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e^+ -H Collisions by the Faddeev Approach

G. Banerji, A. S. Ghosh, and N. C. Sil

*Department of Theoretical Physics, Indian Association for the Cultivation of Science,
Calcutta-32, India*

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The positron-hydrogen collision problem has been investigated by the Faddeev formalism as used by Sloan and Moore. The cross sections for the elastic scattering and the positronium formation have been calculated above the positronium-formation threshold for the incident positron energy up to 1.36 keV, and the results have been compared with those of other theoretical calculations. Appreciable differences have been found between the present results for the elastic-scattering cross sections and the corresponding results obtained by the first-order Born approximation at energies as high as the order of keV. The proton-positronium elastic-scattering cross sections are also reported. These cross sections which vanish in the first-order Born approximation are found to be significant at low incident proton energies.

I. INTRODUCTION

In view of the significant physical differences between positron-atom and electron-atom interactions, the study of positron-atom collisions deserves special attention. The scattering of the positron by a hydrogen atom has been extensively investigated theoretically. Below the positronium-formation threshold some refined calculations have been performed by Schwartz,¹ Kleinman *et al.*,² Drachman,³ Perkins,⁴ and recently by Kramer and Chen.⁵ Above this threshold energy, Smith *et al.*⁶ have calculated the elastic e^+ -H-scattering cross sections by the close-coupling method. They have retained only the $1s$, $2s$, and $3s$ states of the hydrogen atom in their expansion and neglected the Ps formation. Burke *et al.*⁷ have also investigated the same problem. In their close-coupling method they have, however, considered the $1s$, $2s$, and $2p$ states of the hydrogen atom. They have obtained the values of the cross sections which are less than those of Smith *et al.*⁶ Recently Garibotti and Massaro⁸ have applied the rational Padé approximants to calculate the cross sections for the elastic scattering of electrons and positrons by a hydrogen atom. They have also neglected the effects of the rearrangement channels in both cases. The importance of the Ps-formation channel even in the

elastic scattering process has been emphasized by several authors.^{9,10} Few theoretical calculations have so far been made on the e^+ -H collision problem including the effect of the Ps formation, and the results of these calculations do not agree among themselves. Bransden and Jundi¹¹ have investigated the e^+ -H collision problem in the close-coupling approximation taking the ground states of the hydrogen atom and the positronium in their eigenfunction expansion for the incident energy varying from 6.8 to 11.1 eV. They have considered the partial waves for $l=0$ and $l=1$ only. As they have concentrated on the low-energy region, they have also taken into account the effects of polarization in both the channels. Fels and Mittleman¹² have also considered the same problem, making allowance for the effect of polarization of the hydrogen atom and the positronium through phenomenological potentials. They have considered four partial waves ($l=0, 1, 2$, and 3) and obtained the values of the Ps-formation cross sections much smaller as compared to the first-Born-approximation (FBA) results of Massey and Mohr.¹³

The scattering of the positron by a hydrogen atom is a three-body problem, and this can be better investigated by the rigorous and elegant formulation of Faddeev.¹⁴ Sinfailam and Chen¹⁵ have used the Faddeev-Watson multiple-scatter-

ing¹⁶ (FWMS) approximation, suitable for high energies, to obtain the cross sections for e^+ -H collision. There is appreciable difference between their results and the FBA results for the differential cross sections for e^+ -H scattering, even at an incident energy of several keV. In the present paper we have applied the approximate form of the Faddeev equations as used by Sloan and Moore¹⁷ to investigate the e^+ -H collision problem, taking into account the direct and rearrangement channels. This formalism, which is rather suitable for high energies, can include the rearrangement channels and the effect of coupling to all physical states. Further, the unitarity condition is preserved by this approximation below the breakup threshold.¹⁸ However, this formalism cannot take the effect of virtual excitations and strong distortions. In our calculations we have taken into account both the elastic and Ps-formation channels. Sil and Ghosh¹⁹ have successfully applied the same formalism to the e^- -H scattering problem, taking the exchange effect and the effects of couplings to 1s and 2s states only.

II. THEORY

Here we would not go into the details of the Faddeev formalism as used by Sloan and Moore.¹⁷ Following them, we may write the formally exact equations for the three-body scattering as (notations are same as used by them)

$$\langle \beta \vec{k}' \eta' | Y | \alpha \vec{k} \eta \rangle = \langle \beta \vec{k}' \eta' | Y^{(1)} | \alpha \vec{k} \eta \rangle + \sum_{\gamma} \sum_{\eta''=1}^{N_{\gamma}} \int d\vec{k}'' \times \frac{\langle \beta \vec{k}' \eta' | Y^{(1)} | \gamma \vec{k}'' \eta'' \rangle \langle \gamma \vec{k}'' \eta'' | Y | \alpha \vec{k} \eta \rangle}{s - E''}, \quad (2.1)$$

where Y and $Y^{(1)}$ denote the three- and two-body operators, and $\langle \vec{k}' \eta' | Y | \vec{k} \eta \rangle$ and $\langle \vec{k}' \eta' | Y^{(1)} | \vec{k} \eta \rangle$ are their corresponding matrix elements, respectively. The summation over γ indicates the different channels and the summation over η'' stands for the different bound states in a particular channel. Now, the pole term in (2.1) (with $s = E + i\epsilon$) may be expressed as a sum of δ function and principal-value parts:

$$(E - E'' + i\epsilon)^{-1} = -i\pi\delta(E - E'') + P(E - E'')^{-1}.$$

The pole term is then approximated^{16,17} for the high-energy region by retaining only the δ function, and this means that only the physical amplitudes are taken into account in the formalism. Equation (2.1) then takes the form

$$\langle \vec{k}' \eta' | Y_{\beta\alpha} | \vec{k} \eta \rangle = \langle \vec{k}' \eta' | Y_{\beta\alpha}^{(1)} | \vec{k} \eta \rangle - i\pi \sum_{\gamma} \sum_{\eta''=1}^{N_{\gamma}} \int d\vec{k}'' \times \langle \vec{k}' \eta' | Y_{\beta\gamma}^{(1)} | \vec{k}'' \eta'' \rangle \delta(E - E'') \langle \vec{k}'' \eta'' | Y_{\gamma\alpha} | \vec{k} \eta \rangle. \quad (2.2)$$

For the positron-hydrogen system, we choose particle 1 to be the positron, particle 2 to be the atomic electron, and particle 3 to be the proton so that the potentials are given by

$$V_{13} = \frac{1}{r_1}, \quad V_{23} = -\frac{1}{r_2}, \quad \text{and} \quad V_{12} = -\frac{1}{|\vec{r}_1 - \vec{r}_2|}.$$

Here V_{13} produces no bound states. In performing the actual calculations, we have included the Ps channel and retained only the ground states of the positronium and the hydrogen atom. Then we have the following equations for the three-body scattering amplitudes:

$$\begin{aligned} \langle \vec{k}' 1s | Y_{11} | \vec{k} 1s \rangle &= \langle \vec{k}' 1s | Y_{11}^{(1)} | \vec{k} 1s \rangle - i\pi \int d\vec{k}'' \langle \vec{k}' 1s | Y_{11}^{(1)} | \vec{k}'' 1s \rangle \delta(E - E'') \langle \vec{k}'' 1s | Y_{11} | \vec{k} 1s \rangle \\ &\quad - i\pi \int d\vec{k}_1'' \langle \vec{k}' 1s | Y_{13}^{(1)} | \vec{k}_1'' 1s \rangle \delta(E - E'') \langle \vec{k}_1'' 1s | Y_{31} | \vec{k} 1s \rangle, \end{aligned} \quad (2.3a)$$

$$\begin{aligned} \langle \vec{k}' 1s | Y_{31} | \vec{k} 1s \rangle &= \langle \vec{k}' 1s | Y_{31}^{(1)} | \vec{k} 1s \rangle - i\pi \int d\vec{k}_1'' \langle \vec{k}' 1s | Y_{31}^{(1)} | \vec{k}_1'' 1s \rangle \delta(E - E'') \langle \vec{k}_1'' 1s | Y_{11} | \vec{k} 1s \rangle \\ &\quad - i\pi \int d\vec{k}'' \langle \vec{k}' 1s | Y_{33}^{(1)} | \vec{k}'' 1s \rangle \delta(E - E'') \langle \vec{k}'' 1s | Y_{31} | \vec{k} 1s \rangle; \end{aligned}$$

$$\begin{aligned} \langle \vec{k}' 1s | Y_{13} | \vec{k} 1s \rangle &= \langle \vec{k}' 1s | Y_{13}^{(1)} | \vec{k} 1s \rangle - i\pi \int d\vec{k}_1'' \langle \vec{k}' 1s | Y_{13}^{(1)} | \vec{k}_1'' 1s \rangle \delta(E - E'') \langle \vec{k}_1'' 1s | Y_{33} | \vec{k} 1s \rangle \\ &\quad - i\pi \int d\vec{k}'' \langle \vec{k}' 1s | Y_{11}^{(1)} | \vec{k}'' 1s \rangle \delta(E - E'') \langle \vec{k}'' 1s | Y_{13} | \vec{k} 1s \rangle, \end{aligned} \quad (2.3b)$$

$$\begin{aligned} \langle \vec{k}' 1s | Y_{33} | \vec{k} 1s \rangle &= \langle \vec{k}' 1s | Y_{33}^{(1)} | \vec{k} 1s \rangle - i\pi \int d\vec{k}'' \langle \vec{k}' 1s | Y_{33}^{(1)} | \vec{k}'' 1s \rangle \delta(E - E'') \langle \vec{k}'' 1s | Y_{33} | \vec{k} 1s \rangle \\ &\quad - i\pi \int d\vec{k}_1'' \langle \vec{k}' 1s | Y_{31}^{(1)} | \vec{k}_1'' 1s \rangle \delta(E - E'') \langle \vec{k}_1'' 1s | Y_{13} | \vec{k} 1s \rangle. \end{aligned}$$

The Eqs. (2.3a) and (2.3b) are two sets of coupled equations. On neglecting the double scattering and

higher-order terms of the multiple-scattering series, the two-body operators may be approxi-

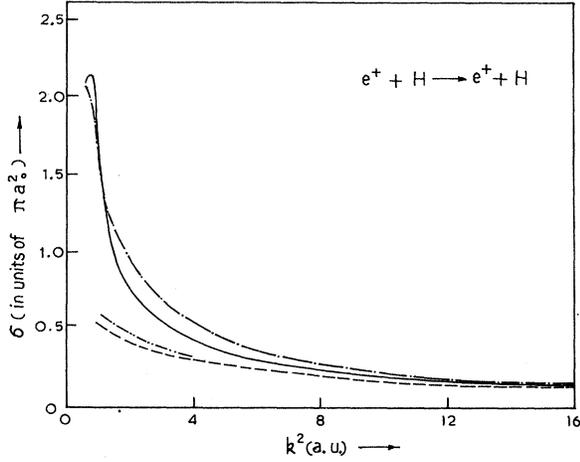


FIG. 1. Total cross sections (in units of πa_0^2) for the positron-hydrogen elastic scattering are plotted against k^2 (a. u.), the incident positron energy being $13.6 k^2$ eV. Solid line: present calculation; single-chained curve: Born results; double-chained curve: Burke *et al.* (Ref. 7); and dashed curve: Garibotti and Massaro (Ref. 8).

mated¹⁷ in the high-energy limit as

$$Y_{11}^{(1)} \simeq V_{13} + V_{12}, \quad Y_{31}^{(1)} \simeq V_{23} + V_{13},$$

$$Y_{13}^{(1)} \simeq V_{12} + V_{13}, \quad Y_{33}^{(1)} \simeq V_{13} + V_{23}.$$

With this approximation, the matrix elements for the two-body operators may be written in terms of the corresponding FBA amplitudes:

$$\langle \vec{k}' \eta' | Y_{\beta\alpha}^{(1)} | \vec{k} \eta \rangle = -(1/4\pi^2 \mu_\beta) f_{\beta\alpha}^B(\hat{k}' \cdot \hat{k}),$$

where μ_β is the reduced mass in the channel β . In a similar way we write the three-body matrix elements as

$$\langle \vec{k}' \eta' | Y_{\beta\alpha} | \vec{k} \eta \rangle = -(1/4\pi^2 \mu_\beta) f_{\beta\alpha}(\hat{k}' \cdot \hat{k}).$$

We now use the partial-wave form for $f_{\beta\alpha}^B(\hat{k}' \cdot \hat{k})$:

$$f_{\beta\alpha}^B(\hat{k}' \cdot \hat{k}) = \frac{1}{k} \sum_{l=0}^{\infty} (2l+1) T_l^B(\beta\alpha) P_l(\hat{k}' \cdot \hat{k}).$$

Similar expressions have been used for $f_{\beta\alpha}(\hat{k}' \cdot \hat{k})$. After the partial-wave analysis, we have obtained two sets of coupled algebraic equations:

$$T_l(11) = \frac{T_l^B(11)}{1 - iT_l^B(11)} + i \frac{T_l^B(13)}{1 - iT_l^B(11)} T_l(31), \quad (2.4a)$$

$$T_l(31) = \frac{T_l^B(31)}{1 - iT_l^B(33)} + i \frac{T_l^B(31)}{1 - iT_l^B(33)} T_l(11);$$

$$T_l(13) = \frac{T_l^B(13)}{1 - iT_l^B(11)} + i \frac{T_l^B(13)}{1 - iT_l^B(11)} T_l(33), \quad (2.4b)$$

$$T_l(33) = \frac{T_l^B(33)}{1 - iT_l^B(33)} + i \frac{T_l^B(31)}{1 - iT_l^B(33)} T_l(13).$$

It may be noted that $T_l^B(31) = T_l^B(13)$ and $T_l^B(33) = 0$ for all values of l . When $T_l(31)$ and $T_l(13)$ are ex-

pressed completely in terms of the two-body FBA amplitudes, we find that $T_l(31) = T_l(13)$. Now, the differential cross sections are given by the relation

$$\frac{d\sigma_{\beta\alpha}}{d\Omega} = \frac{\mu_\alpha}{\mu_\beta} \frac{k'}{k} |f_{\beta\alpha}(\hat{k}' \cdot \hat{k})|^2, \quad (2.5)$$

where μ_α and μ_β are the reduced masses of the channels α and β , respectively. The total cross sections $\sigma_{\beta\alpha}$ are obtained as usual by the integration of the expression (2.5) over the solid angle.

III. RESULTS AND DISCUSSION

The present formalism has been applied to the three-body systems for the following elastic and rearrangement processes:

$$e^+ + H(1s) \rightarrow e^+ + H(1s), \quad (3.1a)$$

$$e^+ + H(1s) \rightarrow \text{Ps}(1s) + H^+. \quad (3.1b)$$

The total cross sections are calculated for these processes for $k^2 = 0.6$ to 100 a. u. (atomic units have been used throughout except where otherwise stated). We have also obtained the differential cross sections at 0° for all energies. As inputs, we require the FBA partial-wave amplitudes $T_l^B(11)$ and $T_l^B(31)$ for the processes (3.1a) and (3.1b). For the elastic collision, we have taken $T_l^B(11)$ as given by Mott and Massey.²⁰ For the rearrangement channel, we have used the integral expression for the corresponding FBA amplitudes found by Cheshire.²¹ To get the required partial-wave amplitudes $T_l^B(31)$, we have multiplied the integrand of this expression by $P_l(\hat{k}' \cdot \hat{k})$ and integrated first

TABLE I. Total cross sections (in units of πa_0^2) for the positron-hydrogen elastic scattering. (The number in the parentheses in each entry is the exponent of 10 by which the cross-section value should be multiplied.)

k^2	Born results	Present calculations
0.6	2.061	2.111
0.75	1.831	2.142
0.85	1.703	1.982
0.88	1.668	1.926
0.92	1.624	1.849
0.95	1.592	1.792
1.00	1.542	1.697
1.25	1.330	1.299
2.00	9.383(-1)	7.390(-1)
4.00	5.227(-1)	4.122(-1)
5.00	4.275(-1)	3.471(-1)
10.00	2.234(-1)	1.957(-1)
18.00	1.265(-1)	1.160(-1)
26.00	8.826(-2)	8.265(-2)
34.00	6.776(-2)	6.427(-2)
40.00	5.771(-2)	5.510(-2)
60.00	3.861(-2)	3.737(-2)
100.00	2.323(-2)	2.276(-2)

with respect to $(\hat{k}' \cdot \hat{k})$ analytically: The original one-dimensional integration is next performed numerically with the help of the Gauss-Legendre quadrature formula.

In Fig. 1 we have plotted our results for the total cross sections for the e^+ -H elastic scattering from $k^2 = 0.6$ to 16 along with the FBA results and compared them with other theoretical results found by Burke *et al.*⁷ and Garibotti and Massaro.⁸ Our results near the Ps-formation threshold are slightly greater than the FBA values. For $k^2 > 1$ (i. e., 13.6 eV), our curve lies below the FBA curve. With the increase of energy, the difference between the FBA and the present curve diminishes. Sloan and Moore¹⁷ have also obtained a similar feature for the e^- -H scattering. The curves found by Burke *et al.*⁷ and Garibotti and Massaro⁸ lie below the FBA and the present curves. However, the difference between the present curve and that of Garibotti and Massaro⁸ has diminished appreciably with the increase of energy. The lower values of Burke *et al.*⁷ compared to ours may be attributed to the fact that they have taken a greater number of states in the direct channel, but neglected completely the rearrangement channel, which has a pronounced effect at low energies. For e^- -H scattering, Sil and Ghosh¹⁹ have shown that the effect of couplings to 1s and 2s states in the direct channel causes a reduction in the cross section, and this reduction is appreciable in the low-energy region. It has been pointed out²² that the cross-section values decrease with the increase of the number of states included in the direct channel. Further, Sil and Ghosh¹⁹ have observed that in the low-energy region the effect of the rearrangement channel ap-

preciably enhances the elastic-scattering cross-section values in e^- -H scattering.

In Table I we have displayed the present theoretical results for the total cross section in e^+ -H elastic scattering and have compared them with the corresponding FBA values. The differences between our results and those of FBA decrease with the increase of energy. However, even at $k^2 = 100$ (i. e., $E = 1.36$ keV) our value for the total cross section differs from that of FBA by about 2%. This feature has also been noticed by Sloan and Moore¹⁷ and Sil and Ghosh¹⁹ for e^- -H scattering. More recently Sinfailam and Chen¹⁵ have also found appreciable differences between their results obtained by the first-order FWMS approximation and the FBA values for e^\pm -H systems at energies as high as the keV order. These findings contradict the conventional belief that FBA is supposed to be accurate for e^\pm -H scattering at energies above 100 eV. We have presented our results for the differential cross section in the forward direction for the e^+ -H elastic scattering in Fig. 2. It is to be noted that the corresponding FBA cross sections are unity for all k^2 .

In Table II we have shown our results for the total cross section for the Ps formation for the energy range $0.6 \leq k^2 \leq 100$ along with the corresponding FBA results and have compared them with the values obtained by Cheshire.²¹ Throughout the energy range considered, the results of the present calculation are always lower than the FBA values, while the values obtained by Cheshire²¹ are always greater than both these results. At low energies there is a marked disagreement among the three sets of results. In the range $0.75 < k^2 < 1$, for

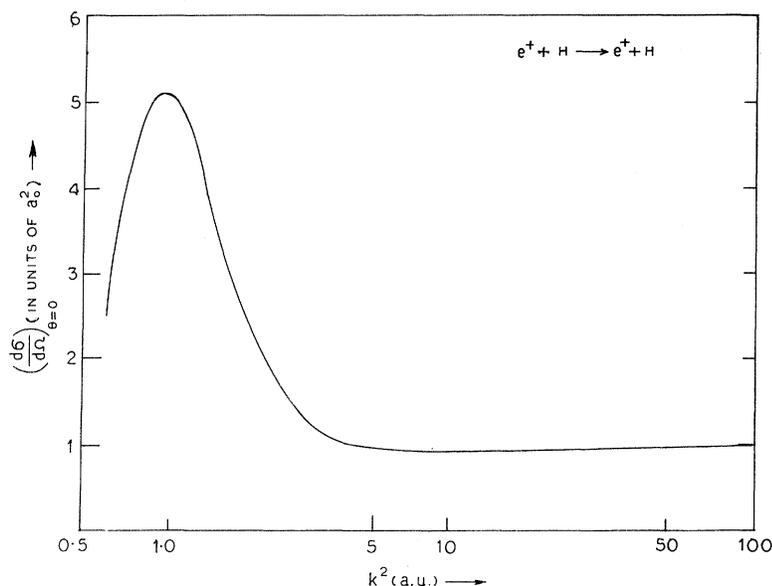


FIG. 2. Differential cross sections (in units of a_0^2) for the positron-hydrogen elastic scattering in the forward direction as a function of k^2 (a. u.).

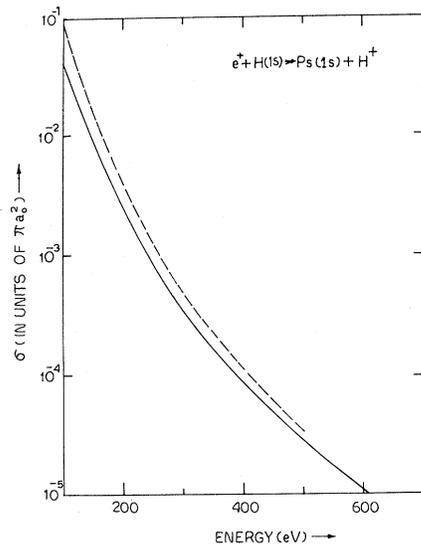


FIG. 3. Comparison of the Chen-Kramer and the present results for the total cross section (in units of πa_0^2) for the positronium formation in hydrogen as a function of the laboratory energy of the projectile in eV.

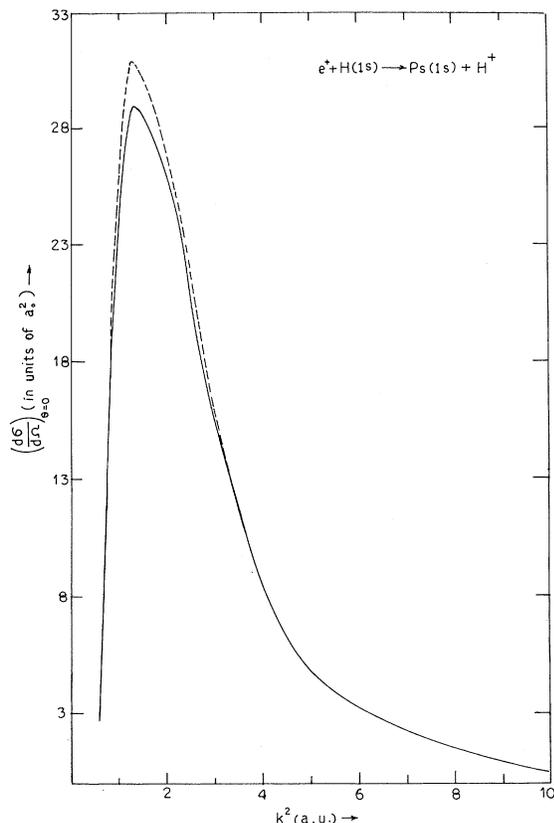


FIG. 4. Comparison of the FBA and the present results for the differential cross section (in units of a_0^2) for the positronium formation in hydrogen in the forward direction as a function of k^2 (a.u.).

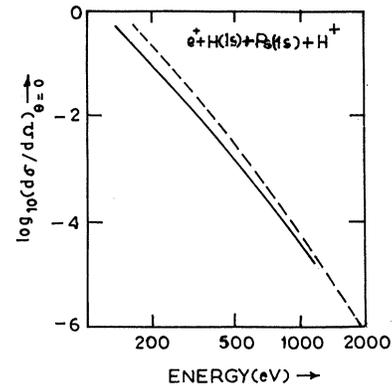


FIG. 5. Comparison of the Chen-Kramer and the present results for the differential cross section (in units of a_0^2) for the positronium formation in hydrogen in the forward direction as a function of the laboratory energy of the positron in eV.

example, our results are lower by about 30% than the FBA values which, in turn, are more than 10 times smaller than the values given by Cheshire.²¹ All the three sets have a maximum at about the same energy region, though the peak values are widely different. Our peak value is about 1.4 times smaller, while that obtained by Cheshire²¹ is about 14 times larger, than the FBA peak value. With the increase in energy our values tend more and more towards the FBA values, and the difference is negligible at $k^2 = 10$ and above. The values obtained by Cheshire,²¹ on the other hand, show a

TABLE II. Total cross sections (in units of πa_0^2) for the positronium formation in hydrogen. (The number in parentheses in each entry is the exponent of 10 by which the cross-section value should be multiplied.)

k^2	Born results	Present calculations	Results of Cheshire ^a
0.6	2.661	1.632	...
0.75	4.474	2.992	6.8(1)
0.85	4.843	3.377	...
0.88	4.875	3.438	...
0.92	4.876	3.489	...
0.95	4.853	3.508	...
1.00	4.778	3.510	4.8(1)
1.25	4.063	3.190	3.3(1)
2.00	2.007	1.765	1.2(1)
4.00	3.626(-1)	3.486(-1)	...
5.00	1.800(-1)	1.753(-1)	5.9(-1)
10.00	1.348(-2)	1.334(-2)	2.9(-2)
18.00	9.794(-4)	9.726(-4)	1.4(-3)
26.00	1.626(-4)	1.616(-4)	2.0(-4)
34.00	4.132(-5)	4.106(-5)	4.5(-5)
40.00	1.765(-5)	1.754(-5)	1.8(-5)
60.00	1.994(-6)	1.982(-6)	...
100.00	1.166(-7)	1.159(-7)	...

^aReference 21.

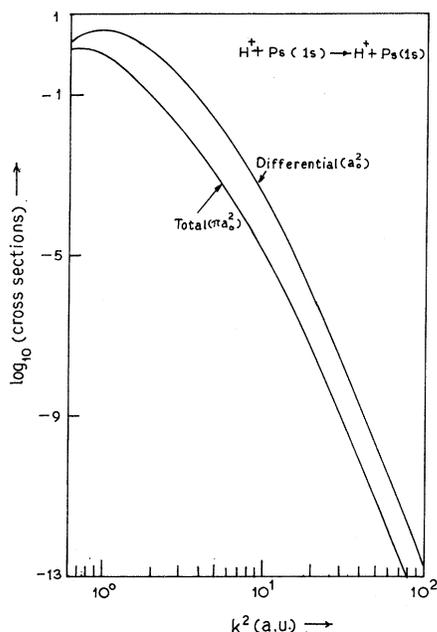


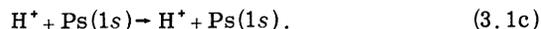
FIG. 6. Total cross sections (in units of πa_0^2) and the differential cross sections (in units of a_0^2) in the forward direction for the elastic proton-positronium scattering as a function of k^2 (a. u.), where the incident proton energy $\approx 6.24 (2k^2 - 1)$ keV.

marked difference with the FBA results at the above energy, even at $k^2 = 40$ (i. e., 544-eV) the difference is about 2.5%. However, the reliability of the impulse approximation below $k^2 = 10$ is doubtful, as pointed out by Cheshire himself. Akerib and Borowitz²³ have also shown for the e^- -H scattering that the impulse approximation is not applicable below 150 eV. The results obtained by them for the excitation processes are inferior to the FBA values when compared with the experimental findings.

Majumdar and Rajagopal²⁴ have also obtained the Ps-formation cross sections using an impulse-type approximation. Their formalism is rather suitable for a high-energy region. The cross-section values obtained by them are higher than the FBA values at low energies up to 66 eV and then fall below the FBA values. They have obtained a maximum at $k^2 = 0.85$; the peak value is about 1.4 times greater than that obtained by FBA. In Fig. 3 we have compared our results for the total cross section of the Ps formation with those obtained by

Chen and Kramer.²⁵ The difference between the two curves decreases slowly with the increase in energy and is expected to become negligible in the keV region. In Fig. 4 we have shown our results for the differential cross section of the Ps formation in the forward direction along with the corresponding FBA values for $0.6 \leq k^2 \leq 10$. Each of the two curves shows a peak almost in the same region; our peak value, however, is lower than that of FBA. For $k^2 \geq 4$ our curve coincides with the FBA curve. (Detailed numerical values may be available from the authors on request.) In Fig. 5 we have displayed our results for the differential cross section for the Ps formation in the forward direction in the energy region 100–1360 eV along with the corresponding results of Chen and Kramer.²⁵ Similar to the case of total cross sections we note here as well that the results of the present calculation are always lower than the corresponding values obtained by them.

From the second set of coupled equations, (2.4b), we have obtained the cross sections for the elastic process:



It is to be mentioned that the FBA amplitude for the above process vanishes, since the positronium target is made of equal-mass particles having charges which are equal, but opposite in sign. From Fig. 6, where we have shown the values of the total cross sections and the differential cross sections in the forward direction for this process, one can easily find that the cross-section values are appreciable at low energies; at $k^2 = 2$ (i. e., incident proton energy ≈ 18.75 keV) the value of the total cross section for this process is about $0.05\pi a_0^2$. Sinfailam and Chen¹⁵ have also obtained the differential cross sections for nonzero scattering angle for this process using FWMS approximation.

In our investigations we have found appreciable differences between our results and the FBA values for the elastic e^- -H scattering at energies as high as in the keV region. The present calculations take care of the unitarity but neglect the effects of virtual excitations and multiple scattering. However, these effects are not expected to have significant influence on the results at sufficiently high energies ($E \geq 500$ eV). Some more investigations may be required to ascertain the exact behavior of these cross sections.

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PHYSICAL REVIEW A

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Variational Technique for Scattering Theory

Herschel Rabitz*

Department of Chemistry, Princeton University, Princeton, New Jersey 08540

and

Robert Conn

Department of Nuclear Engineering, University of Wisconsin, Madison, Wisconsin 53706

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A stationary variational functional for the T matrix that uses trial T matrices rather than trial wave functions is discussed. Taking a trial T matrix expressed as a general linear combination of matrices leads to a Fredholm integral equation of the first kind for the coefficient vector. The special case of a trial function having the same form as the Born series, except with variable coefficients, is treated in detail. Requiring the functional to be stationary with this trial form leads to the previously established result of Padé approximants to the scattering amplitude. Approximate techniques are used to evaluate the high-order Born integrals, and the behavior of the Padé approximants and the Born series is investigated for a Yukawa potential. An upper bound on the series is used to estimate its radius of convergence as a function of energy and potential strength. The variational calculations converge rapidly even for cases where the Born series diverges.

I. INTRODUCTION

The use of variational methods for obtaining scattering amplitudes has always been an attractive procedure.¹ For a particular trial function with variable coefficients, it is possible to obtain a "best" amplitude by varying the coefficients in an appropriate variational principle. Two well-known stationary variational functionals for the T matrix¹ are those of Kohn² and Schwinger.³ Saraph and Seaton^{4,5} have developed an iteration-variation method which employs the Kohn principle. Burke and Seaton⁶ and Harris and Michels⁷ have recently reviewed the use of these and related procedures for electron-atom scattering. Such procedures, as with most that have been used previously, employ variational functionals that require trial wave

functions. Since we ultimately want the T matrix from a collision calculation, it can be advantageous to have procedures that deal directly with T and bypass the use of wave functions. Approximate solutions to the Lippmann-Schwinger equation for T [Eqs. (2) and (3) below] can be constructed by a variety of methods,^{1,8,9} and these solutions can be further improved by treating them as trial variational functions. In this paper we shall explore the use of a functional presented by Newton that uses trial T matrices.¹⁰ In Sec. II the general approach to obtaining the scattering amplitude from trial functions with linear variational coefficients is reviewed with particular emphasis on the functional using trial T matrices. In Sec. III trial T matrices first suggested by Cini and Fubini¹¹ are used to illustrate the formalism. In the particular case of