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**LETTER TO THE EDITOR**

# Evidence of two-channel distortion effects in positronium formation reactions

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**Abstract**

The formation of ground-state positronium in collisions of positrons on hydrogen-like atoms is considered. In previous theoretical works, two-centre distorted wavefunctions were employed to approximate either the initial or the final channel. Here we report results obtained by means of the eikonal final state continuum distorted wave approximation for which asymptotically correct distorted wavefunctions are used for both the initial and final states of the scattering system. Comparison of the present theoretical total cross sections with experimental data reveals that distortion effects become important in both channels as the impact energy decreases. This work also shows that distorted-wave theories may be extended from their usual domain of high impact energies to lower ones.

## 1. Introduction

The system $e^+ e^- p^+$ is a fundamental three-particle system of great physical interest. It contains three distinguishable particles and has two two-particle bound states: $H = (e^-, p^+)$, $Ps = (e^-, e^+)$, related by the charge transfer or rearrangement reaction

$$e^+ + H \rightarrow Ps + p^+. \tag{1}$$

The positronium atom (Ps) is an exotic atom compound of one electron and one positron and may be considered as an isotope of H in which the proton is replaced by a positron. The Ps ground state (triplet state) has a mean life of $1.4 \times 10^{-7}$ s, decaying by annihilation into three photons. Ps atoms attract a great deal of interest in many fields. In quantum electrodynamics, Ps atoms offer the possibility of studying a fundamental bound system containing only leptons (i.e., particles not affected by the strong interactions). In astrophysics, the study of annihilation

  

radiation from outer space gives information about otherwise inaccessible parts of the universe. Moreover, positron annihilation can be used to probe the Fermi surface of solids as well as to obtain scans of the human brain through positron emission tomography techniques.

Since the pioneering work of Massey and Mohr [1] using the first order of the Born (B) approximation for the initial and final states, the understanding of the fundamental process (1) has been a formidable theoretical task [2]. The presence in the system of two light particles introduces coordinate transformations which significantly complicate the description of the process. This is in contrast to the theoretical considerations for electron capture by heavy ions where, in addition, another important approximation is also possible: the relative motion of nuclei can be treated classically at all but very low energies and, for the computation of total cross section, can be straightforwardly ignored. No such simplification occurs in positron–atom collisions since the positron–nucleus interaction plays a decisive role even at high energies.

The continuum distorted wave (CDW) approximation was originally proposed in 1964 by Cheshire [3] to deal with ion–atom charge exchange. It has proved to be fairly successful in describing experiments over a wide range of collision velocities and target-projectile combinations. However, the CDW total cross sections become unrealistic as the collision speed decreases and even fail to show the observed maximum at intermediate energies ($\mathbf{v}_\mathrm{i} \simeq \mathbf{v}_\mathrm{e}$, $v_\mathrm{i}$ and $v_\mathrm{e}$ being the collision and electron orbital velocities, respectively). As Crothers realized [4], one of the reasons for this behaviour is that the CDW function is not properly normalized. In order to avoid these undesirable features, the introduction of normalized eikonal states to describe the entrance and/or the exit channel was proposed. The continuum distorted wave eikonal initial state (CDW-EIS) [5–7], and the eikonal final state-continuum distorted wave (EFS-CDW) [8, 9] are examples of such approximations.

The unique antecedent of a two-centre distorted-wave theory for both the initial and final channels applied to a light projectile collision was presented in the work of Jones and Madison [10], who successfully employed the CDW-EIS approximation for an $(\mathrm{e}^-, 2\mathrm{e}^-)$ process. For Ps formation collisions, one-channel two-centre distorted-wave theories were developed by Bransden *et al* for neutral targets [11] and by Fojón *et al* for initially charged targets [12]. In this work, we go a step further and calculate for the first time the charge transfer reaction by positron impact on hydrogen-like atoms using the two-channel distorted-wave EFS-CDW approximation. Since our approach takes into account the correct Coulomb boundary conditions in both initial and final channels, we can describe the capture process independently of the charge state of the target.

## 2. Theory

We consider a general system formed by an incoming positron of mass $M_\mathrm{P}$ and charge $Z_\mathrm{P}$ colliding with a hydrogen-like atom composed of one electron and a nucleus target of charge $Z_\mathrm{T}$ and mass $M_\mathrm{T}$. In the centre of mass system, the problem can be described by any of the pairs of Jacobi coordinates $(\mathbf{r}_\mathrm{T}, \mathbf{R}_\mathrm{P})$, $(\mathbf{r}_\mathrm{P}, \mathbf{R}_\mathrm{T})$, or $(\mathbf{R}, \mathbf{r})$ (see, for example, [2]). The position vectors $\mathbf{R}_\mathrm{T}$, $\mathbf{R}_\mathrm{P}$, $\mathbf{r}$ refer each particle to the centre of mass of the other two ones. The electronic coordinates $\mathbf{r}_\mathrm{T}$ and $\mathbf{r}_\mathrm{P}$ and their associated momenta $\mathbf{k}_\mathrm{T}$, $\mathbf{k}_\mathrm{P}$ refer to the target nucleus and the positron projectile, respectively, while the distance $\mathbf{R}$ and the momentum $\mathbf{K}$ are considered between positron and the target nucleus. We use atomic units throughout, unless explicitly stated otherwise.

In this context, we can readily write the EFS-CDW transition amplitude as

$$T^{\text{EFS-CDW}} = \left\langle \Psi_\mathrm{f}^{\text{EFS}} \middle| W_\mathrm{i} \middle| \Psi_\mathrm{i}^{\text{CDW}} \right\rangle, \tag{2}$$

with the initial and final states defined by

$$\Psi_{\rm i}^{\rm CDW} = \Psi_{\rm i}^{\rm B}(\mathbf{R}_{\rm P}, \mathbf{r}_{\rm T}) F^{+}(a_{\rm P}, -\mathbf{v}_{\rm i}/2, \mathbf{r}_{\rm P}) F^{+}(a_{\rm i}, \mathbf{v}_{\rm i}, \mathbf{R}), \tag{3}$$

$$\Psi_{\rm f}^{\rm EFS} = \Psi_{\rm f}^{\rm B}(\mathbf{R}_{\rm T}, \mathbf{r}_{\rm P}) E^{-}(a_{\rm T}, \mathbf{v}_{\rm f}, \mathbf{r}_{\rm T}) E^{-}(a_{\rm f}, \mathbf{v}_{\rm f}, \mathbf{R}), \tag{4}$$

$\mathbf{v}_{\rm f}$ being the Ps velocity. Here we denote with $\Psi_{\rm i,f}^{\rm B}$ the undistorted Born initial and final states

$$\Psi_{\rm i,f}^{\rm B} = \Phi_{\rm i,f}(\mathbf{R}_{\rm P,T}) \psi_{\rm i,f}(\mathbf{r}_{\rm T,P}), \tag{5}$$

where $\Phi$ and $\psi$ represent a plane wave and a bound state wavefunction, respectively. The distortion effects of the Coulomb potentials are contained in the functions

$$F^{\pm}(a, \mathbf{p}, \mathbf{r}) = \exp\left(\frac{\pi a}{2}\right) \Gamma(1 \mp {\rm i}a)\, {}_1F_1(\pm {\rm i}a; 1; \pm {\rm i}kr - {\rm i}\mathbf{k}\cdot\mathbf{r}), \tag{6}$$

$$E^{\pm}(a, \mathbf{p}, \mathbf{r}) = \exp[\mp {\rm i}a \ln(pr \mp \mathbf{p}\cdot\mathbf{r})]. \tag{7}$$

with the Sommerfeld factors $a_{\rm P} = Z_{\rm P}/v_{\rm i}$, $a_{\rm T} = Z_{\rm T}/v_{\rm f}$ and $a_{\rm i,f} = -Z_{\rm T}Z_{\rm P}/v_{\rm i,f}$.

The choice of multiplicative continuum factors and eikonal phases to distort the initial and final bound states, respectively, is based on physical grounds. It was demonstrated [4] that for heavy ion–atom collisions, at finite separation between the collision partners, continuum distorted waves are not normalized. This defect is more severe as the impact energy diminishes, provoking in general an overestimation of the total cross sections. Formal theory demands only normalization of the distorted wavefunctions at large interaggregate distances. Considering that only a first order of a *distorted-wave series* is used, the initial or final distorted wavefunction must approximate the behaviour of the initial or final exact wavefunction (which is normalized at all internuclear distances) if the *post* or the *prior* version of the transition matrix element is used, respectively. Thus, a *compromise* was made in choosing the distorted wavefunctions [8]. With this choice, the inclusion of the projectile and the target nucleus fields in the initial and exit channels, respectively, was also preserved as well as the two-centre character of the initial and final electronic wavefunctions. It is well known that the projectile–target nucleus interaction can be taken into account through a phase factor not affecting total cross sections. Therefore, the CDW-EIS and EFS-CDW models were introduced with success to represent experimental cross sections for H targets (i.e. in a three-body reaction), depending on the relative strength of the projectile and target nuclear fields in the entry and exit channels [8]. In CDW-EIS (EFS-CDW), the exact outgoing (incoming) wavefunction is approximated as a product of the target (projectile) bound wavefunction and a multiplicative projectile (target nucleus)–electron continuum eikonal phase, preserving thus its normalization at all internuclear distances. In the final (initial) channel, the distorted wavefunction was chosen as a simple product of the projectile (target) bound wavefunction and a target nucleus (projectile)–electron Coulomb continuum factor, considering thus normalization only at infinite internuclear distances. We must remark that for the case of ion impact the relative velocities between the aggregates of the collision are almost the same in the initial and final channels $v_{\rm i} \simeq v_{\rm f}$. A main difference between protons and positrons as projectiles must be kept in mind at the time of choosing the distortion factors. This fact is related to the different masses of both projectiles giving place to a dynamical effect, breaking the projectile–target criterion valid for ion impact [8]. For reaction (1) at all impact energies,

$$v_{\rm f} = \sqrt{v_{\rm i}^2/2 + (\epsilon_{\rm i} - \epsilon_{\rm f})}$$

so the final collision velocity is smaller than the initial one, this behaviour being more evident close to the threshold of the process. As a consequence, the failure in the normalization of

distorted wavefunctions will be more notable using Coulomb continuum factors in the exit channel rather than in the entry channel. Therefore, we choose to distort the final wavefunction with eikonal phases, assuring its normalization for all interparticle velocities and distances. On the other hand, continuum distortions must be used in the entry channel to take into account the Thomas multiple scattering mechanisms at high energies and at the same time to preserve the normalization of the whole initial wavefunction at infinite separation of the aggregates.

We complete the description of equation (2), writing the residual interaction $W_i$, which is the sum of two mass-polarization terms ($M_T \gg 1$)

$$W_i \Psi_i^{CDW} = (H - E)\Psi_i^{CDW}, \tag{8}$$

$$= \Phi_i(\mathbf{R}_P)\left(\frac{1}{M_P}\nabla_{\mathbf{R}} \cdot \nabla_{\mathbf{r}_P} - \nabla_{\mathbf{r}_T} \cdot \nabla_{\mathbf{r}_P}\right)\psi_i(\mathbf{r}_T)F^+(a_P, -\mathbf{v}_i/2, \mathbf{r}_P)F^+(a_i, \mathbf{v}_i, \mathbf{R}). \tag{9}$$

In this notation, previous theoretical approximations can be easily expressed. The B approximation takes the form $T^B = \langle \Psi_f^B | V_i | \Psi_i^B \rangle$, the B-CDW approximation reads $T^{B\text{-}CDW} = \langle \Psi_f^B | W_i | \Psi_i^{CDW} \rangle$ while the CDW-B approximation results as $T^{CDW\text{-}B} = \langle \Psi_f^{CDW} | V_i | \Psi_i^B \rangle$, where the perturbation potential is $V_i = Z_P Z_T/R - Z_P/r_P$. For initially charged targets, Fojón *et al* [12, 13] introduced the Coulomb–Born approximation (CBA) and the continuum distorted wave final state (CDW-FS) approximation respectively, where the initial B state is distorted by a one-centre Coulomb wavefunction

$$\Psi_i^C = \Psi_i^B(\mathbf{R}_P, \mathbf{r}_T)F^+(b_i, \mathbf{v}_i, \mathbf{R}), \tag{10}$$

with $b_i = -Z_P(Z_T - 1)/v_i$, which takes into account the movement of the positron in the field of the net charge of the target. In this way, the transition amplitudes read $T^{CBA} = \langle \Psi_f^B | U_i | \Psi_i^C \rangle$ and $T^{CDW\text{-}FS} = \langle \Psi_f^{CDW} | U_i | \Psi_i^C \rangle$ where the perturbing potential is $U_i = 1/R - 1/r_P$.

We present here a computational method developed to evaluate the different distorted-wave models considered before. We concentrate on the computation of the $T^{EFS\text{-}CDW}$ matrix element, but the evaluation of the $T$-matrix for other approximations follow the same lines. Since one-channel two-centre distorted-wave models were calculated in previous works, their results will serve as a check of the method employed here. The evaluation of the $T$-matrix elements implies, in principle, the computation of a six-dimensional numerical quadrature as Jones and Madison [10] performed. However, we can readily reduce it to three dimensions by Fourier transformation of the integrand part which depends only on the coordinate $\mathbf{r}_P$ as

$$\tilde{\mathbf{G}}(\mathbf{Q}) = \int \frac{d\mathbf{r}_P}{(2\pi)^{3/2}} \exp(-i\mathbf{Q} \cdot \mathbf{r}_P)\psi_f(\mathbf{r}_P)\nabla_{\mathbf{r}_P} E^+(a_P, \mathbf{v}_i/2, \mathbf{r}_P), \tag{11}$$

and then integrating separately on the coordinates $\mathbf{r}_T$ and $\mathbf{R}$. This procedure leads to the following momentum-space vectorial integrals

$$\mathbf{J}_T(\mathbf{Q}) = \int d\mathbf{r}_T \exp[-i(\mathbf{v}_f + \mathbf{Q}) \cdot \mathbf{r}_T]F^{-*}(a_T, \mathbf{v}_f, \mathbf{r}_T)\nabla_{\mathbf{r}_T}\psi_i(\mathbf{r}_T), \tag{12}$$

$$\mathbf{J}_{TP}(\mathbf{Q}) = \int d\mathbf{R} \exp\{i[(\mathbf{v}_i - \mathbf{v}_f) + \mathbf{Q}] \cdot \mathbf{R} - \epsilon R\}F^{-*}(a_f, \mathbf{v}_f, \mathbf{R})\nabla_{\mathbf{R}} F^+(a_i, \mathbf{v}_i, \mathbf{R}), \tag{13}$$

and scalar integrals

$$I_T(\mathbf{Q}) = \int d\mathbf{r}_T \exp[-i(\mathbf{v}_f + \mathbf{Q}) \cdot \mathbf{r}_T]\psi_i(\mathbf{r}_T)F^{-*}(a_T, \mathbf{v}_f, \mathbf{r}_T), \tag{14}$$

$$I_{TP}(\mathbf{Q}) = \int d\mathbf{R} \exp\{i[(\mathbf{v}_i - \mathbf{v}_f) + \mathbf{Q}] \cdot \mathbf{R} - \epsilon R\}F^+(a_i, \mathbf{v}_i, \mathbf{R})F^{-*}(a_f, \mathbf{v}_f, \mathbf{R}), \tag{15}$$

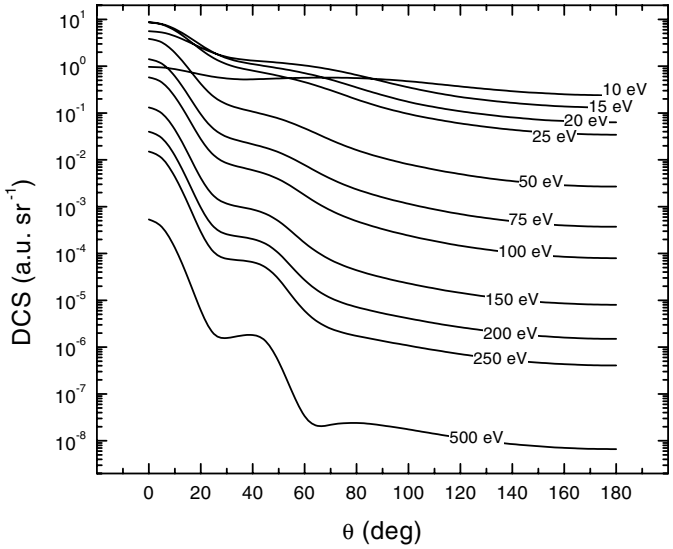


**Figure 1.** EFS-CDW DCS for Ps formation reactions on H, at positron impact energies between 10 eV and 500 eV.

in terms of which we can write $T^{\text{EFS-CDW}}$ as

$$T^{\text{EFS-CDW}} = \int \frac{\mathrm{d}\mathbf{Q}}{(2\pi)^{3/2}} \tilde{\mathbf{G}}(\mathbf{Q}) \cdot [\mathbf{J}_{\text{T}}(\mathbf{Q}) I_{\text{TP}}(\mathbf{Q}) - \mathbf{J}_{\text{TP}}(\mathbf{Q}) I_{\text{T}}(\mathbf{Q})]. \tag{16}$$

Here $\epsilon$ appears as a part of a convergence factor for the integrals $\mathbf{J}_{\text{TP}}(\mathbf{Q})$ and $I_{\text{TP}}(\mathbf{Q})$. We note that all the integrals given by equations (12)–(15) can be evaluated in closed forms [14]. We have developed a program to compute numerically the remaining three-dimensional integral in the variable $\mathbf{Q}$. The relative integration error was kept below 1%. Final results require to take the limit $\epsilon \to 0^+$. We observed that this limit can be achieved considering $\epsilon = 0.005$.

## 3. Results

We have obtained differential and total cross sections for the reaction (1) employing the distorted-wave models introduced above. In figure 1, we present differential cross sections (DCS) for Ps formation in the framework of the EFS-CDW approximation for a wide range of positron impact energies between 10 eV and 500 eV. The results show two outstanding features in the angular spectra. First, there is a peak in the forward direction for all DCSs. While at higher energies, the scattering of the positron at $0^\circ$ dominates the angular distribution, at lower energies it spreads over a wider angular domain, as expected from collision dynamics. This behaviour becomes more evident for impact energies lower than 15 eV in correspondence with a decrease of the total cross section as the energy decreases (see figure 3). This decrease is provoked by a dramatic reduction in the forward scattering. Second, a shoulder appears at low energies in the vicinity of $45^\circ$, which progressively becomes a perfectly well-defined peak as the impact energy increases. The presence of this peak can be understood as a classical two-step Thomas mechanism in the process of Ps formation [15]: in the first encounter the positron transfers half of its energy to the electron, and the two particles go out under $\pm 45^\circ$. In the second encounter either the electron or the positron is deflected through $90^\circ$ in the field of the proton. In this way, both particles leave with equal speed and direction allowing the formation of Ps.

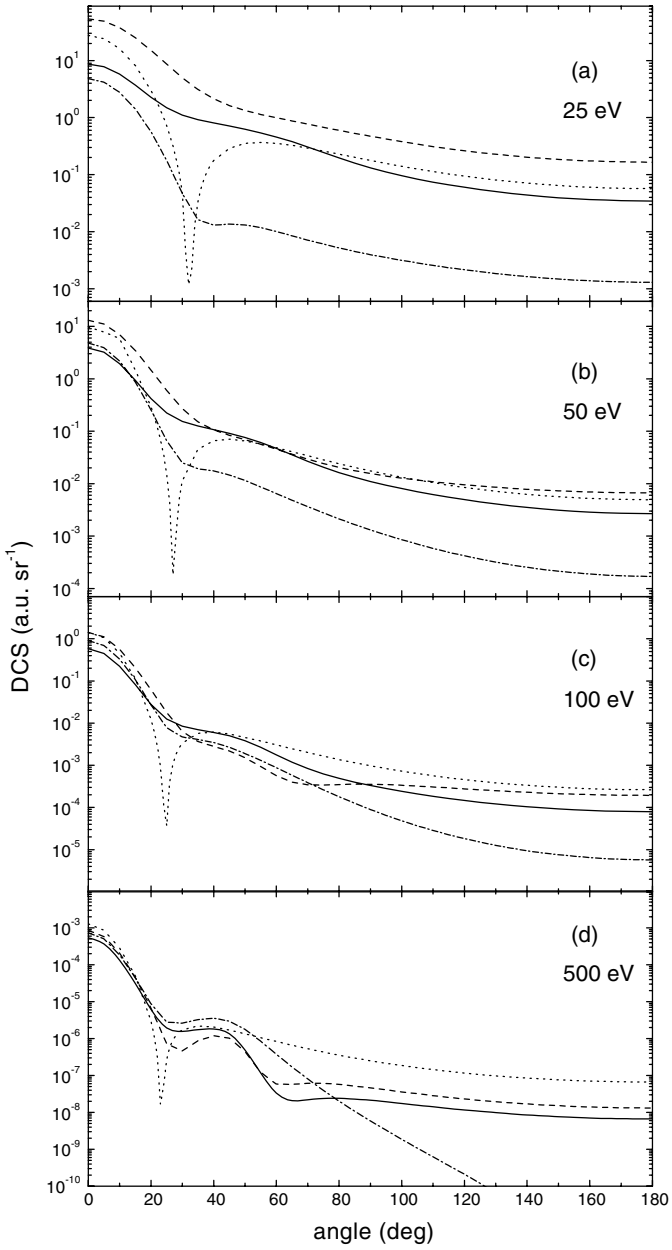


**Figure 2.** Ps formation DCS for collisions of positrons on H at impact energies of: (a) 25 eV, (b) 50 eV, (c) 100 eV and (d) 500 eV. EFS-CDW, full line; B-CDW, dashed line; CDW-B, dot-dashed line and B, dotted line.

In order to study the Thomas peak in more detail, in figure 2(d) we compare DCS for the EFS-CDW theory with results obtained using the B, B-CDW and the CDW-B approximations for collisions of 500 eV positrons on H. We observe that the B approximation presents a dip at 25° as a consequence of the cancellation of the contributions corresponding to the attractive and repulsive parts of the residual perturbation. Besides this dip and the forward peak,

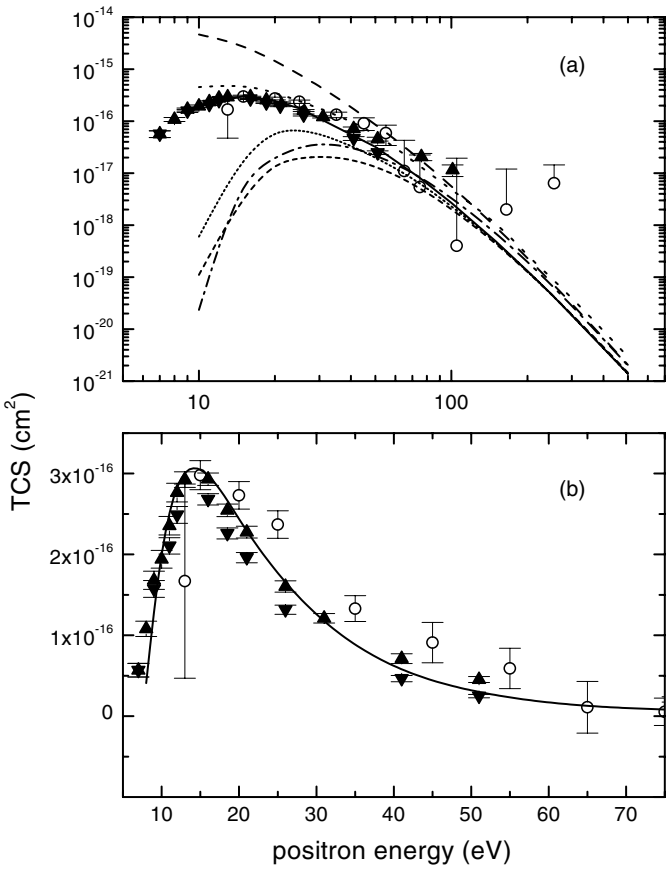


**Figure 3.** TCS for positronium formation reaction on H. In (a) results for the EFS-CDW (full line) model are compared with the CDW-CDW (short-dotted line) CDW-EIS (short-dashed line), B-CDW (dashed line), CDW-B (dot-dashed line) and B (dotted line) theories and with Weber *et al* [17] (hollow symbols) and Zhou *et al* [18] (full symbols) experiments. In (b) EFS-CDW results are compared on a more detailed linear scale with experiments.

B theory does not show any other structure. Double collision process cannot be represented, since it is a first-order theory. On the other hand, CDW-B, B-CDW and EFS-CDW do not present the 25° dip, but show clearly the Thomas peak. Differences between them come from the sharpness of the peak. For CDW-B the angular width $\Delta\vartheta$ is of the order of $Z_T/v_f$, for B-CDW $\Delta\vartheta$ is of the order of $Z_P/v_i$, while for EFS-CDW $\Delta\vartheta$ behaves as $\sqrt{Z_P Z_T/v_i v_f}$. This discrepancy persists even at higher energies since $v_f \to v_i/\sqrt{2}$. In the forward direction, there is agreement between all the distorted-wave theories at high enough energies. However, B calculations overestimate the other theoretical predictions as the collision velocity increases.

Differences between the models become more severe at lower energies as can be seen in figures 2(a)–(c) for positron impact energies of 25 eV, 50 eV and 100 eV respectively. We found quantitative discrepancies at the lowest energies, which can be as great as a factor of ten for the forward direction, and a factor of hundred for the back direction. This will have an immediate consequence on total cross sections as we show below.

In figure 3, we present results for total cross sections (TCS) using atomic H as a target which has been measured by Weber *et al* [17] and by Zhou *et al* [18]. In figure 3(a), we

compare in a log–log scale the theoretical and experimental data from the threshold to high energies. As experiments do not discriminate the final Ps bound state, we have multiplied all the theoretical 1s–1s TCS by the factor 1.202 to estimate roughly the capture to excited states at high energies. We should note that this estimation is not valid at low energies. We see that the B approximation gives a rough sketch of the Ps formation with an overestimation of the TCS maximum around 15 eV. On the other hand, the comparison of the one-channel distorted-wave theories B-CDW and CDW-B with experiments confirm the generally accepted sentence that distorted-wave theories are not expected to be valid at low energies. As previously discussed, the failure in the normalization of the distorted wavefunction is more dramatic if the CDW is used in the final channel. This behaviour is put in evidence in the proximity of the threshold where $v_f$ annulates, while $v_i$ remains always different from zero for the studied reaction. Comparing, for example, B-CDW and CDW-B approximations at 10 eV we can observe a discrepancy of greater than five orders of magnitude. The question is if a double distortion can give a better description through the CDW-CDW or the CDW-EIS theory. As shown in figure 3(a), the presence of the CDW function in the final state leads, as in the case of the CDW-B theory, to an underestimation of the experiments. Fortunately, we show here that this shortcoming can be remedied including the normalized and also boundary correct EFS through the EFS-CDW approximation, which enables us to extend distorted-wave theories to unexpected low energies. In figure 3(b), we show on a linear scale how the EFS-CDW theory represents precisely the position, width and intensity of the capture peak and describes the general behaviour of TCS. However, the agreement of EFS-CDW and experimental data must be taken with care in the proximities of the threshold due to the perturbative character of the EFS-CDW model. In this way, we find in the EFS-CDW model a theory accurate at high energies which can be extrapolated to a lower energy regime where coupled channel results are reliable [19–22].

## 4. Summary

In conclusion, in this work for the first time a perturbative theoretical model able to describe Ps formation experiments from relatively low to high (non relativistic) energies has been introduced. In this distorted-wave model, which is formulated on physical grounds, the importance of distorting both the initial and final channels has been shown. The success of the use of eikonal phases instead of Coulomb waves to distort the final bound state is supported by a correct normalization which leads to the proper scale and shape of the TCS even at low energy. Coulomb distortions affect the results less when they are used in the initial state and, on the other hand, they must be taken into account to describe the Thomas multiple scattering mechanisms at high energies. Calculations for other targets appear as necessary. They are the subjects of our future interest.

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