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Use of single-body potentials to accurately describe virtual positronium formation in positron collisions

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Abstract

We present a single-body adiabatic potential to investigate the role of virtual Positronium (Ps) formation in positron scattering with atoms at energies below the Ps formation threshold. Our model is applied to positron scattering by hydrogen and noble-gas atoms. The potential is decomposed into two components: the correlation-polarization (CP) potential, derived from perturbation theory for the positron-hydrogen system and generalized for other atoms, and the virtual Positronium (VPs) potential. The VPs potential is modeled as a short-ranged attractive term based on the CP component but shifted toward the atom's vicinity, with its strength controlled by a semiempirical parameter fine-tuned to match the scattering length to reference values. Our results show that the inclusion of the VPs term is essential for reproducing experimental measurements and results from other theoretical models for both integrated and differential cross-sections.

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I. INTRODUCTION

The interactions of positrons with atoms and molecules are important in medical applications like positron emission tomography [1] and in the localization of defects in material sciences [2]. For simulations of the microscopic processes, a large amount of data in the form of cross sections for collisions between positrons and different atoms and molecules at many different collision energies are required [3]. However, obtaining accurate cross sections for collision with energies below a few eV remains challenging, both experimentally and theoretically [4, 5].

One of the main challenges for theoretical models lies in describing the Positronium (Ps) formation [6]. Ps formation is *real* when the incident positron has sufficient energy to remove the electron from the target, and *virtual* when it lacks the energy to do so [7]. It has been showed that elastic cross sections from theory are likely to be too low in magnitude when the virtual Ps interactions are not taken into account [8]. Gribakin and King [9] addressed this problem by introducing a method to account for the contribution of virtual Ps within the Many-Body Theory (MBT) approach.

An alternative approach to MBT and other *ab initio* methods is the use of single-body potentials [10–19]. These kind of potentials have proven to be a powerful and efficient tool to model positron interactions with atoms and molecules. This methodology aims to simplify the complex many-body problem by describing the positron-target interaction through an effective single-body potential, which may include adjustable parameters [20]. Despite their simplified nature, these models are remarkably capable of providing reasonable results for scattering and annihilation of positrons by atoms and molecules [10].

In this paper we propose a single-body adiabatic potential to model the effects of virtual Ps in positron-atom scattering. With this potential, which depends on a single adjustable parameter, we obtain elastic cross sections which are comparable to those from high-level *ab initio* calculations [21–24]. By decomposing the full interaction potential into correlation-polarization and virtual Ps components, we investigate important questions, such as the impacts of virtual Ps formation on both integral and differential cross sections. We also discuss the limitations of the adiabatic approximation.

Results for the hydrogen and noble-gas atoms are presented for energies below the Ps formation threshold. Positron scattering by the H atom has been extensively investigated

in previous studies, such as in the variational calculations from Schwartz [25], Bhatia *et al.* [26, 27] and Register and Poe [28]. Another notable study is that of Humberston *et al.* [29], in which the authors applied the Kohn variational method (KVM) to investigate the effects of Ps formation on the elastic cross section. These variational calculations employed a Hylleraas basis to accurately describe the correlation between the positron and the H atom, yielding results that are nearly exact. Consequently, these results serve as a benchmark for validating any newly developed methodologies. Other examples of successful non-variational calculations for this system include the Convergent Close-Coupling (CCC) method by Bray and Stelbovics [30], MBT approach by Gribakin and Ludlow [31], the R-matrix method by Kernoghan *et al.* [32] and the T-matrix formalism of Mitroy and Ratnavelu [33].

For the He atom, the effects of virtual Ps formation were extensively studied by Van Reeth and Humberston using the KVM [34–37]. Additionally, the Confined Variational Method (CVM) has been successfully applied to calculate s-wave phase shifts for the positron-helium system [38–40]. Non-variational *ab initio* methods have also been successfully applied to noble gas systems, ranging from helium to xenon. Notable examples include the CCC [41–43], the MBT [21, 44], and the Polarized Orbital Method (POM) calculations [45–47].

This article is organized as follows: In Section II we describe the differences between electron and positron collision, the various terms of our model potential and introduce the model potential for virtual Ps. In Section III we present results for phase shifts, potentials, differential and integral elastic cross sections for positron collisions with hydrogen and krypton atoms. For both targets we discuss the effect of including the model potential for virtual Ps. In addition we show differential and integral elastic cross sections for the noble-gases helium, neon and argon. In Section IV we finish the article presenting our conclusions. In the appendix we give more details about the matrix elements of the model potential. Phase shifts as a function of positron momentum for all targets studied in this work are included in the supplementary material. Atomic units are used throughout this article, unless otherwise stated.

II. METHODOLOGY

One conventional way to discuss the optical potential is through the close-coupling approximation. In this section, we provide a basic overview of the close-coupling methodol-

ogy. We then examine the fundamental differences between electron and positron scattering problems, emphasizing how the nature of positron interactions, particularly the formation of virtual Ps, introduces complexities absent in electron scattering.

For the electron scattering by the hydrogen atom, in the close-coupling approximation, the wave-function is expanded in terms of the eigenfunctions of the target (ψ_α) [20]:

$$\Psi(\mathbf{r}_1, \mathbf{r}_2) = \sum_{\alpha} (\psi_{\alpha}(\mathbf{r}_2) F_{\alpha}^{(\pm)}(\mathbf{r}_1) \pm \psi_{\alpha}(\mathbf{r}_1) F_{\alpha}^{(\pm)}(\mathbf{r}_2)) \quad (1)$$

where $\mathbf{r}_1$ and $\mathbf{r}_2$ are the coordinates of the electrons in respect to the nucleus, which is considered to be at the coordinate origin. The sum in α runs over all the states of the target, also including the continuum spectra. By substituting this scattering wave-function into the Schrödinger equation, one obtains:

$$\left(E + \frac{\nabla_{\mathbf{r}_1}^2}{2} - \varepsilon_{\alpha} \right) F_{\alpha}^{(\pm)}(\mathbf{r}_1) = \sum_{\alpha'} V_{\alpha\alpha'}(\mathbf{r}_1) F_{\alpha'}^{(\pm)}(\mathbf{r}_1) \pm \sum_{\alpha'} \int K_{\alpha\alpha'}(\mathbf{r}_1, \mathbf{r}_2) F_{\alpha'}^{(\pm)}(\mathbf{r}_2) d^3r_2, \quad (2)$$

where $V_{\alpha\alpha'}(\mathbf{r}_1) \equiv \langle \psi_{\alpha} | (-1/r_1 + 1/|\mathbf{r}_1 - \mathbf{r}_2|) | \psi_{\alpha'} \rangle$, ε_{α} is the energy of the α state of the target, $E = k^2/2 + \varepsilon_1$ is the total energy, and $K_{\alpha\alpha'}(\mathbf{r}_1, \mathbf{r}_2) = \psi_{\alpha'}(\mathbf{r}_2)(H - E)\psi_{\alpha}(\mathbf{r}_1)$ with H being the full electron-atom Hamiltonian operator, is the exchange potential, which is a direct consequence of the antisymmetrization of the wave-function (1). The main idea of the optical potential technique lies on, instead of solving the complicated system of coupled equations (2), to reduce the problem into a simple mono-channel approximation. This is accomplished by restricting the wave-function expansion to the target's ground state ($\alpha = 1$) in the wave-function expansion (1). In doing so, the correlation-polarization effects that arises from the first term of the right hand side of eq. (2) are, initially, not included. To compensate for this omission, it is assumed that the optical potential will include an effective adiabatic potential capable of describing the correlation-polarization effects. Consequently, we obtain:

$$\left(\frac{k^2}{2} + \frac{\nabla_{\mathbf{r}}^2}{2} - \mathcal{V}_{opt}(\mathbf{r}) \right) F_1^{(\pm)}(\mathbf{r}) = 0, \quad (3)$$

with:

$$\mathcal{V}_{opt}(\mathbf{r}) \equiv \mathcal{V}_{st}(\mathbf{r}) + \mathcal{V}_{cp}(\mathbf{r}) + \mathcal{V}_{ex}(\mathbf{r}). \quad (4)$$

where $\mathcal{V}_{st}(\mathbf{r}) \equiv V_{11}(\mathbf{r})$ is the static (ST) potential that emerges from the mono-channel expansion, $\mathcal{V}_{ex}(\mathbf{r})$ is the exchange potential, and $\mathcal{V}_{cp}(\mathbf{r})$ is the effective correlation-polarization potential introduced to account for the missing correlation-polarization effects from the simplified wave-function expansion.

For the positron case, following Mitroy [6], considering that $\mathbf{r}$ localizes the electron and $\mathbf{x}$ the positron, the scattering wave-function for the positron-H system within the close-coupling expansion framework is expressed as:

$$\Psi(\mathbf{r}, \mathbf{x}) = \sum_{\alpha} \psi_{\alpha}(\mathbf{r}) F_{\alpha}(\mathbf{x}) + \sum_{\beta} \phi_{\beta}(\boldsymbol{\rho}) G_{\beta}(\mathbf{R}), \quad (5)$$

where $\mathbf{R} = (\mathbf{r} + \mathbf{x})/2$ denotes the position of the center of mass of the Ps in respect to the atomic nucleus, and $\boldsymbol{\rho} = \mathbf{r} - \mathbf{x}$ is the internal Ps coordinate. The $G_{\beta}(\mathbf{R})$ describes the movement of the Ps and $\phi_{\beta}(\boldsymbol{\rho})$ is the eigenfunction of the Ps Hamiltonian with eigenenergy $\tilde{\varepsilon}_{\beta}$. Substituting this expansion into the Schrödinger equation, we obtain the set of coupled equations:

$$\left(E + \frac{\nabla_{\mathbf{r}}^2}{2} - \varepsilon_{\alpha} \right) F_{\alpha}(\mathbf{x}) = \sum_{\alpha'} V_{\alpha\alpha'}(\mathbf{x}) F_{\alpha'}(\mathbf{x}) + \sum_{\beta} \langle \Psi_{\alpha} | (H - E) | \phi_{\beta} G_{\beta} \rangle, \quad (6)$$

$$\left(E + \frac{\nabla_{\mathbf{R}}^2}{4} - \tilde{\varepsilon}_{\beta} \right) G_{\beta}(\mathbf{R}) = \sum_{\beta'} V_{\beta\beta'}(\mathbf{R}) G_{\beta'}(\mathbf{R}) + \sum_{\alpha'} \langle \phi_{\beta} | (H - E) | \psi_{\alpha'} F_{\alpha'} \rangle, \quad (7)$$

with $V_{\alpha\alpha'}(\mathbf{x}) \equiv \langle \psi_{\alpha} | (1/x - 1/|\mathbf{r} - \mathbf{x}|) | \psi_{\alpha'} \rangle$, $V_{\beta\beta'}(\mathbf{R}) \equiv \langle \phi_{\beta} | (1/x - 1/r) | \phi_{\beta'} \rangle$ and H being the full Hamiltonian of the system. Solving this system of equations is remarkably difficult, and it requires the inclusion of many target and Ps states (and pseudo-states) to reach satisfactory convergence [48]. For any target with more than one electron, the situation is even more difficult, as the ionic states of the target as well as the exchange between the Ps and the electrons of the ion must also be considered in the expansion of the scattering wave-function [49].

As an initial approximation, the effects of the Ps states can be neglected by setting $G_{\beta}(R) = 0$ for any β in eq. (5). This, as expected, leads to significant simplifications. Consequently, equation (6) reduces to a form analogous to the corresponding equation for electron scattering (eq. (2)), but without the exchange term. Therefore, in this case, the optical potential takes the form:

$$\mathcal{V}_{opt}(x) = \mathcal{V}_{st}(x) + \mathcal{V}_{cp}(x), \quad (8)$$

where $\mathcal{V}_{cp}(x)$ is similar with the one from the electron scattering case, and $\mathcal{V}_{st}(x)$ is also similar but with an opposite sign. Throughout this article, we will refer to this approximation as the "CP model," which indicates that the optical potential includes not only the static term but also the correlation-polarization potential.

It is not expected that converged results can be achieved with the CP approximation alone, as this model completely neglects the virtual Ps (VPs) effects that are specially relevant at low energies [9, 50]. To incorporate these essential contributions, we assume that the optical potential takes the following form:

$$\mathcal{V}_{opt}(x) = \mathcal{V}_{st}(x) + \mathcal{V}_{cp}(x) + \mathcal{V}_{Ps}(x), \quad (9)$$

where $\mathcal{V}_{Ps}(x)$ is introduced as an adiabatic potential that effectively accounts for the VPs interactions. This potential depends on a free parameter that is determined according to the scattering length (SL). By solving the scattering problem with this potential, as defined in the expression above, we estimate the phase shifts, which are then used to compute both the elastic cross section and the differential elastic cross section. Throughout this article, we refer to this approximation as CP+VPs.

Since exchange and Ps formation can be rearrangement processes, in a given sense, neglecting the VPs contribution is somewhat similar to not account for the exchange effect in electron scattering: while this simplification may be sufficient at high projectile speeds, it significantly breaks down at lower energies. For electron scattering, it is well-established that the exchange interaction can be effectively modeled using a single-body potential [51–53]. Following this reasoning, we assume that a similar treatment can be applied to the VPs interaction in positron scattering.

A. The ST potential

The ST potential for the positron-H system is exact, and takes the form:

$$\mathcal{V}_{st}(x) = e^{-2x} \left(1 + \frac{1}{x} \right). \quad (10)$$

For the noble-gas atoms studied in this work, we use the ST potential proposed by Salvat *et al.* [54], which is given by:

$$\mathcal{V}_{st}(x) = \frac{Z}{x} \sum_{i=1}^{i_{max}} A_i e^{-a_i x}, \quad (11)$$

where Z is the number of electrons of the atom, $\{A_i\}$ and $\{a_i\}$ are fitting parameters provided in ref. [54], and i_{max} denotes the number of fitting parameters available for each target, which is 2 for He, Ne, and Kr, and 3 for Ar. These parameters are presented in table I for reference.

	A_1	A_2	A_3	a_1	a_2	a_3
He	-0.2259	1.2259	-	5.5272	2.3992	-
Ne	0.0188	0.9812	-	34.999	-2.5662	-
Ar	2.1912	-2.2852	1.0940	5.5470	4.5687	2.0446
Kr	0.4190	0.5810	-	9.9142	1.8835	-

TABLE I. Parameters for the ST potential (11) for the noble-gas according to ref. [54].

B. The CP potential

The first step in constructing the full optical potential is to determine the adiabatic CP potential. As discussed in ref. [20], an expression for the CP potential can be derived using perturbation theory, although its application is only viable to the H atom. Therefore, we begin by focusing on the positron-H system, with the primary objective of establishing an analytical form for the CP potential. Once this form is obtained, we proceed to generalize the CP potential using atomic parameters, thereby extending the methodology to treat noble-gas atoms.

As discussed, we start from the adiabatic CP potential for the positron-H [20]:

$$\mathcal{V}_{cp}(x) = - \sum_{\lambda \neq 1} \frac{|V_{1\lambda}(\mathbf{x})|^2}{\varepsilon_{\lambda} - \varepsilon_1}, \quad (12)$$

where:

$$V_{1\lambda}(\mathbf{x}) \equiv \langle \psi_1^{\xi} | V(\mathbf{r}, \mathbf{x}) | \psi_{\lambda}^{\xi} \rangle. \quad (13)$$

where $V(\mathbf{r}, \mathbf{x})$ is the electrostatic potential between the positron and the H atom. The $\psi_i^{\xi}(\mathbf{r})$ is the H atom wave-function, with a scale factor ξ considered (this function is presented in further details at appendix A). The introduction of this scale factor aims to generalize the CP potential to other atoms, as previously mentioned. This will be discussed in greater detail shortly.

The matrix element defined in (13) can be easily solved if we consider only the discrete spectra of the H atom. In this case, we have:

$$\mathcal{V}_{cp}(x) \approx \sum_{l=0}^{l_{max}} \mathcal{V}_l(x), \quad (14)$$

where we defined:

$$\mathcal{V}_l(x) \equiv -\frac{(2l+1)}{4\pi} \sum_{\substack{n=l+1 \\ n \neq 1}}^{n_{max}} \frac{v_{nl}(x)^2}{\varepsilon_n - \varepsilon_1}. \quad (15)$$

In the expressions above, l_{max} and n_{max} represents the maximum values of l and n accounted in the calculation, and $\varepsilon_n = 1/\xi n^2$. The function $v_{nl}(x)$ is presented in appendix A (see eq. (A5)).

Neglecting the states of the continuum in the CP potential (14) will impact on the polarization of the target, leading to polarizability values lower than the expected. This can be showed through the asymptotic behaviour of CP potential for $x \rightarrow +\infty$:

$$\mathcal{V}_l(x \rightarrow \infty) \approx -\frac{\alpha'_l}{2x^{2l+2}}, \quad (16)$$

where α'_l is the effective polarizability obtained from (15):

$$\alpha'_l = \sum_{n=1+l}^{n_{max}} \frac{(2l+1)c_{nl}^2}{2\pi(\varepsilon_n - \varepsilon_1)}, \quad (17)$$

where the c_{nl} coefficient is also calculated and presented in the appendix A. Due to the fact that the $c_{nl} \propto l$ (see eq. (A5)), it follows that $\alpha'_0 = 0$. This implies that the $\mathcal{V}_0(x)$ component of the potential is purely short-ranged.

For the H atom ($\xi = 1$), the dipolar effective polarizability sufficiently converges with $n_{max} = 10$ to the value of $\alpha'_1 \approx 11/3 a_0^3$. This corresponds to only $\approx 81\%$ of the exact value of $\alpha_1 = 9/2 a_0$, and, therefore, the asymptotic CP potential (14) does not behave as it should. To deal with this problem, while keeping the calculation simple, we propose to introduce a l dependent rescaling factor (γ_l) to account for the continuum spectra contribution:

$$\mathcal{V}_{cp}(x) = \sum_{l=0}^{l_{max}} \gamma_l \mathcal{V}_l(x), \quad (18)$$

For $l > 0$, it is easy to conclude that:

$$\gamma_l = \frac{\alpha_l}{\alpha'_l}. \quad (19)$$

where α_l is the correct value of the polarizability. The numerical value of the polarizabilities, which are now input parameters for the CP potential (18), are usually known or can be calculated by means of quantum chemistry programs. The value of γ_0 , however, is not so obvious. The $l = 0$ term is a pure correlation contribution to the total CP potential, as

$\mathcal{V}_0(x \rightarrow \infty) = 0$. Thus, there are no direct information that helps to attribute a value for this factor. Faced with this problem, for the H atom we kept the original form of the derived potential, meaning setting $\gamma_0 = 1$. The comparison with external results was encouraging, supporting this choice.

Finally, having knowledge of the γ_l factors and with expression (18), the CP potential is completely known for positron-H. We now turn our attention to the generalization of this CP potential for other atoms.

To achieve that goal, we assume that the CP potential found for positron-H can be extended to other targets. This is where the ξ factor, previously introduced, becomes useful. It seems logical to consider ξ as the numerical value of the atomic radius r_a ($\xi = r_a/a_0$). This choice is justified noting that electronic probability density $r^2|\psi_1^\xi(r)|^2$ is maximum at $r = \xi a_0$ and this point is used to define the H atomic radius. It is important to observe that our intention with this is not to find eigenfunctions that describe the atom, but rather to modify the CP potential derived for positron-H to effectively represent another target, while keeping its simplicity.

The γ_l factor for $l > 0$ is still obvious, as we can simply use the polarizabilities of the studied target. We are, then, left with the γ_0 factor. As discussed, this term corresponds to the correlation between the positron and the electrons of the target. Thus, it seems reasonable to multiply it by the number of electrons of the target Z . This led, however, to a overcorrelation problem, especially as the number of electrons of the target increased. This implied that a screening effect is playing a role, and in fact, when we considered $\gamma_0 = Z^*$, where Z^* is the effective nuclear charge of the outmost shell, the results came into reasonable agreement with MBT calculations in the CP-approximation [9, 21, 50]. Thus, based on this reason, we impose:

$$\gamma_0 = Z^*. \quad (20)$$

Finally, we have the CP potential generalization desired. It does not have any free parameter, as it only depends on atomic parameters such as the atomic radius, the effective nuclear charge and the polarizability. The table II presents these required parameters, as used in this work. As shown in this table, only the dipole polarizability is provided, which means that the calculation in this article were performed with $l_{max} = 1$ for the CP potential (18). This approach was chosen because the inclusion of higher-order terms demands additional input data, such as the numerical values of higher-order polarizabilities,

	H	He	Ne	Ar	Kr
Z^*	1.000	1.688	5.758	6.764	9.380
r_a	1.000	0.585	0.718	1.341	1.663
α_1	4.500	1.383	2.670	11.10	16.80
r_w	2.26	2.64	2.91	3.55	3.82

TABLE II. Required parameters for the CP potential model in a.u. Z^* is the effective nuclear charge of the outmost shell, obtained from ref. [55]; r_a is the atomic radius obtained from ref. [56]; α_1 is the dipole polarizability, obtained from ref. [57]; Van der Waals radius r_w values from [58].

yet it did not lead to any significant changes in the calculated results.

C. The virtual Ps potential

To effectively describe the impact of VPs formation, we model this interaction as a short-ranged attractive potential. It is well-known that VPs formation results in a significant increase in electron density around the atom [7]. Therefore, we expect the VPs interactions to have the greatest influence on the overall potential in this region. On the other hand, the VPs potential at very short distances may be less relevant due to the dominance of the static potential near the nucleus.

For these reasons, we model the VPs potential as the purely short-ranged component of the CP-potential ($l = 0$), but shifted towards the vicinity of the atom. While using this component of the CP-potential as the VPs potential is not accurate, it remains a reasonable approximation. This is because the $l = 0$ component already captures the essential positron-electron correlation in the atom's inner region, allowing us to approximate the VPs interaction more effectively in the outer regions where these effects are more prominent.

The ξ factor introduced in the CP-potential can also be used here for this purpose. This raises an interesting question: what value of ξ should be chosen to effectively characterize the "vicinity" of the atom? One suitable option for this task is the Van de Waals radius, r_w . Unlike the atomic radius, the Van de Waals radius is defined at a distance where the electronic density is already very low [58], making it an ideal candidate to represent the "vicinity" of the atom. Furthermore, it has been observed that the transition from the

short-range potential to the long-range asymptotic behavior in model potential applications tends to occur near this radius [59, 60].

Therefore, considering $\xi = r_w/a_0$, we propose:

$$V_{Ps}(x) = \rho \mathcal{V}_0^{\xi=\frac{r_w}{a_0}}(x), \quad (21)$$

where ρ is the semiempirical parameter of the model. The r_w values used in this work are also presented in table II.

As previously discussed, the $\mathcal{V}_0^\xi(x)$ function is the same as defined in eq. (15). From the analysis of the convergence of the results with the value of n_{max} , we found that using a value of n_{max} as low as 2 is already enough to reach convergence in this case (the inclusion of more states only impacts the numerical value of the ρ parameter). This allows us to simplify the VPs potential to the simple and convenient form:

$$V_{Ps}(x) \approx -\rho e^{-3x/r_w} \left(1 + \frac{3x}{2r_w}\right)^2. \quad (22)$$

From this expression, it becomes clear that the ρ parameter exclusively controls the depth of the potential, and plays no role in determining the range or shape of the interaction.

By fine-tuning ρ , we can modulate the strength of the VPs potential to match experimental or theoretical results. In this work, we follow the approach of Arretche *et al.* [16, 61] where the parameter is adjusted using the SL values found in literature. For this study, we have considered the SL values obtained through MBT [21], as well as those from the POM calculations [22, 45–47]. These values are listed in Table III, along with the corresponding ρ values required to reproduce these SL values. Additionally, alternative SL values are available, including the experimentally estimated values of -4.9 a.u. for Ar [62] and -10.3 a.u. for Kr [63]. However, since these values fall within the range obtained using the POM and MBT methodologies, we report only the results obtained with MBT-SL and POM-SL in this work.

For comparison, we also include the SLs obtained from the CP approximation (A_{cp}) in Table III. Notably, the SL magnitudes in the CP approximation are consistently lower than the reference values, indicating that the potential is under-correlated when the VPs contribution is not taken into account, as expected. The potential proposed here is valid for energies up to the real Ps formation threshold. For reference, the Ps formation threshold values are also provided in Table III.

	H	He	Ne	Ar	Kr
A_{cp}	-1.13	-0.36	-0.37	-1.87	-4.21
A	-2.1 ^a	-0.435 ^b /-0.53 ^c	-0.467 ^b /-0.61 ^c	-4.41 ^b /-5.3 ^c	-9.71 ^b /-10.4 ^c
ρ	5.581[-2]	3.790[-3]/7.790[-3]	3.955[-3]/9.618[-3]	3.480[-2]/4.304[-2]	3.186[-2]/3.430[-2]
E_{Ps} (eV)	6.8	17.79	14.76	8.80	7.20

TABLE III. The A_{cp} values were obtained within the CP approximation (8); The scattering length values A were taken from: [31] for a ; [21] for b and [22, 45–47] for c . The semiempirical parameter ρ was fine-tuned to reproduce the corresponding scattering length values listed in the row above; The values for the Ps formation threshold (E_{Ps}) were taken from ref. [64].

III. RESULTS AND DISCUSSION

A. Validation of the Model

In this section, we evaluate the validity of the potentials proposed in this work. Equally important to the VPs is the CP potential, as drawing meaningful conclusions from the inclusion of the VPs term requires a good description of the correlation-polarization term. It is important to notice that, unlike the VPs term, the CP potential contains no free parameter, as discussed in section IIB. After discussing the results obtained within the CP approximation, we proceed to analyze the implications of incorporating the VPs contribution. The phase shifts (up to $l = 8$) as a function of positron momentum, calculated using the CP and CP+VPs approximations for all targets considered in this work, are provided in tabular format as supplementary material.

Fig. 1 presents the s -, p - and d -wave phase shifts for the CP and CP+VPs models for momentum below the Ps formation threshold. The top-left panel presents the results for positron-H compared to the MBT results of Gribakin and King [9] within the same level of approximation. For the s -wave phase shift (δ_0), good agreement for k from threshold up to ≈ 0.2 a.u. is found. For larger values of k , our result differs from the MBT by a small margin. Similar conclusions can be drawn for the p -wave phase shift (δ_1), where very good agreement is observed up to $k \approx 0.5$ a.u. For the d -wave phase shift (δ_2) the agreement is observed for the whole region. Given the high accuracy of the MBT calculation within the

polarization approximation, as discussed by Gribakin and King [9], it can be concluded that the CP potential proposed in this work effectively captures the polarization interactions for this system below the Ps formation threshold.

In the bottom-left panel of the same figure, the positron-Kr results for the s -, p - and d -wave phase shifts within the CP approximation are compared with those obtained from the MBT [21]. Overall, the conclusions are consistent with those drawn from the positron-H system. For the s -wave phase shift strong agreement is observed up to $k \approx 0.4$ a.u., with some discrepancies appearing for higher values of k . For the p - and d -wave phase shifts, strong agreement are observed, with only minor discrepancies. This suggests that the proposed generalization of the CP potential developed in this work is also adequate for treating the noble-gas atoms. In fact, similar agreements are also observed with the elastic cross section reported for He in [9], and for Ne and Ar in [50].

In the top-right panel of Fig. 1 it is presented the phase-shifts in the CP+VPs approximation for positron-H system. The MBT results with VPs from Gribakin and Ludlow [31] are also shown in the figure for comparison. Very good agreement for the s -wave phase shift with the MBT one is observed. This is an encouraging result for the proposed VPs potential. For the p -wave phase shift the agreement remains good up to $k \approx 0.3$ a.u. For larger values, the MBT predicts a significantly higher phase-shifts compared to our result. For the d -wave phase shift the agreement holds up to $k \approx 0.5$ a.u., and, similarly to the p -wave, the MBT result exhibits a higher magnitude compared to ours beyond this point. The observed discrepancies in the p - and d -wave phase shifts are not surprising. As Gribakin and Ludlow discussed [31], the sudden increase in the contribution of the higher-order partial waves are related to the VPs becoming more “real” as it approaches the threshold. This energy-dependent effect cannot be accurately described by a simple adiabatic potential such as the one proposed in this work.

The bottom-right panel of Fig. 1 shows the phase shifts for the CP+VPs approximation for the positron-Kr system. The results are compared with those obtained from the MBT [21] and the POM [47]. Our model’s results, incorporating the POM-SL and MBT-SL approximations as shown in Table III, are very similar, with the largest discrepancy being approximately 4% at the peak of the s -wave phase shift. For this reason, only the POM-SL results for Kr are shown, as they demonstrate slightly better overall agreement with the reference data. Similarly to the positron-H case, the s -wave phase shift (δ_0) shows excellent

agreement with the reference data. For the p - and d - phase shifts, our results compare well with the MBT calculations up to $k \approx 0.3$ a.u. and ≈ 0.5 a.u., respectively. Beyond these values, the MBT results are higher than ours, though the discrepancies are smaller compared to the positron-H results. However, when compared to the POM, our phase shifts exhibits very good agreement, which is expected since the POM also employs an adiabatic approach. Interesting conclusions may be drawn from these results: First, it confirms that the VPs potential proposed in this work is capable of describing the effective interaction of the virtual Ps for targets other than the H atom. Second, the fact that this simple adiabatic potential offers good results suggests that the impact of virtual Ps as it approaches the Ps formation threshold is more subtle for the Kr atom compared to the H atom.

One of the key advantages of a single-body potential, as the one proposed in this work, is the possibility of analysing each component of the optical potential individually. This is illustrated in Fig. 2, where the potential is plotted as a function of the positron's distance from the atomic nucleus. In panel (a), the CP potential is decomposed into its $l = 0$ and $l = 1$ components, along with the VPs potential for positron-H. The comparison between the VPs with the CP- $l = 0$ component clearly demonstrates the impact of using the Van der Waals radius in (22): it extends the range of the correlation function. Interestingly, the VPs resembles the CP- $l = 1$ component, which describes the long range dipole polarizability interaction. The same pattern is observed for the positron-Kr in the panel (b), with the notable exception that the CP- $l = 0$ component is significantly deeper, approaching ≈ -1.0 a.u. for $x \rightarrow 0$ a.u.

Yet in the same figure, the panels (c) and (d) show the potential within the ST only, the ST+CP and the ST+CP+VPs approximations for H and Kr, respectively. As expected, the inclusion of the VPs interaction makes the potential more attractive in regions where the short-range CP- $l = 0$ contribution to the total potential is already minimal ($x \gtrsim 2.0$ a.u. for the H and $x \gtrsim 5.0$ a.u. for the Kr atom). These results, along with those presented in the top panels, elucidate the significant impact of the VPs interaction on the results. Unlike the electron-atom problem, the ST potential is repulsive for positron, which makes the low energy phase shifts to become very sensitive to the attractive part of the potential. Since the VPs potential is modeled here as a correlation function with a relatively long range compared to the CP- $l = 0$ component, its contribution becomes particularly significant as the ST potential approaches zero. Consequently, the VPs interaction is as crucial as the

polarization interaction for the description of the positron-target problem.

To better understand the effects of the VPs potential on physical observables, we analyse both the elastic cross section and the differential elastic cross section (DCS). This analysis is conducted for the Kr atom, as the conclusions drawn are consistent with those for the H atom, thereby avoiding redundant results.

Fig. 3 displays the elastic cross section as a function of the positron momentum for positron-Kr, comparing our results with the ones from MBT [21], POM [47] and CCC [42]. Notably, there is a significant difference between the results obtained with and without the VPs contribution: the CP result shows a much smaller magnitude compared to the CP+VPs approximation. As expected from the phase shifts presented in the bottom-right panel of fig. 1, the CP+VPs results is in good agreement with both reference models up to $k \approx 0.3$ a.u. Beyond this momentum, while our CP+VPs calculation remains consistent with the POM result, the MBT and CCC results exhibits a higher magnitude. As previously discussed, the discrepancies between the models arise from the varying approaches to (or omission of) non-adiabatic VPs effects.

Fig. 4 presents the DCS for $k = 0.1, 0.3, 0.5$ and 0.7 a.u. for positron-Kr. The results are compared with the ones from the MBT and POM. It is important to notice that, unlike the elastic cross section, convergence of the DCS at small angles requires including a large number of partial waves in the calculation. While this is manageable in semiempirical calculations as the one present in this paper, it poses a significant computational challenge for *ab initio* models such as the MBT and POM. Consequently, a common approach is to compute a limited number (l_c) of phase shifts using the *ab initio* formulation and then make use of the modified effective theory equation for phase-shifts with $l \geq 1$ to estimate the contribution from the higher-order partial waves [65], which leads to the scattering amplitude [21]:

$$f(\theta) = \sum_{l=0}^{l_c} (2l+1) \left(\frac{e^{2i\delta_l} - 1}{2ik} - \frac{\pi\alpha_1 k}{(2l-1)(2l+1)(2l+3)} \right) P_l(\cos\theta) - \frac{\pi\alpha_1 k}{2} \sin \frac{\theta}{2} \quad (23)$$

The DCS for the MBT and POM models were derived using the phase shifts reported in their respective studies (l_c up to 2 for the MBT and l_c up to 6 for POM).

For a momentum of 0.1 a.u. (panel (a)), all models with VPs show good agreement. At this momentum, the *s*-wave contribution is the dominant partial wave, so the absence of VPs results in a DCS with considerably lower magnitude. For $k = 0.3$ a.u. (panel (b)), including

the VPs increases the DCS at small angles compared to the CP model. The addition of the VPs correlation also alters the position and depth of the minimum in the DCS: the minimum shifts from ≈ 83 to ≈ 101 degrees and becomes shallower. However, for angles greater than ≈ 130 degrees, the DCS for the CP and CP+VPs models are relatively similar. The comparison between the VPs and the DCS from the MBT and POM shows reasonable agreement, though small differences are noted, primarily in the position of the minimum. Similar trends are observed for $k=0.5$ a.u. (panel (c)) and $k=0.7$ a.u. (panel (d)). As k increases, the discrepancies between the CP and CP+VPs models only become evident at progressively smaller angles, where the VPs contributes with a significant increase in the DCS. Furthermore, the differences between the CP+VPs model and POM with the MBT due to non-adiabatic effects become more pronounced, especially for angles greater than 70 degrees.

The analysis of the DCS of fig. 4 highlights both the strengths and limitations of using adiabatic potentials for positron. On the positive side, our results satisfactory matches the accuracy of established *ab initio* methodologies for low momentum. These potentials offer a large advantage in terms of computational speed, on the cost of requiring an additional parameter, such as the SL. However, as the momentum approaches the real Ps formation threshold, the inclusion of the VPs term did not affect the back-scattering and only showed considerable differences at small and intermediate angles. This suggests that the high-angle region is predominantly influenced only by the ST potential in our model. In contrast, the MBT result demonstrate that the VPs interaction have a substantial impact on back-scattering, enough to alter the integral elastic cross section, as shown in Fig. 3.

To analyze the sensitivity of the results to the adjustable parameter ρ , the SL and the zero-angle DCS for various momenta are presented as functions of ρ in Table IV. The DCS at $\theta = 0$ degrees is selected to emphasize its pronounced increase at small angles as the potential becomes more attractive. Considering the experimental SL of -10.3 ± 1.5 for positron-Kr, as measured by Zecca *et al.* [63], the results obtained for $0.03 \lesssim \rho \lesssim 0.04$ remain within a reasonable range. By assuming $\rho = 3.5$ as a value close to the optimal one, the zero-angle DCS may vary by approximately $\pm 15\%$ for $k = 0.1$ a.u., and by approximately $\pm 11\%$ for $k = 0.3, 0.5$ and 0.7 a.u.. When the interaction potential becomes sufficiently attractive, the Hamiltonian supports a bound state, causing the scattering length to change sign [10]. In this case, the transition occurs for ρ values between 0.08 and 0.09. In contrast to the

zero-angle DCS for $k = 0.3, 0.5$ and 0.7 a.u., which consistently increase as ρ increases, the result for $k = 0.1$ a.u. increases up to $\rho \approx 0.1$, after which it starts to decrease.

$\rho/10^{-2}$	A	DCS($\theta = 0^\circ$)			
		$k = 0.1$	$k = 0.3$	$k = 0.5$	$k = 0.7$
0.0	-4.21	12.96	12.81	13.24	13.28
1.0	-5.45	18.79	17.17	17.50	17.45
2.0	-7.06	26.38	22.26	22.41	22.22
3.0	-9.22	35.98	28.09	27.94	27.60
3.5	-10.62	41.57	31.29	30.95	30.51
4.0	-12.32	47.68	34.67	34.12	33.57
5.0	-17.11	61.21	42.00	40.92	40.15
6.0	-25.60	75.78	50.06	48.34	47.33
7.0	-44.75	90.03	58.82	56.36	55.09
8.0	-129.60	102.23	68.29	64.97	63.44
9.0	191.34	110.79	78.41	74.15	72.37
10.0	59.53	114.87	89.14	83.87	81.86
11.0	36.70	114.57	100.44	94.10	91.90
12.0	27.21	110.74	112.23	104.82	102.48
13.0	21.99	104.53	124.45	116.00	113.58
14.0	18.68	97.04	137.01	127.59	125.19
15.0	16.38	89.09	149.79	139.57	137.28
17.5	12.83	70.37	181.89	170.98	169.53
20.0	10.77	55.75	212.22	204.01	204.35

TABLE IV. The scattering length A and the zero-angle differential elastic cross section for $k = 0.1, 0.3, 0.5$ and 0.7 are tabulated as a function of the adjustable parameter ρ for the $e^+ + \text{Kr}$ system. All values are expressed in atomic units.

B. Helium

Fig. 5 shows the elastic cross section for positron-helium system. Overall, theoretical models for this system exhibit relatively good agreement with each other, as well as with experimental data of Sullivan *et al.* [66]. We observe that our CP approximation already shows good agreement with the experimental results for energies above ≈ 3 eV, reflecting a likely weak VPs effects on this atom. For the CP+VPs approximation, we consider two different SL values to fine tune the ρ parameter (see Table III). Notably, the differences between the CP and CP+VPs models are only significant at low energies (below ≈ 5 eV). Furthermore, the result using the MBT-SL is in great agreement with the experimental measurements, accurately describing the Ramsauer-Townsend minimum, which is highly sensitive to the potential used. Excellent agreement is also observed with the theoretical results obtained from the MBT [21], CCC [41] and KVM [36]. In contrast, the results obtained using the POM-SL shows a elastic cross section with a higher magnitude in the minimum region, possible indicating a over-correlation problem.

Fig. 6 presents the DCS at 2 eV and 12 eV in the top and bottom panels, respectively. At 2 eV, the VPs term significantly increases the DCS for angles below ≈ 60 degrees compared to the CP model. The greater the VPs contribution to the overall potential, the more pronounced the increase in the DCS at small angles, as evidenced by the comparison between the results using the MBT-SL and the POM-SL. A similar pattern is observed for 12 eV. However, in this case, the DCS increase is restricted to angles below ≈ 30 degrees. Additionally, the DCS for the CP+VPs model is close to the one obtained by the CP model for angles above ≈ 35 degrees.

These observations leads us to conclude that for high energies, the impact of the VPs for this system is only appreciable at small angles, and these differences are suppressed by the sine function when integrating the DCS to obtain the elastic cross section. This explains why all the models presented in fig. 5 have similar elastic cross section at higher energies.

C. Neon

Positron interactions with the neon atom is an interesting case. One notable peculiarity is its annihilation parameter at low energies, which is lower than its number of electrons.

In Fig. 7, we present the elastic cross sections obtained in this work with the experimental measurements of Jones *et al.* [23] and with the theoretical results from the POM [45], MBT [21] and CCC [43]. For energies above ≈ 1 eV, the CP and CP+VPs models yield similar results, all of which are in good agreement with the experimental and theoretical data. However, at lower energies, similarly to the He atom, the CP model underestimates the experimental data. In contrast, the CP+VPs model, particularly when fine-tuned with the POM-SL, aligns more closely with the experimental data at the Ramsauer minimum than the version with the MBT-SL. As expected, the MBT-SL results align more closely with the MBT data, while the POM-SL results exhibit better agreement with the POM and CCC data. Interesting conclusion may be drawn from the results in this figure: the early agreement of the CP model with the measurements indicates that the VPs effects are modest for neon. This modest effect likely explains why the annihilation parameter is unusually low for this atom, as VPs formation is known to significantly enhance annihilation [67].

In Fig. 8, the Folded Differential Cross Sections (FDCS) obtained in this work are compared with both experimental and theoretical results reported by Cheong *et al.* [24] for energies of 1, 2, 3 and 5 eV. The FDCS is defined as the DCS symmetrically folded around 90 degrees to account for experimental limitations that prevent the resolution of forward and backward scattering directions separately. Given that our POM-SL model showed better agreement with the experimental total cross section in Fig. 7, only the results for this model is presented here. The effect of the VPs manifests as a sharp increase in the FDCS at small angles, and a decrease at larger angles. This decrease at larger angles is associated with the shift of the minimum in the unfolded DCS toward angles closer to 90 degrees. For the 1 and 2 eV cases, our CP+VPs model shows very good agreement with the CCC results of Jones *et al.* [23], except at small angles, where the CCC results becomes higher. Good agreement is also found with the Relativistic Optical Potential (ROP) model across all energies. A more recent theoretical investigation with the CCC methodology for this system was performed by Mori *et al.*, where the results obtained are very similar to the ROP ones (see fig. 5 of ref. [43]), and, for this reason, these results are omitted from this figure. Regarding the comparison with the experimental data, good agreement is only found for 1 eV, and some marginal agreement is observed for 2 eV. The reasons of the discrepancy between the theoretical predictions and this experimental data are not yet understood [24, 43].

D. Argon

Fig. 9 shows the elastic cross section as a function of energy for the positron argon system. As it can be seen in the CP model and in the MBT without Ps calculation of [50], one notable characteristic of the lack of VPs for this system is the presence of a Ramsauer minimum in the results. This minimum vanishes when the VPs effects are included, as shown in the CP+VPs calculations. Similar to the Kr atom case, the elastic cross section at higher energy is influenced by non-adiabatic effects, as evident when comparing with the MBT, POM, and CCC results from [21] [46] and [43], respectively. These non-adiabatic contributions likely explain the discrepancies observed between our results and the experimental data of Jones *et al.* [23] for energies above 3 eV, although the CP+VPs model shows better agreement in this region when compared to the experimental measurements reported by Karwasz *et al.* [68]. This suggests that non-adiabatic VPs effects play a crucial role in describing the positron-argon interaction at higher energies, influencing both the magnitude and shape of the elastic cross section, differently from the He and Ne cases.

IV. CONCLUSIONS

In this work, we decomposed the positron-target interaction single-body adiabatic potential into two distinct components: the pure Correlation-Polarization and the virtual Ps formation terms. For the CP term, we employed a potential initially derived for positron-hydrogen interactions, which we then generalized to account for multi-electron targets. This potential only depends on well-known target parameters, and presented strong agreement with results from Many-Body Theory under similar approximation.

For the virtual Ps term, we introduced a simple attractive potential, derived from the short-ranged component of the Correlation-Polarization potential. This potential depends on the Van der Waals radius, which reflects on that fact that virtual Ps effects are expected to be significant at regions beyond the target's valence shell. Additionally, the potential's depth is controlled by an adjustable parameter, which is fine-tuned to match scattering lengths consistent with established theoretical calculations. This approach allows for an effective representation of virtual Ps interactions without over-complicating the potential's formulation.

Results were obtained for the hydrogen and the noble-gas atoms. We have shown that the inclusion of the virtual Ps potential produces results in good agreement with other theoretical models and experimental measurements. The exceptions occurs at energies near the virtual Ps formation threshold, where non-adiabatic effects become significant, leading to some deviations from expected results, specially for the p and d -wave phase-shifts. This highlights the limitations of the adiabatic approximation in such regimes and suggests the need for more sophisticated approaches to fully capture the dynamics near the threshold.

We also examined how the inclusion of the virtual Ps term impacts on the differential elastic cross sections. Our analysis revealed that the incorporation of the virtual Ps primarily enhances the scattering at small angles for all the studied targets. The comparison of results from this work with those obtained from Many-Body Theory indicates that non-adiabatic effects can significantly influence the back-scattering.

Interestingly, while the virtual Ps formation poses a significant challenge for many-body methodologies, in approaches based on a single-body optical potential it can be effectively described using a simple additional correlation term, leading to results that align well with experimental measurements.

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Appendix A: Matrix element

In this appendix, we present the solution of the matrix element given in eq. (13), which is given by:

$$V_{1\lambda}(\mathbf{x}) \equiv \langle \psi_1^\xi | V(\mathbf{r}, \mathbf{x}) | \psi_\lambda^\xi \rangle = \int \psi_{100}^{\xi*}(\mathbf{r}) \left(\frac{1}{x} - \frac{1}{|\mathbf{r} - \mathbf{x}|} \right) \psi_{nlm}^\xi(\mathbf{r}) d^3r \quad (\text{A1})$$

where $\psi_{nlm}^\xi(\mathbf{r}) = R_{nl}^\xi(r)Y_{lm}(\hat{r})$, with $Y_{lm}(\hat{r})$ being the spherical harmonic function, and:

$$R_{nl}^\xi(r) = N_{nl}^\xi e^{-r/\xi n} \left(\frac{2r}{\xi n}\right)^l L_{n-l-1}^{(2l+1)}\left(\frac{2r}{\xi n}\right), \quad (\text{A2})$$

being $L_b^{(a)}(r)$ the associated Laguerre function. The normalization factor is:

$$N_{nl}^\xi = \sqrt{\left(\frac{2}{\xi n}\right)^3 \frac{(n-l-1)!}{2n(n+l)!}}. \quad (\text{A3})$$

Using the multi-polar expansion in (A1) and solving the angular integral, the matrix element reduces to $V_{1\lambda}(\mathbf{x}) = -v_{nl}(x)Y_{lm}(\hat{x})$, with:

$$v_{nl}(x) \equiv \int_0^\infty r^2 R_{10}^\xi(r) \frac{r_{\leq}^l}{r_{>}^{l+1}} R_{nl}^\xi(r) dr. \quad (\text{A4})$$

The solution of the above integral is:

$$\begin{aligned} v_{nl}(x) = & \frac{\sqrt{4\pi}}{2l+1} N_{10}^\xi N_{nl}^\xi \sum_{i=0}^{n-l-1} \frac{(-1)^i}{i!} \left(\frac{2}{\xi n}\right)^{i+l} \binom{n+l}{n-l-1-i} \\ & \times \left[\frac{(2+2l+i)!}{\left(\frac{1}{\xi} + \frac{1}{\xi n}\right)^{3+2l+i} x^{l+1}} \left(1 - e^{-(\frac{1}{\xi} + \frac{1}{\xi n})x} \sum_{j=0}^{2+2l+i} \frac{[(\frac{1}{\xi} + \frac{1}{\xi n})x]^j}{j!}\right) \right. \\ & \left. + \frac{(1+i)! x^l e^{-(\frac{1}{\xi} + \frac{1}{\xi n})x}}{\left(\frac{1}{\xi} + \frac{1}{\xi n}\right)^{2+i}} \sum_{j=0}^{1+i} \frac{[(\frac{1}{\xi} + \frac{1}{\xi n})x]^j}{j!} \right], \end{aligned}$$

The asymptotic form of the $v_{nl}(x)$ for x sufficiently large reduces to $v_{nl}(x \rightarrow \infty) = c_{nl}/x^{l+1}$, with:

$$c_{nl} \equiv l \frac{\sqrt{4\pi}}{2l+1} N_{10}^\xi N_{nl}^\xi \left(\frac{2}{\xi n}\right)^l \frac{(n+l)!}{(n-l-1)!} \frac{\left(\frac{1}{\xi} - \frac{1}{\xi n}\right)^{n-l-2}}{\left(\frac{1}{\xi} + \frac{1}{\xi n}\right)^{n+l+2}} \frac{2}{\xi}. \quad (\text{A5})$$

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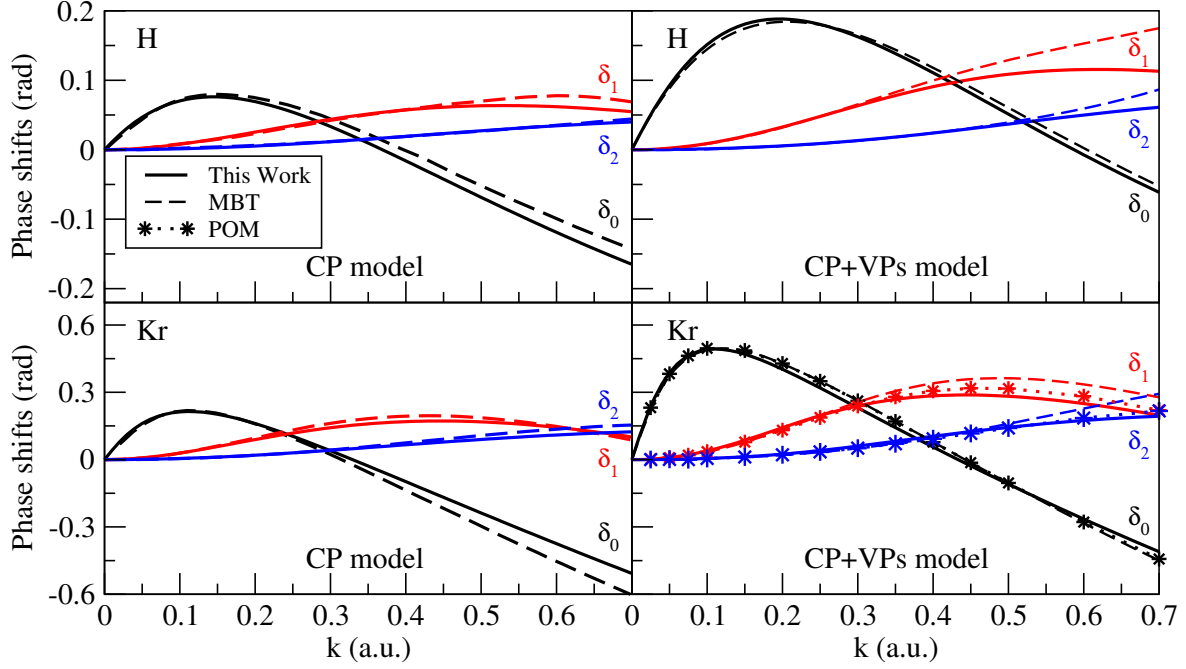


FIG. 1. Phase Shifts as a function of momentum within the CP and CP+VPS approximations. Top-left panel: results within the CP model for positron-H compared with the MBT results from Gribakin and King [9]; Bottom-left panel: results within the CP model for positron-K compared with the MBT results from Green *et al.* [21]. Top-right panel: results within the CP+VPS model for positron-H compared with the MBT results from Gribakin and Ludlow [31]; Bottom-right panel: results within the CP+VPS model for positron-Kr compared with the MBT results from Green *et al.* [21] and POM results from McEachran *et al.* [47]. Legends in figure.

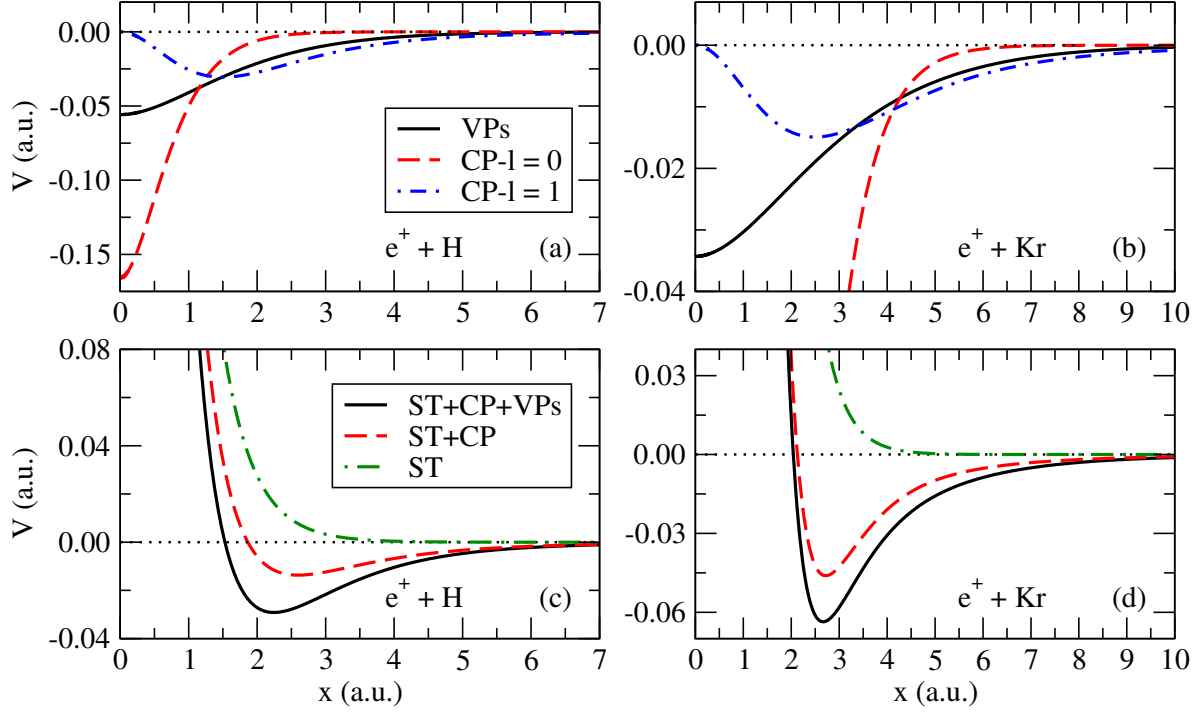


FIG. 2. Potential energy as a function of positron's distance from the atomic nucleus. Panel (a): VPs, CP- $l=0$ and CP- $l=1$ components for positron-H; Panel (b): same as a panel (a), but for positron-Kr; Panel(c): full potential in the ST, ST+CP and ST+CP+VPs approximations for positron-H; Panel (d): same as panel (c), but for positron-Kr. Legends in figure.

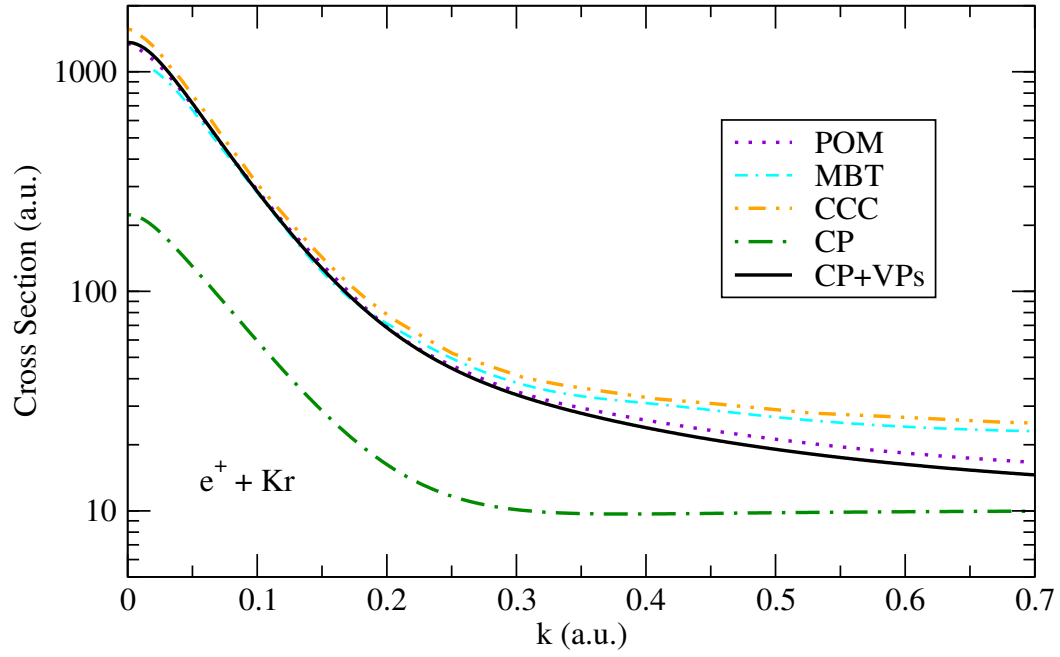


FIG. 3. Elastic cross section as a function of momentum for the positron-Kr system. Legends in figure. The MBT, POM and CCC results were taken from references [21], [47] and [42], respectively.

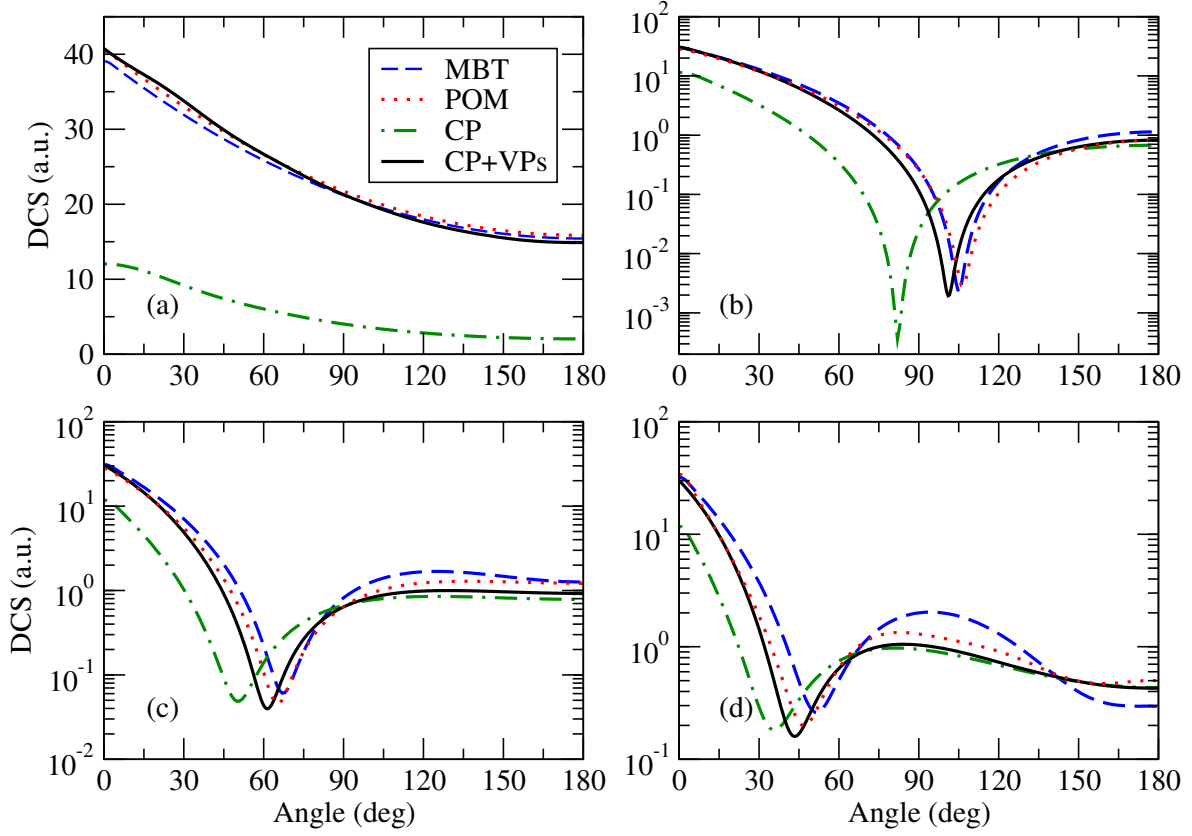


FIG. 4. Differential elastic cross sections as a function of the angle for positron-Kr. Panel (a): results for $k = 0.1$ a.u.; Panel (b): results for $k = 0.3$ a.u.; Panel (c): results for $k = 0.5$ a.u.; Panel (d): results for $k = 0.7$ a.u. The MBT and POM results were calculated as described in the text, with the phase-shifts taken from references [21] and [47], respectively.

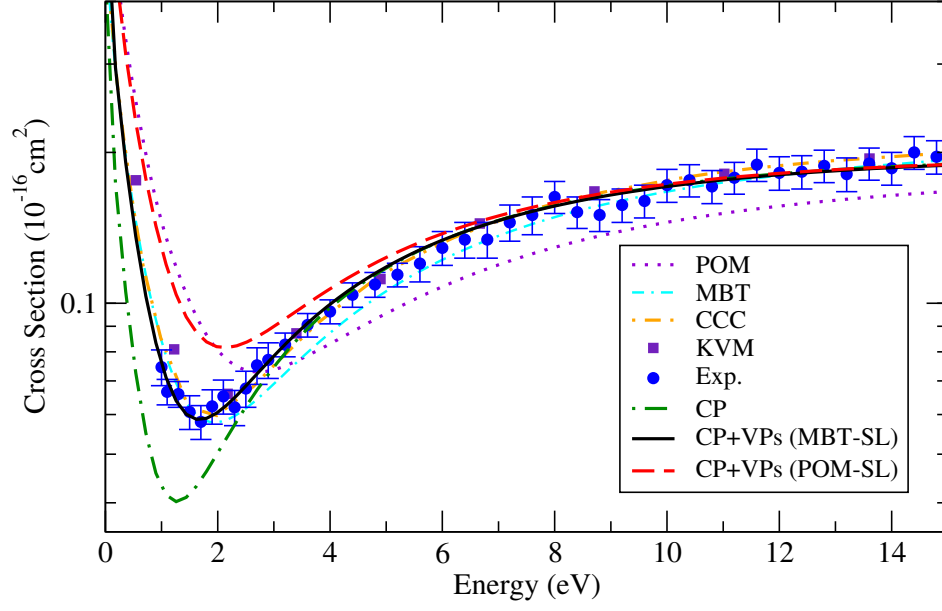


FIG. 5. Elastic cross section as a function of energy for positron-He. Legends in figure. The MBT-SL and POM-SL indicate that the results were obtained by fine-tuning the free parameter to match the SL with those from the MBT and POM, respectively (see Table III). The experimental results were taken from ref. [66]. The POM, MBT, CCC and KVM results were taken from references [22], [21], [41] and [36], respectively.

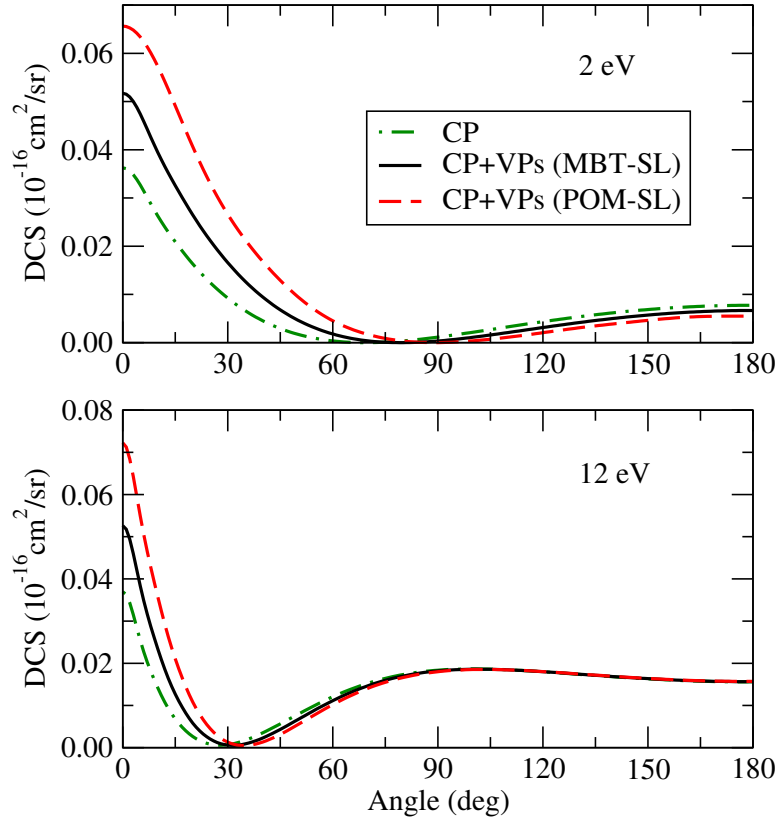


FIG. 6. Differential elastic cross sections as a function of the angle for positron-He. Top panel: results for 2 eV; Bottom Panel: results for 12 eV. Legends in figure. The MBT-SL and POM-SL indicate that the results were obtained by fine-tuning the free parameter to match the SL with those from the MBT and POM, respectively (see Table III).

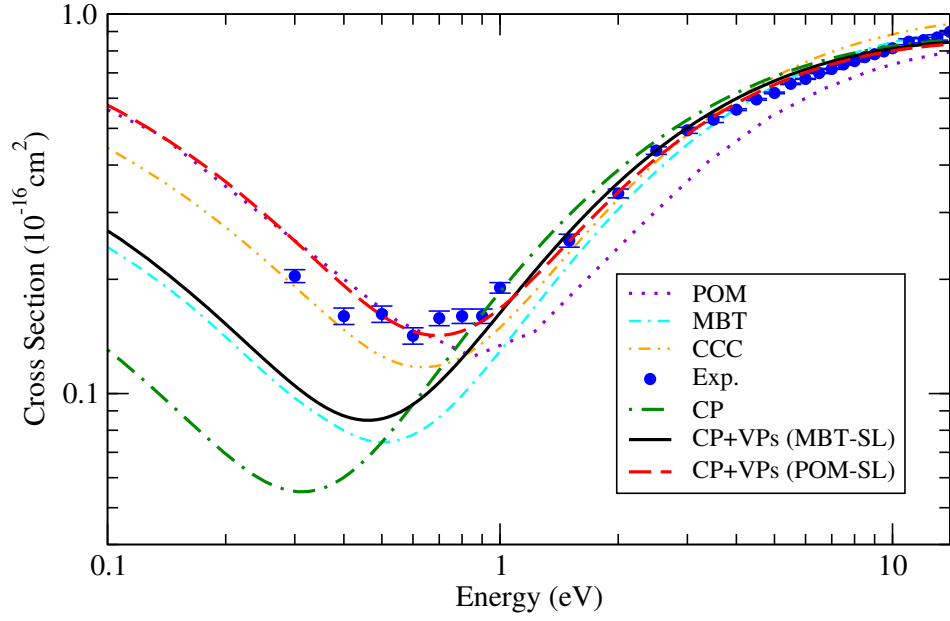


FIG. 7. Elastic cross section as a function of energy for positron-Ne up to 14 eV. Legends in figure. The MBT-SL and POM-SL indicate that the results were obtained by fine-tuning the free parameter to match the SL with those from the MBT and POM, respectively (see Table III). The experimental results were taken from ref. [23]. The POM, MBT and CCC results were taken from references [45], [21] and [43], respectively.

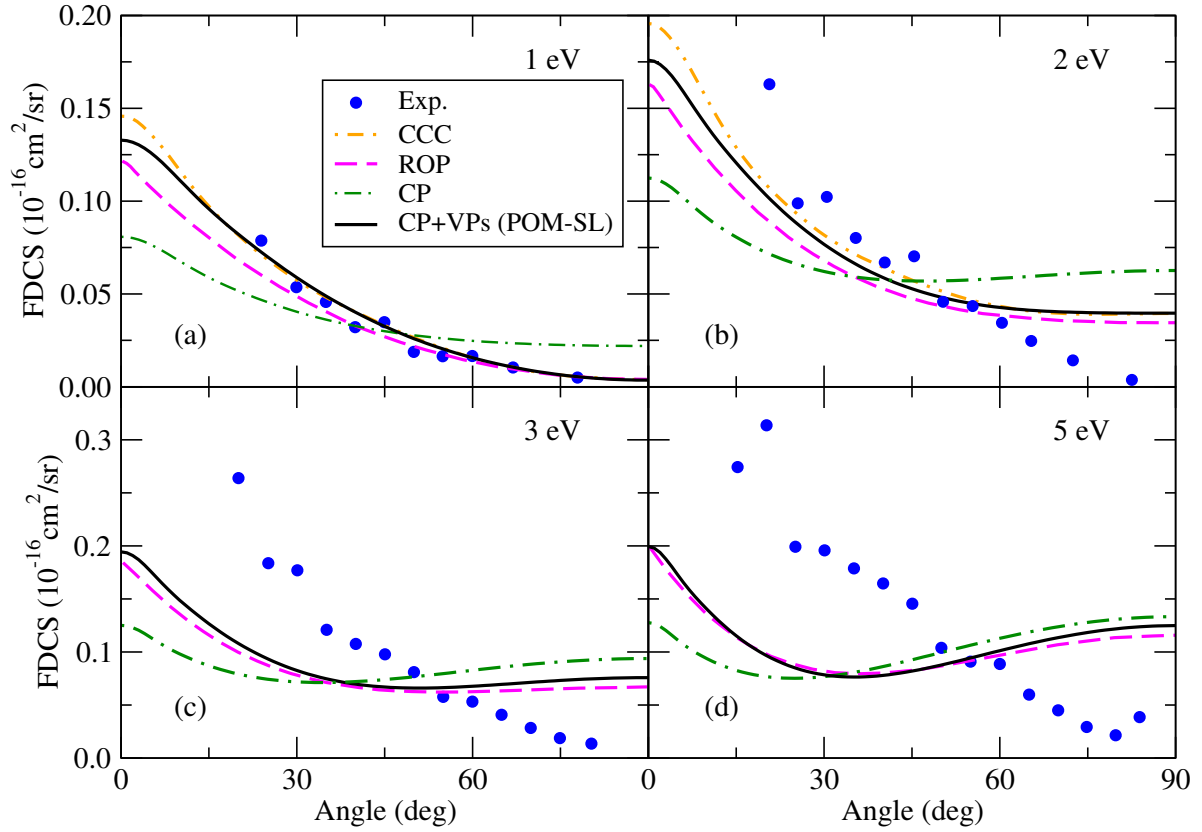


FIG. 8. Folded Differential Cross Sections (FDCS) as a function of the angle for positron-Ne. The FDCS is defined as the DCS symmetrically folded around 90 degrees. Panel (a): results for 1 eV; Panel (b): results for 2 eV; Panel (c): results for 3 eV; Panel (d): results for 5 eV. Legends in figure. The experimental and ROP results were taken from ref. [24], and the CCC results was taken from ref. [23].

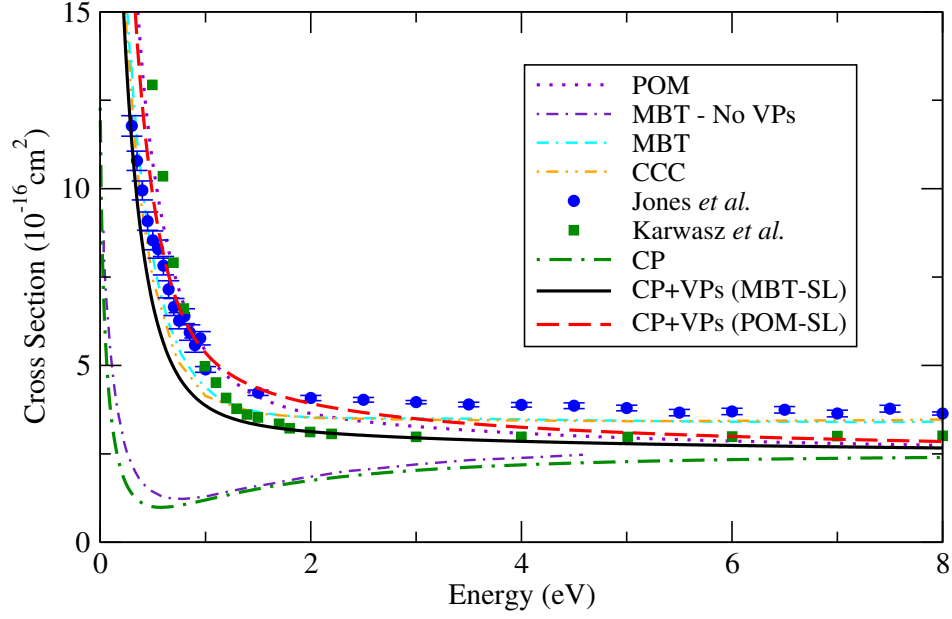


FIG. 9. Elastic cross section as a function of energy for positron-Ar. Solid line: present CP+VPs result obtained with the MBT-SL; Dashed line: present CP+VPs result obtained with the POM-SL; Dash-dotted line: present CP result; Double-dash-dotted line: MBT result from ref. [21]; Dash-dotted short line: MBT results without VPs from ref. [50]; Dotted line: POM result from ref. [46]; Double-dot-dashed line: CCC from ref. [43]; Squares: experimental measurements from ref. [68]; Circles: experimental measurements from [23].