Electron capture by positrons from atomic hydrogen using the second Born and Padé approximations

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(Received 7 January 1974)

The cross sections for electron capture by positrons from atomic hydrogen are calculated using the second Born approximation and the method of Padé approximants for incident positron energy ranging from 12 to 500 eV. The results are compared with those obtained in the first Born approximation and other theoretical calculations. The contributions from the intermediate states higher than the first to the second-order rearrangement scattering amplitude are found to be significant. The nature of the variation of the second Born and the Padé differential cross sections with the angle of scattering is discussed.

I. INTRODUCTION

Electron capture by positrons from atomic hydrogen is one of the simplest rearrangement collision processes where the wave functions of the initial and the final unperturbed states are exactly known. A study of the process offers a good opportunity for making a comparison among the different approximation methods available for dealing with a rearrangement. Massey and Mohr[1] used the first Born approximation (FBA) to calculate the cross section for positronium formation in atomic hydrogen. As is well known, the first Born approximation to the rearrangement scattering amplitude is the leading term of the Born series for the amplitude. The second term of the series involves a sum over an infinite number of intermediate states and the evaluation of the contribution of even the first state is laborious.[2] There is also the problem of the convergence of the Born series for the rearrangement scattering amplitude and that of making a reliable estimate of the amplitude from the first few terms of the series. A suitable approach for the solution of the last problem is to use the rational Padé approximants[3] which can be used to represent functions to a good approximation even in cases where the convergence properties of the power-series expansions are poor.

In the present work we have used the second Born approximation (SBA) and the Padé-approximant method to investigate the positronium formation process in atomic hydrogen. The summation over the infinite number of intermediate states occurring in the second term of the Born series is done following a method of approximation used by Holt and Moiseiwitsch[4] for some direct scattering processes. This method and the Padé-approximant method are explained in Secs. II and III. In Sec. IV we have compared our results with those obtained by other workers.

Atomic units will be used throughout the present work.

II. SECOND BORN APPROXIMATION

The proton will be assumed to be at rest and the position vectors of the positron and the electron from the proton will be denoted by $\vec{r}_1$ and $\vec{r}_2$, respectively. The electron is initially bound to the proton, forming the hydrogen atom in its ground state. It is captured by the incident positron and a positronium is formed, again in its ground state. The Born series for the rearrangement scattering amplitude for the process is

$$g(\theta, k_i) = g_1(\theta, k_i) + g_2(\theta, k_i) + \cdots , \tag{1}$$

where θ is the angle of scattering, $\vec{k}_i$ is the momentum of the incident positron, and the first two terms on the right-hand side are given, respectively, by

$$g_1(\theta, k_i) = -\frac{1}{\pi} \int e^{-i\vec{k}_f \cdot \vec{r}_f} \varphi_1^*(\vec{r}_{12}) \left(\frac{1}{r_1} - \frac{1}{r_2}\right) \times e^{i\vec{k}_i \cdot \vec{r}_1} \psi_1(\vec{r}_2)\, d\vec{r}_f\, d\vec{r}_{12} \tag{2}$$

and

$$g_2(\theta, k_i) = \sum_n g_2^{(n)}(\theta, k_i) , \tag{3}$$

with

$$g_2^{(n)}(\theta,k_i)=\lim_{\epsilon\to 0}\frac{1}{4\pi^4}\int e^{-i\vec{k}_f\cdot\vec{r}_f}\varphi_1^*(\vec{r}_{12})\left(\frac{1}{r_1}-\frac{1}{r_2}\right)\frac{\exp[i\vec{q}\cdot(\vec{r}_1-\vec{r}_1')]}{q^2-k_n{}^2-i\epsilon}\psi_n(\vec{r}_2)\psi_n^*(\vec{r}_2')$$
$$\times\left(\frac{1}{r_1'}-\frac{1}{|\vec{r}_1'-\vec{r}_2'|}\right)e^{i\vec{k}_i\cdot\vec{r}_1'}\psi_1(\vec{r}_2')d\vec{r}_f\,d\vec{r}_{12}\,d\vec{r}_1'\,d\vec{r}_2'\,d\vec{q}\ . \tag{4}$$

The summation on the right-hand side of Eq. (3) implies a summation and an integration over all the discrete and continuum states of the hydrogen atom. Here $\vec{r}_f=\frac{1}{2}(\vec{r}_1+\vec{r}_2)$, $\vec{r}_{12}=\vec{r}_1-\vec{r}_2$, and $\vec{k}_f$ is the momentum of the final positronium in its ground state. $\varphi_1(\vec{r}_{12})$ is the wave function of the ground state of the positronium and is given by

$$\varphi_1(r_{12})=(1/8\pi)^{1/2}e^{-(1/2)r_{12}}\ . \tag{5}$$

ψ_n represents the wave function of the hydrogen atom in the state n (discrete or continuous) with eigenenergy E_n, and k_n is given by

$$\tfrac{1}{2}k_n{}^2+E_n=\tfrac{1}{2}k_i{}^2+E_1\ . \tag{6}$$

If we retain only the first two terms in Eq. (1) we get the second Born approximation to the rearrangement scattering amplitude and the corresponding differential cross section for positronium formation in atomic hydrogen becomes

$$I(\theta,k_i)=\frac{k_f}{2k_i}\,|g_1(\theta,k_i)+g_2(\theta,k_i)|^2. \tag{7}$$

The difficulty lies in calculating the sum occurring on the right-hand side of Eq. (3). Majumdar and Rajagopal[2] have calculated the cross section for positronium formation by neglecting all terms with $n>1$. In order to estimate the effect of these terms, we have followed a method used by Holt and Moiseiwitsch[4] for direct scattering of electrons and protons by hydrogen atoms. We have replaced Eq. (3) by

$$g_2(\theta,k_i)=\sum_{n=1}^{N}g_2^{(n)}(\theta,k_i)+\sum_{n>N}g_2^{(n),k_{N+1}}(\theta,k_i), \tag{8a}$$

where $g_2^{(n),k_{N+1}}$ is given by the right-hand side of Eq. (4) but with k_{N+1} substituted for k_n. Because of the computational difficulty involved in the evaluation of the terms $g_2^{(n)}$, we have, for the present, taken $N=1$. Equation (8a) can then be written as

$$g_2(\theta,k_i)=g_2^{(1),k_1}(\theta,k_i)-g_2^{(1),k_2}(\theta,k_i)+\sum_n g_2^{(n),k_2}(\theta,k_i)\ . \tag{8b}$$

The third term on the right-hand side of Eq. (8b) can be reduced to a simplified form by using the closure relation

$$\sum_n\psi_n(\vec{r}_2)\psi_n^*(\vec{r}_2')=\delta(\vec{r}_2-\vec{r}_2')\ , \tag{9}$$

and is given by

$$\sum_n g_2^{(n),k_2}(\theta,k_i)=\lim_{\epsilon\to 0}\frac{1}{4\pi^4}\int e^{-i\vec{k}_f\cdot\vec{r}_f}\varphi_1^*(r_{12})\left(\frac{1}{r_1}-\frac{1}{r_2}\right)\frac{\exp[i\vec{q}\cdot(\vec{r}_1-\vec{r}_1')]}{q^2-k_2^2-i\epsilon}$$
$$\times\left(\frac{1}{r_1'}-\frac{1}{|\vec{r}_1'-\vec{r}_2|}\right)e^{i\vec{k}_i\cdot\vec{r}_1'}\psi_1(\vec{r}_2)d\vec{r}_f\,d\vec{r}_{12}\,d\vec{r}_1'\,d\vec{q}\ . \tag{10}$$

In the evaluation of the integrals occurring in Eqs. (2), (4), and (10) we first make a change of variable from $\vec{r}_f$, $\vec{r}_{12}$ to $\vec{r}_1$, $\vec{r}_2$. Using then the method of Fourier transform to separate some of the variables, we arrive at the following expressions for $g_1(\theta,k_i)$, $g_2^{(1),k}(\theta,k_i)$ $(k=k_1,k_2)$, and $\sum_n g_2^{(n),k_2}(\theta,k_i)$:

$$g_1(\theta,k_i)=-\frac{2\sqrt{8}}{\pi^2}\left(\int\frac{d\vec{p}}{(\vec{p}+\vec{k}_i-\frac{1}{2}\vec{k}_f)^2(p^2+\frac{1}{4})^2[(\vec{p}+\frac{1}{2}\vec{k}_f)^2+1]^2}-\frac{\pi^2}{[(\vec{k}_i-\frac{1}{2}\vec{k}_f)^2+\frac{1}{4}]^2[(\vec{k}_i-\vec{k}_f)^2+1]}\right), \tag{11}$$

$$g_2^{(1),k}(\theta,k_i)=\lim_{\epsilon\to 0}\frac{2\sqrt{8}}{\pi^4}\left(\int\frac{d\vec{q}\,d\vec{p}\,[(\vec{q}-\vec{k}_i)^2+8]}{(q^2-k^2-i\epsilon)(\vec{p}+\vec{q}-\frac{1}{2}\vec{k}_f)^2(p^2+\frac{1}{4})^2[(\vec{p}+\frac{1}{2}\vec{k}_f)^2+1]^2[(\vec{q}-\vec{k}_i)^2+4]^2}\right.$$
$$\left.-\pi^2\int\frac{d\vec{q}\,[(\vec{q}-\vec{k}_i)^2+8]}{(q^2-k^2-i\epsilon)[(\vec{q}-\frac{1}{2}\vec{k}_f)^2+\frac{1}{4}]^2[(\vec{q}-\vec{k}_f)^2+1][(\vec{q}-\vec{k}_i)^2+4]^2}\right), \tag{12}$$

$$\sum_n g_2^{(n),k_2}(\theta,k_i)=\lim_{\epsilon\to 0}\frac{2\sqrt{8}}{\pi^4}\Bigg[\int\frac{1}{(q^2-k_2^2-i\epsilon)(\vec{p}+\vec{q}-\frac{1}{2}\vec{k}_f)^2(p^2+\frac{1}{4})^2(\vec{q}-\vec{k}_i)^2}$$
$$\times\left(\frac{1}{[(\vec{p}+\frac{1}{2}\vec{k}_f)^2+1]^2}-\frac{1}{[(\vec{p}+\vec{q}-\vec{k}_i+\frac{1}{2}\vec{k}_f)^2+1]^2}\right)d\vec{q}\,d\vec{p}$$
$$-\pi^2\int\frac{1}{(q^2-k_2^2-i\epsilon)[(\vec{q}-\frac{1}{2}\vec{k}_f)^2+\frac{1}{4}]^2(\vec{q}-\vec{k}_i)^2}\left(\frac{1}{[(\vec{q}-\vec{k}_f)^2+1]}-\frac{1}{[(\vec{k}_i-\vec{k}_f)^2+1]}\right)d\vec{q}\Bigg]\,. \tag{13}$$

Using the Feynman parametrization technique and the method of Dalitz[5] one can reduce the above integrals to one- or two-dimensional integrals with the variables ranging from 0 to 1. The final integrations are done numerically. Substituting the values of $g_1(\theta,k_i)$ and $g_2(\theta,k_i)$ [Eq. (8b)] in Eq. (7) we get the differential cross section $I(\theta,k_i)$. The total cross section for positronium formation is now obtained from

$$Q(k_i)=2\pi\int_0^\pi I(\theta,k_i)\sin\theta\,d\theta\,. \tag{14}$$

This integral has also been evaluated numerically taking proper care of the nature of the variation of the differential cross section with the angle of scattering.

III. METHOD OF PADÉ APPROXIMANT

If $g(z)$ is a function with a formal power-series expansion

$$g(z)=a_0+a_1z+a_2z^2+\cdots, \tag{15}$$

then its $[N, M]$ Padé approximant is defined[3] as the ratio of a polynomial $P(z)$ of degree M and a polynomial $Q(z)$ of degree N, the coefficients of the polynomials being uniquely determined by equating like powers of z in the equation

$$f(z)Q(z)-P(z)=Az^{M+N+1}+Bz^{M+N+2}+\cdots \tag{16}$$

and taking

$$Q(0)=1\,. \tag{17}$$

The $[1,1]$ approximant to $g(z)$, for example, is

$$\frac{a_0a_1+(a_1^2-a_0a_2)z}{a_1-a_2z}\,. \tag{18}$$

In many cases of physical importance it has been found that the convergence properties of some sequences of Padé approximants are much better than that of a sequence consisting of partial sums of the series (15). Garibotti and Massaro[6] have found that for the elastic scattering of electrons and positrons by hydrogen atoms, even the $[1,1]$ approximant is satisfactory. We have used the $[1,1]$ Padé approximant to the series (1) to get an approximation to the rearrangement scattering amplitude,

$$g_P(\theta,k_i)=\frac{g_1^2(\theta,k_i)}{g_1(\theta,k_i)-g_2(\theta,k_i)}\,. \tag{19}$$

For $g_1(\theta,k_i)$ and $g_2(\theta,k_i)$ we take the expressions given in Eqs. (2) and (8b), respectively. The corresponding differential cross section for positronium formation is given by

$$I_P(\theta,k_i)=\frac{k_f}{2k_i}\,|g_P(\theta,k_i)|^2\,, \tag{20}$$

and the total cross section can be obtained from Eq. (14) by replacing $I(\theta,k_i)$ by $I_P(\theta,k_i)$.

IV. RESULTS AND DISCUSSION

We have calculated the total cross section Q for electron capture by positrons from atomic hydrogen using the SBA and the Padé-approximant method for incident positron energy ranging from 12 to 500 eV. Our results are shown in Figs. 1 and 2. In these figures, we have also displayed the energy dependence of the total cross section obtained in the first Born approximation. The FBA differential cross sections are calculated by simply omitting the term g_2 occurring on the right-hand side of Eq. (7); the total cross sections are then determined by using Eq. (14). As is evident from Figs. 1 and 2, the SBA total cross sections are lower than the FBA values for all incident energies above 13 eV. With the increase in the incident energy the SBA curve first comes closer to the FBA curve, but afterwards the two curves separate out. At 100 eV the total cross section obtained by the SBA differs from the FBA result by about 3.3%, but the percentage difference increases to about 8.7% at 500 eV. The total cross sections calculated by the Padé-approximant method are considerably lower than those obtained by the SBA or the FBA in the entire energy range considered. At 12 eV the Padé cross section is less than half the value obtained by the FBA method. A similar lowering of the cross section for positronium formation was obtained by Massey and Mohr[1] at 13.54 eV when, in the initial positron

wave function, the distortion of the $l = 0$ partial wave owing to the repulsive static field of the hydrogen atom was taken into account.

In Fig. 1, extending up to the incident energy of 100 eV, we have also shown the total cross sections obtained by a truncated second Born approximation (TSBA) and those calculated by Banerji, Ghosh, and Sil[7] (BGS). The TSBA total cross section at any energy is determined by integrating the corresponding differential cross section, the latter being calculated by replacing g_2 in Eq. (7) by $g_2^{(1)}$ [see Eqs. (3) and (4)]. The assumption in the TSBA is that the second-order Born term in the rearrangement scattering amplitude is dominated by only one intermediate state, namely, the ground state of the hydrogen atom, and hence the contributions from other intermediate states can be neglected.[2] The SBA results include the effect of all the intermediate states. It is seen from Fig. 1 that the contributions of the intermediate states higher than the first are significant and have, in general, an effect of lowering the total cross sections by considerable amounts. Banerji *et al.*[7] have calculated the total cross section for positronium formation in atomic hydrogen by applying an approximate form of the Faddeev equations as used by Sloan and Moore.[8] Their results lie between the FBA and the SBA cross sections for all incident energies above 16 eV.

Chen and Kramer[9] (CK) have used the first-order Faddeev-Watson multiple-scattering approximation for finding the electron transfer cross section in positron-hydrogen-atom collisions. The CK total cross sections for incident positron energy ranging between 100 and 500 eV are compared in Fig. 2 with our SBA and Padé results. Unlike the cross sections obtained by the last two methods the CK cross sections lie always above the corresponding FBA values.

Figure 3 shows the SBA and the Padé differential cross sections for positronium formation in atomic hydrogen for two different incident energies (12 and 100 eV). While the differential cross sections are all peaked in the forward direction, the nature of the variation with the angle of scattering in the Padé-approximant method is different from that obtained in the SBA. The

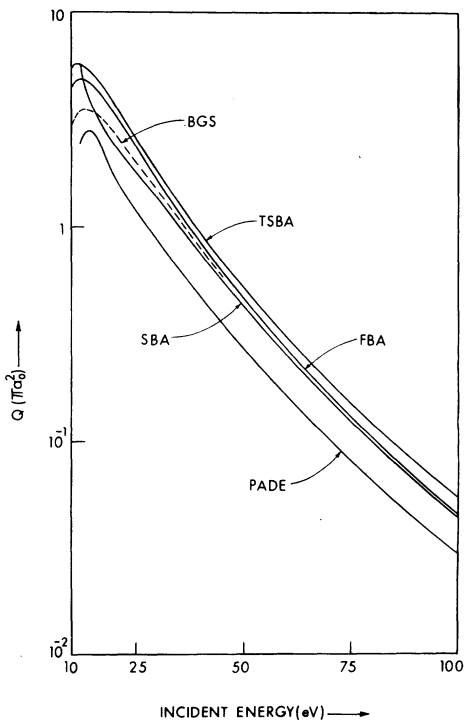

FIG. 1. Comparison of the second Born approximation (SBA) and the Padé total cross sections for positronium formation in atomic hydrogen with those obtained in the first Born approximation (FBA), a truncated second Born approximation (TSBA), and by Banerji *et al.* (BGS) for incident positron energies up to 100 eV.

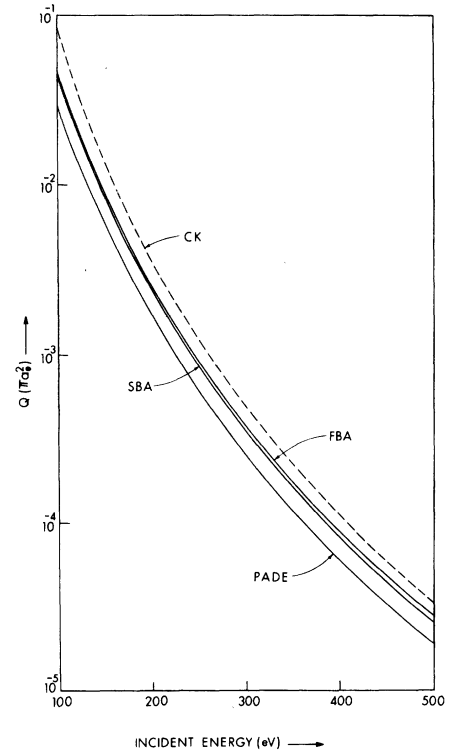

FIG. 2. Comparison of the second Born approximation (SBA) and the Padé total cross sections for positronium formation in atomic hydrogen with those obtained in the first Born approximation (FBA) and the first-order Faddeev-Watson multiple-scattering approximation (CK) for incident positron energies ranging from 100 to 500 eV.

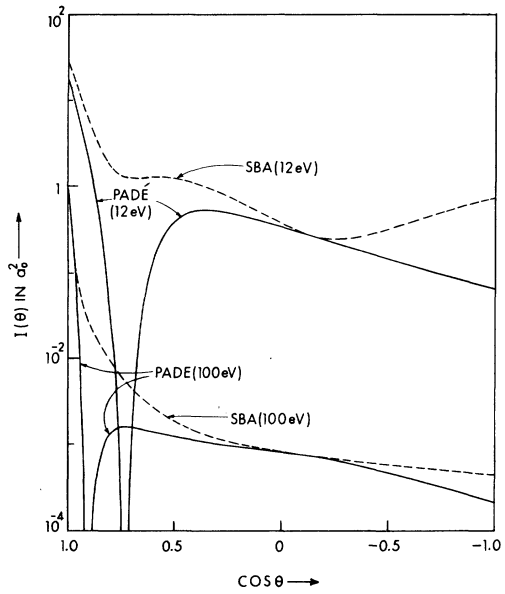

FIG. 3. Comparison of the nature of the variation of the second Born approximation (SBA) and the Padé differential cross sections for positronium formation in atomic hydrogen with the cosine of the angle of scattering θ for two different incident positron energies (12 and 100 eV).

Padé differential cross section goes to zero at an angle whose value decreases from about 44° to about 23° as the incident energy increases from 12 to 500 eV. This feature is similar to that obtained in the FBA and, as can be seen from the expression for the [1, 1] Padé amplitude given in Eq. (19), really reflects the behavior of the first Born amplitude g_1 which vanishes at an angle where the contribution of the positron-electron interaction cancels exactly the contribution of the positron-proton interaction. The SBA differential cross section does not have this characteristic, as the second-order Born term in the rearrangement scattering amplitude gives a nonvanishing contribution when the first-order term is exactly zero.

In the absence of any experimental results for electron capture by positrons from hydrogen atoms there is no unambiguous way of speaking in favor of one theory or the other. But in any second-order calculation the summation over the infinite number of intermediate states must be carried out and our approach is convenient for this purpose. There is scope for improving the result by taking the effect of a few more intermediate states exactly and by modifying the value of k_{N+1} [see Eq. (8a)] judiciously in the light of experimental results, when available. In another approach Kramer[10] has used the free-particle Green's function in the second-order Born term [this amounts to the replacement of the intermediate states ψ_n occurring in Eq. (4) by plane-wave intermediate states] and has given numerical results for the total cross section for the proton-hydrogen rearrangement process. In cases where the second-order Born term in the rearrangement scattering amplitude is not small compared to the first, the [1, 1] Padé-approximant method is expected to give better results. It is desirable to make the calculation with the higher approximants, but this necessitates the computation of Born terms of order higher than the second and the task, for the present, seems arduous.

ACKNOWLEDGMENT

We thank Santanu Pal for help in numerical computation in the course of this work.

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