering. The method is equally applicable to medium-energy nuclear scattering of protons and pions off nuclei.[7,14] Provided the approximate amplitude in the form (2.30) is valid, the method seems to be much simpler to apply than the Glauber-type calculations when more complicated targets are involved. The separation of the amplitude into different parts makes the present approach especially useful in studying the static (density) effect and the dynamic properties of the target systems (arising from the inelastic processes).

The theory as formulated can also be applied to inelastic scattering, since we essentially have the total-scattering function Ψ in terms of the Green's functions g^P and g_φ. Thus, the projection of $V\Psi$ onto a given final state with $\psi_n u_{0f}^{(0)}$ will give the inelastic amplitude for the $0\to n$ transition. However, this may not be so effective if that final-state channel is strongly coupled to the initial channel. In such cases, the explicit inclusion of both initial- and final-state channels may be necessary, with proper modifications of the effective-channel parameters. Appropriate extensions of the present approach to inelastic scattering are being formulated, and will be reported on later with applications. As we have noted, the dominance of the Born amplitude in the elastic scattering makes if difficult to obtain the structure information on the target from the elastic-scattering data, except for the static size of the target and the total inelastic contribution. A more sensible way to study the target structure seems therefore to analyze the inelastic-scattering data.

Notes added in proof: Very recently, Teubner *et al.* [J. Phys. B 6, L134 (1973)] have redone the e^-H elastic-scattering experiment at 50 eV in the small angle region, and compared the cross section with the various theoretical calculations. Although the validity of our calculation at this low energy is marginal, the cross section in Table IV fits well for the angular region $\Theta\gtrsim 60°$, while it is too low for smaller angles.

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APPENDIX

Explicit evaluation of the quantities which appear in (2.17) is given here. We take the units with $m=e^2=\hbar=1$, which give $a_0=1$; the energy is given in Ry units. Thus, for the e^+H system

$$V=\frac{2}{r}-\frac{2}{|\vec{r}-\vec{R}|} \tag{A1}$$

and

$$V^a=\frac{2}{r+a}-\frac{2}{|\vec{r}-\vec{R}|+a}\,. \tag{A2}$$

With the notation

$$\langle\mathcal{O}\rangle\equiv\int d\vec{r}\,\psi_0^*\mathcal{O}\psi_0, \tag{A3}$$

we have

$$\langle V\rangle=2e^{-2R}\left(1+\frac{1}{R}\right), \tag{A4}$$

$$\langle V^a\rangle=\langle V\rangle+\frac{2a}{R}\left(2L_1-\frac{1}{R+a}\right), \tag{A5}$$

$$\langle (V^a)^2 \rangle = \frac{4}{(R+a)^2} - \frac{8}{(R+a)R} + \frac{8}{R(R+a)}(1+R)e^{-2R} + \frac{8}{R}\left(\frac{3a+R}{R+a}\right)L_1 + \frac{8a}{R}N(1,1), \tag{A6}$$

$$\langle V^a V \rangle = -\frac{4}{R^2} + \frac{4(2R+a)}{R^2(R+a)}(1+R)e^{-2R} + \frac{8}{R^2}(R+a)L_1, \tag{A7}$$

$$\langle V^a V V^a \rangle = \frac{2}{R}\langle (V^a)^2 \rangle - \frac{8}{R(R+a)^2} + \frac{8}{R(R+a)^2}(1+R)e^{-2R} + \frac{32L_1}{R(R+a)} + \frac{16}{R}N(1,1), \tag{A8}$$

$$\begin{aligned}\langle V^a H_T V^a \rangle = \frac{8}{R}\Bigg[& -\frac{R}{2(R+a)^2} + \frac{3-e^{-2R}(3+2R)}{2(R+a)} + \left(\frac{R+3a}{R+a}\right)(L_0+L_1) \\ & + N(0,1)\left(\frac{R^2}{R+a} - \frac{a^2}{R+a} - 2a\right) + N(0,2)\left(\frac{a^2}{2} - \frac{R^2}{2}\right) - N(1,1)a^2 + N(1,2)\frac{2a}{R+a} - \frac{1}{R+a}N(2,1) \\ & + \tfrac{1}{2}N(2,2) - \tfrac{4}{3}aN(1,3)\Bigg]\end{aligned} \tag{A9}$$

The special functions used are

$$L_n(R) = \int_0^\infty r^n e^{-2r} \ln\left(\frac{r+R+a}{|r-R|+a}\right) dr, \tag{A10}$$

$$N(m,n) = \int_0^\infty r^m e^{-2r}\left(\frac{1}{(r+R+a)^n} - \frac{1}{(|r-R|+a)^n}\right) dr \equiv N(m,n;R). \tag{A11}$$

The integrals for the e^-H system are obtained by the change of sign for all quantities which involve odd powers of V or V^a. Thus, the entire quantities of interest are parametrized in terms of φ_t with one parameter a. This constant will be fixed by the total-cross-section data.

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