Multiple-Scattering Expansions for Nonrelativistic Three-Body Collision Problems. VII. Differential Cross Section for Elastic Scattering*

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(Received 13 September 1971)

The energy and angular dependences of the differential elastic scattering cross section are investigated in the first-order Faddeev-Watson multiple-scattering (FWMS) approximation for a number of three-body atomic systems. The anomalies in the first-order Born approximation are not present in the first-order FWMS approximation. Significant differences are found between the elastic (e^-, H) and (e^+, H) scattering at energies as high as 10 keV. The elastic (e^+, e^-e^+) and (p^+, e^-e^+) scattering cross sections which are incorrectly predicted to be zero in the first-order Born approximation are calculated. The forward-angle peaking of the elastic scattering cross section is accounted for in the first-order FWMS approximation by allowing the system to participate in the intermediate inelastic scatterings. In general, significant differences are found in the magnitude of the cross sections obtained in the first-order FWMS and Born approximations at energies where the first-order Born approximation has been extensively used for normalizing experimental results. The energy for the first-order Born approximation, to be accurate, can be determined experimentally by locating the energy above which the difference between the (e^-, H) and (e^+, H) scatterings ceases to be appreciable.

I. INTRODUCTION

In Paper IV[1] of this series on the Faddeev-Watson multiple-scattering (FWMS) expansion for three-body collision problems, we have investigated in detail the application of the FWMS expansion to atomic scattering processes. A comparison between the first-order FWMS and Born approximation was then made for the elastic scattering. It was shown that the first-order Born approximation has the following anomalous behavior for elastic scattering: (a) If the target is made of equal-mass particles having charges which are equal but opposite in sign such as positronium, the first-order Born approximation predicts a zero for the elastic scattering amplitude. (b) The first-order Born approximation does not distinguish the sign of the charge of the incident particle and consequently it does not distinguish, for example, the elastic electron scattering from positron scattering. (c) The first-order Born approximation does not allow intermediate inelastic scatterings and is incapable of predicting the forward-angle peaking.[2] These Born anomalies are all removed in the first-order FWMS approximation for elastic scattering.

In the first-order FWMS approximation, the attractive and repulsive pair interactions between the incident and target particles are allowed to go off the energy shell. This then permits the interacting system to participate in the intermediate inelastic scatterings and to distinguish the attractive interaction from the repulsive interaction through their analytic properties. Because of these facts the Born anomalies do not appear in the first-order FWMS approximation. The purpose of the present paper is to present some numerical results of elastic scattering in the first-order FWMS approximation for a number of systems where the first-order Born approximation is anomalous. Excitation scatterings will be considered in subsequent communications.

In Sec. II, a resume of the Faddeev-Watson multiple-scattering expansion for scattering is given. Applications of the FWMS expansion to the investigation of the energy and scattering-angle dependence of the elastic differential scattering cross section are carried out in the first-order approximation. Our results are presented in Sec. III together with a comparison with results obtained in the Born approximation as well as with experimental measurements and the Glauber-eikonal approximation when available. Some concluding remarks are given in Sec. IV.

II. FIRST-ORDER MULTIPLE-SCATTERING APPROXIMATION

The Faddeev-Watson multiple-scattering expansion for scattering processes has been investigated in some detail in Paper IV. In this section we recall only the necessary equations which are used in the present application.

The transition amplitude for the scattering process

$$1+(2,\ 3)\rightarrow 1+(2,\ 3) \tag{2.1}$$

takes the form [Eq. (IV 2.13)]

$$\langle \psi_f^{(1)} \mid T_s \mid \psi_i^{(1)} \rangle$$

$$= (2\pi)^3 \int d\vec{p}_1\, d\vec{q}_1\, d\vec{p}_1'\, d\vec{q}_1'\, \chi_f^{(1)*}(\vec{p}_1)\chi_i^{(1)}(\vec{p}_1') \times \delta(\vec{q}_1 - \vec{\kappa}_f)\delta(\vec{\kappa}_i - \vec{q}_1')\langle \vec{p}_1\vec{q}_1 | T_s | \vec{p}_1'\vec{q}_1' \rangle ,$$

where $\chi_{f,i}^{(1)}$ are the two-body bound-state wave functions for particle pair (2, 3) with quantum numbers collectively denoted by f and i. The mass-scaled momentum variables $(\vec{p}_i,\ \vec{q}_i)$ are defined by Eqs. (IV 2.2). The energy conservation relation in terms of the mass-scaled asymptotic momenta, $\vec{\kappa}_i$ and $\vec{\kappa}_f$, before and after scattering is given by the equation

$$E = \kappa_f^2 + \epsilon_f^{(1)} = \kappa_i^2 + \epsilon_i^{(1)} , \tag{2.3}$$

where E is the total energy of the system and $\epsilon_f^{(i)}$ are the two-body bound-state energies for the ith pair of particles.

The Faddeev-Watson multiple-scattering expansion for the scattering collision operator T_s takes the form[3,4] [see Eq. (I 2.29)]

$$T_s = T_2 + T_3 + T_2 G_0 T_3 + T_3 G_0 T_2 + \cdots , \tag{2.4}$$

with

$$T_i = V_i + V_i G_0 T_i , \tag{2.5}$$

where V_i is the two-body Coulomb potential V_{jk}, G_0 is the Green's function for the three-body system in the absence of interaction, and T_i is the two-body T matrix in the presence of a spectator particle i. The corresponding Born expansion for T_s is

$$T_s^B = \mathcal{U}_1 + \mathcal{U}_1 G_0 \mathcal{U}_1 + \mathcal{U}_1 G_0 \mathcal{U}_1 G_0 \mathcal{U}_1 + \cdots , \tag{2.6}$$

with

$$\mathcal{U}_1 = V_2 + V_3 , \tag{2.7}$$

where superscript B on T_s denotes the Born expansion.

When the Faddeev-Watson expansion is utilized, the differential scattering cross section may be written as

$$\frac{d\sigma_s}{d\Omega} = \frac{\mu_1^2}{4\pi^2}\left(\frac{\kappa_f}{\kappa_i}\right)\left|(2\mu_{23})^{3/2}\left(\frac{\langle\psi_f^{(1)}|T_2|\psi_i^{(1)}\rangle}{(2\mu_{31})(2\mu_2)^{3/2}} + \frac{\langle\psi_f^{(1)}|T_3|\psi_i^{(1)}\rangle}{(2\mu_{12})(2\mu_3)^{3/2}} + \cdots\right)\right|^2 , \tag{2.8}$$

with

$$\mu_{ij} = \frac{m_i m_j}{m_i + m_j} , \quad \mu_i = \frac{m_i(m_j + m_k)}{m_i + m_j + m_k} , \tag{2.9}$$

where m_1, m_2, and m_3 are the masses of the three particles.

In the first-order approximation Eq. (2.8) reduces to the form

$$\frac{d\sigma_s^{(1)}}{d\Omega} = \frac{1}{16\pi^2}\left(\frac{\kappa_f}{\kappa_i}\right)\left|\beta_{12}\langle\psi_f^{(1)}|T_2|\psi_i^{(1)}\rangle + \beta_{31}\langle\psi_f^{(1)}|T_3|\psi_i^{(1)}\rangle\right|^2 , \tag{2.10}$$

with

$$\alpha_{ij}^2 = \frac{m_i m_j}{(m_i + m_k)(m_j + m_k)} , \quad \beta_{ij}^2 = 1 - \alpha_{ij}^2 , \tag{2.11}$$

where α_{ij} and β_{ij} are the mass coefficients.

The matrix element $\langle\psi_f^{(1)}|T_2|\psi_i^{(1)}\rangle$ may be written for elastic scattering as [see Eqs. (IV 4.1) and (IV 4.2)]

$$\langle\psi_{1s}^{(1)}|T_2|\psi_{1s}^{(1)}\rangle = \frac{16 Z_2 e^2(-\epsilon_1^{(1)})^{5/2}}{\pi\beta_{12}\kappa_{fi}^2}\int d\hat{p}_1\, I^{(2)}(\hat{p}_1) , \tag{2.12}$$

with

$$I^{(2)}(\hat{p}_1) = 2\int_0^\infty \frac{dp_1 p_1^2 \tau_2(\vec{p}_1)}{[(p_1 - u_1^{(+)})(p_1 - u_1^{(-)})(p_1 - u_2^{(+)})(p_1 - u_2^{(-)})]^2} , \tag{2.13}$$

$$\tau_2(\vec{p}_1) = \frac{2\pi^2\kappa_{fi}^2}{Z_2 e^2 \beta_{12}^2}\, T_2(\vec{K}_1,\ \vec{K}_2;\ E - K_3^2 + i\eta) , \tag{2.14}$$

where $u_1^{(\pm)}$, $u_2^{(\pm)}$, and $T_2(\vec{K}_1,\ \vec{K}_2;\ E - K_3^2 + i\eta)$ are defined in Eqs. (IV 4.5), (IV 4.6), and (IV 2.20)–(IV 2.23). The momentum transfer κ_{fi} for elastic scattering, $|\vec{\kappa}_f| = |\vec{\kappa}_i| = \kappa$, can be written as

$$\kappa_{fi} \equiv |\vec{\kappa}_f - \vec{\kappa}_i| = 2\kappa \sin\tfrac{1}{2}\theta . \tag{2.15}$$

Similarly, the matrix element $\langle\psi_f^{(1)}|T_3|\psi_i^{(1)}\rangle$ takes, for elastic scattering, the form [see Eqs. (IV 4.8) and (IV 4.9)]

$$\langle\psi_{1s}^{(1)}|T_3|\psi_{1s}^{(1)}\rangle = \frac{16 Z_3 e^2(-\epsilon_1^{(1)})^{5/2}}{\pi\beta_{31}\kappa_{fi}^2}\int d\hat{p}_1\, I^{(3)}(\hat{p}_1) , \tag{2.16}$$

with

$$I^{(3)}(\hat{p}_1) = 2\int_0^\infty \frac{dp_1 p_1^2 \tau_3(\vec{p}_1)}{[(p_1 - u_4^{(+)})(p_1 - u_4^{(-)})(p_1 - u_5^{(+)})(p_1 - u_5^{(-)})]^2} , \tag{2.17}$$

$$\tau_3(\vec{p}_1) = \frac{2\pi^2\kappa_{fi}^2}{Z_3 e^2 \beta_{31}^2}\, T_3(\vec{K}_5,\ \vec{K}_6;\ E - K_7^2 + i\eta) , \tag{2.18}$$

where $u_4^{(\pm)}$, $u_5^{(\pm)}$, and $T_3(\vec{K}_5,\ \vec{K}_6;\ E - K_7^2 + i\eta)$ are defined in Eqs. (IV 4.12), (IV 4.13), and (IV 2.20)–(IV 2.23).

In Paper IV, the integrals $I^{(2)}(\hat{p}_1)$ and $I^{(3)}(\hat{p}_1)$ along the positive real axis were investigated analytically by converting them into integrals around the various singularities of the integrand lying in the upper half of the p_1 plane. It was shown that the integrals consist of contributions coming from (a) the asymptotic two-body bound-state poles in the initial and final wave functions, (b) the intermediate two-body bound- and antibound-state poles, and (c) the branch-point singularities associated both with the continuum (unitarity) and the on-shell Coulomb cuts in the off-shell T matrices. Numerically, it is, however, more convenient to evaluate the integrals $I^{(2)}(\hat{p}_1)$ and $I^{(3)}(\hat{p}_1)$ along the positive real axis. The analytic expressions obtained in Paper IV are used to check our numerical procedures.

To evaluate these integrals along the real axis, we make use of the analytical expression for[5,6] τ_i

$$\tau_i = \tau_i^A + \tau_i^B \tag{2.19}$$

with

$$\tau_i^A = 1 - \frac{1}{(1+\epsilon_i)^{1/2}}\left(1 + \sum_{\lambda=1}^{\infty} \frac{2\nu_i^2}{\lambda^2+\nu_i^2}[t_i^{(+)}]^{\lambda}\right), \tag{2.20}$$

$$\tau_i^B = \frac{2\pi\nu_i}{e^{2\pi\nu_i}-1}\frac{[t_i^{(+)}]^{-i\nu_i}}{(1+\epsilon_i)^{1/2}}, \tag{2.21}$$

$$t_i^{(+)} = \left(1+\frac{2}{\epsilon_i}\right) - \frac{2}{\epsilon_i}(1+\epsilon_i)^{1/2}, \tag{2.22}$$

where ν_2 and ϵ_2 are defined in Eqs. (IV 4.3)–(IV 4.7) and ν_3 and ϵ_3 are defined in Eqs. (IV 4.10)–(IV 4.14).

In taking the $\eta \to 0^+$ limit in the T matrices, care must be exercised in examining how the energy shell is approached since the off-shell Coulomb T matrix does not approach a well-defined limit on the energy shell. Let $T(\vec{p}_1, \vec{p}\,'; k^2)$ denote the T matrix, when $\vec{p} = \vec{K}_1$, $\vec{p}\,' = \vec{K}_2$, and $k^2 = E - K_3^2$, or $\vec{p} = \vec{K}_5$, $\vec{p}\,' = \vec{K}_6$, and $k^2 = E - K_7^2$. There are four regions from which the energy shell may be approached

$$\begin{aligned} &p > k \text{ and } p' > k, && \text{region I} \\ &p > k > p', && \text{region II} \\ &p < k \text{ and } p' < k, && \text{region III} \\ &p < k < p', && \text{region IV}. \end{aligned} \tag{2.23}$$

It can be shown[5-7] that the quantity $t_i^{(+)}$ in these four regions takes on the following different forms in the limit of $\eta \to 0^+$:

$$t_i^{(+)} = |t_i^{(+)}| \times \begin{cases} e^{2i\pi} & \text{region I} \\ e^{i\pi} & \text{regions II and IV} \\ e^{0} & \text{region III.} \end{cases} \tag{2.24}$$

These phase relations must be explicitly considered in carrying out the integration along the positive real axis.

III. SCATTERING-ANGLE AND ENERGY DEPENDENCE OF ELASTIC DIFFERENTIAL SCATTERING CROSS SECTION

Applications of the first-order FWMS approximation ($T_2 + T_3$ terms) of Sec. II to elastic scattering are carried out for the following three-body systems

$$e^+ + (e^-e^+) \to e^+ + (e^-e^+), \tag{3.1a}$$

$$p^+ + (e^-e^+) \to p^+ + (e^-e^+), \tag{3.1b}$$

$$e^{\pm} + \mathrm{H} \to e^{\pm} + \mathrm{H}, \tag{3.1c}$$

$$p^+ + \mathrm{H} \to p^+ + \mathrm{H}, \tag{3.1d}$$

$$p^+ + (e^-\mu^+) \to p^+ + (e^-\mu^+). \tag{3.1e}$$

The results so obtained are compared with the first-order Born approximation ($V_2 + V_3$ terms) as well as with experimental measurements and the Glauber-eikonal approximation when available. These processes are chosen to illustrate the features for which the first-order Born approximation has failed.

In Fig. 1, the differential cross sections for the elastic scattering of p^+ and e^+ by positronium obtained in the first-order FWMS approximation are shown as a function of energy for two fixed scattering angles. As mentioned before, for these elastic-scattering processes the first-order Born approximation yields a zero for the amplitude. In the first-order FWMS approximation, the $e^+ - e^-$ and $e^+ - e^+$ as well as the $p^+ - e^-$ and $p^+ - e^+$ pair interactions between the incident and target particles are distinguishable through their analytic properties in addition to the sign of the interaction. This then prevents the contributions coming from the two pair interactions from cancelling each other, unlike the case in the first-order Born approximation.

In Fig. 2, a comparison of the energy dependence of the differential elastic ($e^{\pm}$, H) scattering cross sections in the first-order FWMS and Born approximations is given for two fixed scattering angles. Significant differences between the (e^-, H) and (e^+, H) scatterings are found in the FWMS approximation even at energies as high as in the keV energy region. The two differential cross sections merge together at $E > 20$ keV. The surprising feature of the first-order FWMS results for the ($e^{\pm}$, H) system lies in the fact that the differential cross sections begin to converge to the first-order Born cross section at energies as high as in the keV region.

This feature is more evident in Fig. 3 where a comparison of the scattering-angle dependence of the differential elastic (e^-, H) scattering cross section in the first-order FWMS and Born approxi-

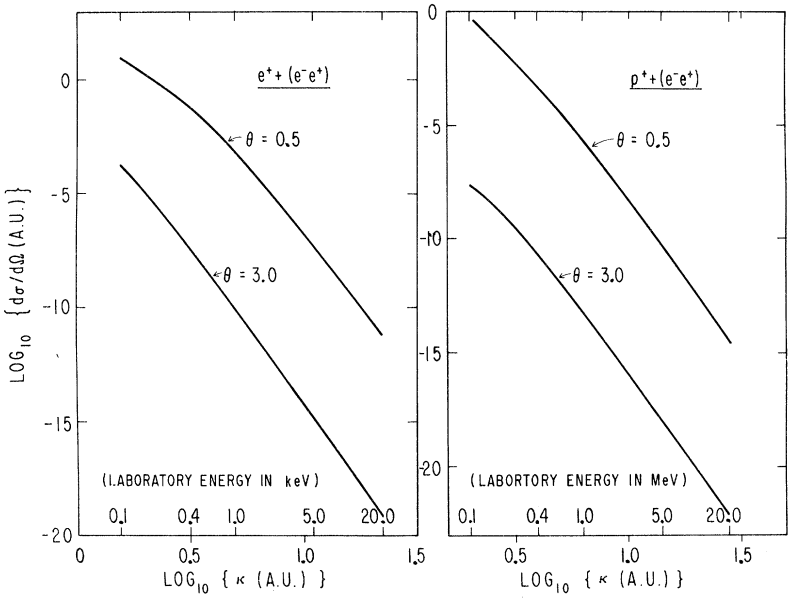

FIG. 1. Energy dependence of the differential elastic (e^+, e^-e^+) and (p^+, e^-e^+) scattering cross section at two fixed c.m. scattering angles in the first-order Faddeev-Watson multiple-scattering approximation.

mations is given for four fixed scattering energies. We have also included in Fig. 3 the results obtained in the Glauber-eikonal approximation.[8] It is seen that the first-order FWMS results are higher than both the first-order Born and Glauber-eikonal results, and approach the Born and Glauber results with increasing energy. The general features of the scattering-angle dependence predicted by the three approximations are, however, very similar except at the small forward angles where the first-order Born approximation fails to account for the forward-angle peaking.[2]

Experimental measurements on the angular dependence of the differential elastic (e^-, H) cross section have been made[9] in relative magnitude for several fixed incident electron energies. Different experimental uncertainties are involved for different incident electron energies.[10] To compare with the theoretical results, the experimental data are normalized to both the first-order FWMS and Glauber-eikonal theoretical results at 60° for each incident energy. We note that the first-order FWMS approximation is consistent with the Glauber-eikonal approximation in predicting the experimental observation at every energy in view of the experimental uncertainties. The magnitudes of the cross section are, however, different. The difference remains significant until in the keV energy region.

It has long been generally believed that at sufficient high energies the first-order Born approximation would be accurate. The Born results in the energy range $E = 100$–500 eV have been used extensively to normalize the relative experimental measurements for electron scattering by atoms (or molecules). In the present investigation, sufficient differences are found between the first-order FWMS and Born approximations for the elastic ($e^\pm$, H) scattering as high as in the keV region and for the elastic (p^+, H) scattering (see Fig. 6 below) as high as in the MeV region. This then raises the serious question of how high the energy should be for the first-order Born approximation to have a desired accuracy.

We are not saying that the differences between the two approximations are necessarily due to the failure of the first-order Born approximation nor

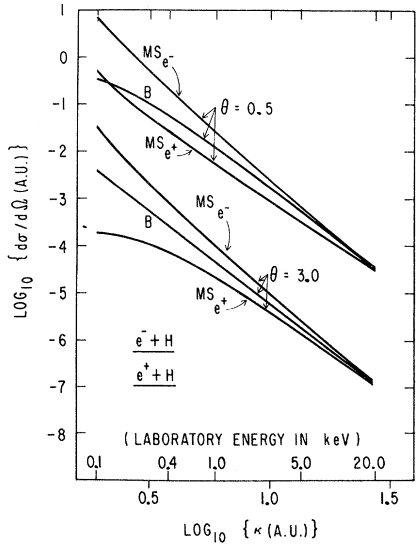

FIG. 2. Comparison of energy dependence of the differential elastic (e^-, H) and (e^+, H) scattering cross section in the first-order Faddeev-Watson multiple-scattering approximation with the Born approximation at two fixed c.m. scattering angles (in rad).

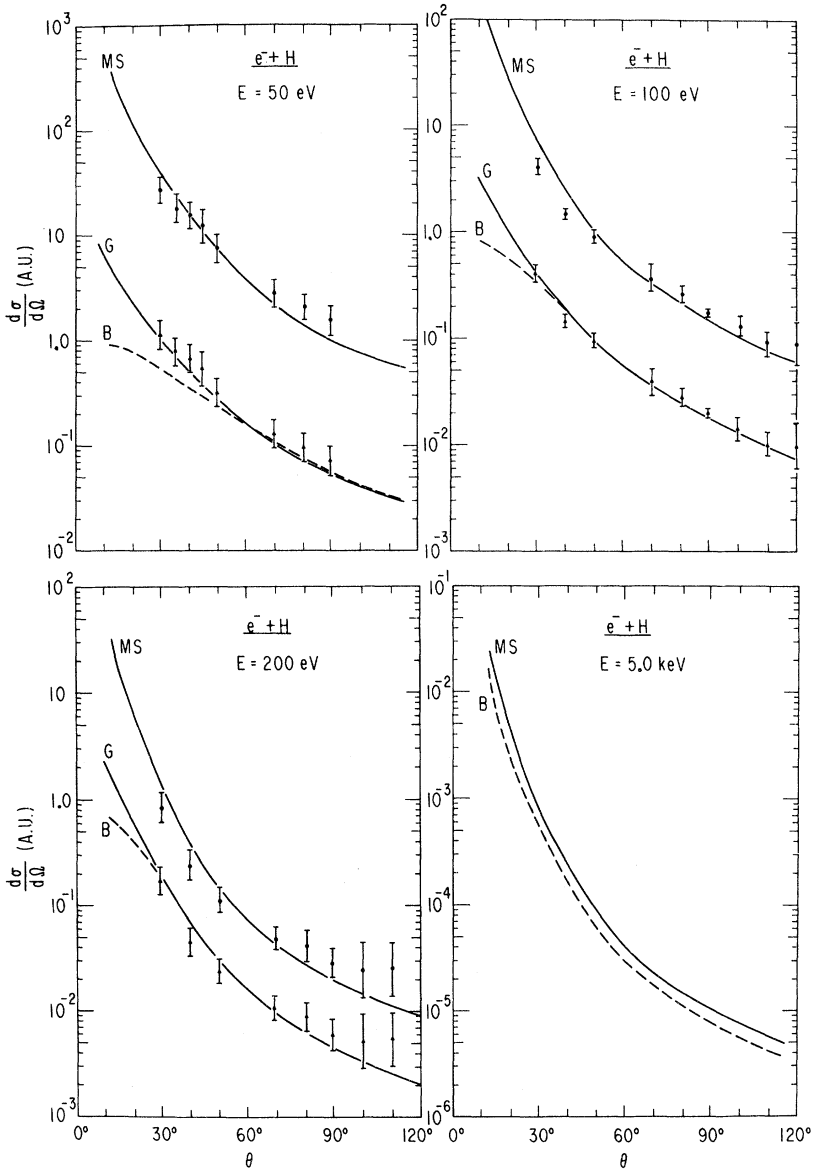

FIG. 3. Comparison of angular dependence of the differential elastic (e^-, H) scattering cross section in the first-order Born and Faddeev-Watson multiple-scattering approximations and in the Glauber-eikonal approximations with the experiment at several fixed laboratory energies. The experimental data are normalized both to the first-order Faddeev-Watson multiple-scattering results and to the Glauber-eikonal results at 60° for each energy.

are we implying that the first-order FWMS approximation is necessarily more accurate. In fact we expect that the magnitude of the cross section predicted in the first-order FWMS approximation could be somewhat reduced if the approximation is modified, to account for the unitarity constraint.[11-13] It is, however, unlikely that such an unitarity modification would bring the two approximations into agreement in the 100–150-eV energy region. It is therefore desirable to have a quantitative answer to the question of how high the energy should be for the first-order Born approximation to be accurate. The 100–500-eV energy region in which the first-order Born approximation has been considered to be accurate was suggested by Massey and Mohr[2] based on a comparison of the Born approximation with a distorted-wave calculation. The validity of the distorted-wave approximation has not been critically assessed.

In Figs. 4 and 5, the energy and angular dependences of the matrix elements in the first-order FWMS and Born approximations are shown for the (e^-, H) system. It is seen from Figs. 4 that for the repulsive $e^- - e^-$ interaction, $\langle \psi_{1s}^{(1)} | T_2 | \psi_{1s}^{(1)} \rangle$ lies below $\langle \psi_{1s}^{(1)} | V_2 | \psi_{1s}^{(1)} \rangle$ and approaches it from below at high energies. For the attractive e^--p^+ interaction, the situation is reversed. We have $\langle \psi_{1s}^{(1)} | T_3 | \psi_{1s}^{(1)} \rangle$ lying above $\langle \psi_{1s}^{(1)} | V_3 | \psi_{1s}^{(1)} \rangle$ and approaching it from above at high energies. Since the e^--p^+ interaction is the leading interaction for the elastic (e^-, H) scattering, its increase does not get cancelled by the decrease in the repulsive e^--e^- interaction. This results in

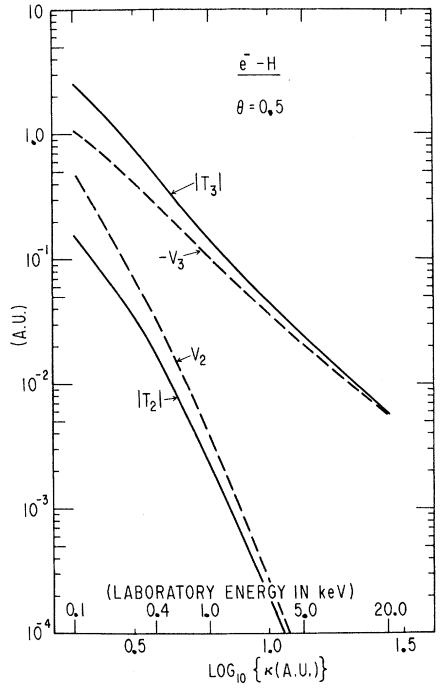

FIG. 4. Comparison of the energy dependence of the matrix elements $\langle\psi_{1s}^{(1)}|T_i|\psi_{1s}^{(1)}\rangle$ and $\langle\psi_{1s}^{(1)}|V_i|\psi_{1s}^{(1)}\rangle$ (denoted by T_i and V_i, respectively) for the (e^-, H) system at a c.m. scattering angle $\theta = 0.5$ rad.

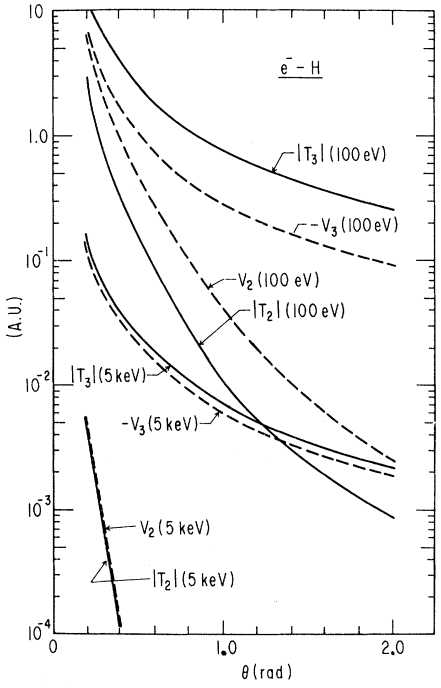

FIG. 5. Comparison of the angular dependence of the matrix elements $\langle\psi_{1s}^{(1)}|T_i|\psi_{1s}^{(1)}\rangle$ and $\langle\psi_{1s}^{(1)}|V_i|\psi_{1s}^{(1)}\rangle$ (denoted by T_i and V_i, respectively) for the (e^-, H) system at two fixed laboratory energies.

a net increase in the differential cross section. From the angular dependence of these matrix elements shown in Fig. 5, it is seen that for a given energy the difference between $\langle\psi_{1s}^{(1)}|T_i|\psi_{1s}^{(1)}\rangle$ and $\langle\psi_{1s}^{(1)}|V_i|\psi_{1s}^{(1)}\rangle$ remains reasonably constant with the scattering angle.

In Paper IV, we have remarked that for certain mass systems, such as the (p^+, H) and (p^+, $e^-\mu^+$) systems, the energy dependence of the differential scattering cross section would change according to the first-order Born approximation from an E^{-2} to an E^{-6} energy dependence with increasing energy. This is particularly noticeable for large-angle scatterings (see Figs. 1 and 2 of Paper IV). In Fig. 6 it is shown that a similar behavior is also predicted in the first-order FWMS approximation for the differential elastic (p^+, H) and (p^+, $e^-\mu^+$) scattering cross sections. From this figure, it is also seen

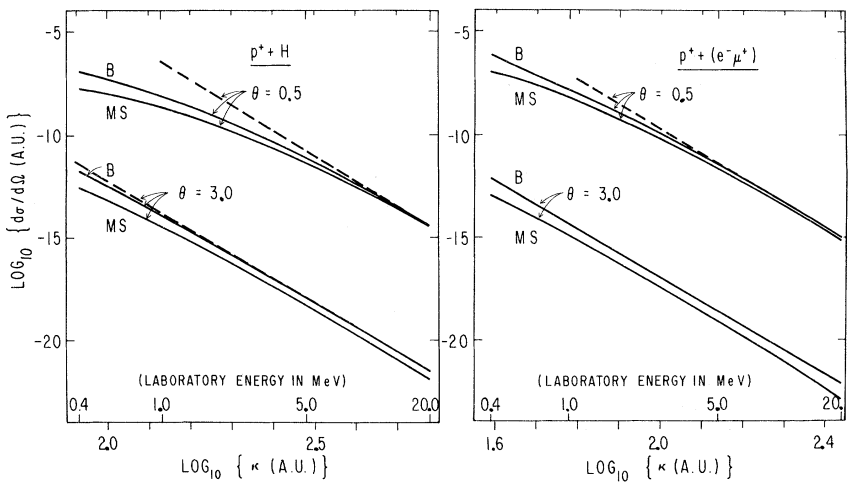

FIG. 6. Energy dependence of the differential elastic (p^+, H) and (p^+, $e^-\mu^+$) scattering cross section in the first-order Born and Faddeev-Watson multiple-scattering approximations at two fixed c.m. scattering angles (in rad). The dashed curves are the cross sections obtained from the high-energy limit of the exact first-order Born approximation given by Eq. (IV 3.24).

that the first-order FWMS and Born approximations approach each other in the MeV energy region at small angles. For large angles, they do not appear to converge into each other. Similar behavior is observed for the differential (p^+, H) and (p^+, $e^-\mu^+$) electron-transfer cross sections as shown in Figs. 4 and 13 of Paper VI.[14]

IV. CONCLUDING REMARKS

In our investigation, we have shown that by allowing the attractive and repulsive pair interactions between the incident and the target particles to go off the energy shell in the first-order FWMS approximation several anomalous features due to the corresponding bare pair interactions in the first-order Born approximations are removed. What we have done in the first-order FWMS approximation amounts to summing up all the disconnected diagrams involving the same pair interactions to all orders in the Born series. The first-order FWMS approximation contains therefore contributions coming from all-order Born approximations involving no cross-pair interactions. Thus the second-order Born terms such as

$$\langle \psi_{1s}^{(1)} | V_2 G_0 V_3 | \psi_{1s}^{(1)} \rangle \quad \text{and} \quad \langle \psi_{1s}^{(1)} | V_3 G_0 V_2 | \psi_{1s}^{(1)} \rangle$$

are not contained in the first-order FWMS approximation. One may ask whether the inclusion of these terms would give rise to cancellation and bring the first-order FWMS approximation in agreement with the first-order Born approximation at a somewhat lower energy. Further investigations are apparently needed. In any event, the differences found in the magnitude of the cross section between the two first-order approximations call for the need to examine quantitatively how high the energy should be for the first-order Born approximation to be accurate. The energy for the first-order Born approximation to be accurate can be determined experimentally by locating the energy above which the difference between the (e^-, H) and (e^+, H) scattering ceases to be appreciable.

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*Research supported by the National Science Foundation, under Grant No. GP-20459 and by the Atomic Energy Commission under Contract No. AT(04-3)-34, PA 196.

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