Positron elastic scattering by a semifilled-shell atom

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Abstract
We theoretically study the positron elastic scattering by an atom with a multielectron semifilled subshell in its structure. We focus on gaining the initial insight into the specifics of such a process. The positron scattering by the Mn(…3d⁵4s²,⁶S) atom with a 3d⁵ semifilled subshell (e⁺ + Mn scattering) is chosen as a case study. We account for both the electron correlation and the formation of a e⁺ + e⁻ virtual positronium (Ps) in the intermediate states of the e⁺ + Mn system. Electron correlation is taken into account in the framework of the self-energy part of the scattering positron Green function generalized for the application to semifilled-shell atoms. The influence of the virtual Ps formation on the positron scattering is taken into account by the reduction of the energy of the virtual positron plus atomic-excited-configuration states by the Ps-binding energy, to a reasonable approximation. We unravel the importance and specificity of the influence of both the virtual Ps and electron correlation on e⁺ + Mn elastic scattering. We demonstrate spectacular differences between the electron and positron scattering processes.

Keywords: positron, elastic, scattering, semifilled, shell, atom

(Some figures may appear in colour only in the online journal)

1. Introduction

Positron-atom (e⁺ + A) scattering is an interesting and important process. Its study has a long history (see, e.g. [1–13], and references therein).

Compared to electron-atom (e⁻ + A) scattering, the e⁺ + A scattering process is, at first glance, much simpler due to the lack of exchange between e⁺ and the atomic electrons. Furthermore, qualitatively, the incident positron is subject to a rapidly increasing static repulsion from a positively charged atomic nucleus as the atom is approached, in contrast, of course, to the case of electron scattering. Note, however, that the positron repulsion is usually attenuated by the atomic polarization potential, which is usually attractive to both incident electrons and positrons. Accordingly, incident electrons usually move in a generally stronger attractive atomic potential than positrons. As a result, one could expect that the scattering cross section for electrons by an atom would be both much larger and qualitatively different than that for scattering of positrons, at a given energy. On the whole, however, even taking into account the atomic polarization potential, the scattering of positrons, as a subject for theoretical understanding and description, may seem to be a much simpler process than the scattering of electrons, due to the absence of exchange between atomic electrons and positrons.

However, in contrast to a would-be simplicity of the e⁺ + A scattering, this process appears to be actually more complicated than the electron scattering. This is due to the possibility of the formation of a e⁺ + e⁻ virtual positronium (Ps) between the incoming positron and a virtually excited electron of one of the atomic shells. This was initially qualitatively recognized and described for the case of e⁺ + He scattering in [1]...
and later detailed in numerous studies; see, e.g. [2–6, 14], (and references therein to many other works on the subject).

The Ps formation—virtual or real—is itself a multielectron process. This significantly complicates the description of the $e^+ + A$ scattering, because this process is an essentially multielectron process even without taking into account the formation of a virtual Ps. It turns out that this formation strongly affects the scattering of positrons by atoms to such an extent that in some cases the $e^+ + A$ elastic scattering cross section strongly deviates from that for an electron—from almost complete suppression to a strong increase in the cross section. Hence, the $e^+ + A$ elastic scattering cross section may even prevail over the $e^- + A$ scattering cross section, in some cases.

Although a number of methods have been developed in recent time and attempts have been made to study $e^+ + A$ scattering with varying success, the main focus has been on positron scattering by inert and alkali atoms.

As far as we know, the scattering of positrons by atoms belonging to another group of atoms—the atoms with the highest spin multiplicity—has remained unexplored both theoretically and experimentally. These atoms have a multielectron semifilled subshell in their ground states, such as, for example, a 3$d^5$ semifilled subshell in the Mn(...3$d^5$4$s^2$, 6$S$) atom, which is a 3$d$-transition-metal atom. Although studies were carried out on the interaction of positrons with a number of transition metal atoms [8], they were aimed at detection of bound states of the $e^+ + A$ system, rather than on elastic scattering of positrons by these atoms, at least not by transition-metal atoms with a semifilled multielectron shell. We are not aware of experimental studies of positron scattering by transition atoms with a semifilled shell, including Mn, in contrast to (only two) experiments on electron scattering at electron energies of 20 eV [15, 16], the agreement between which leaves much to be desired. Possible experimental difficulties when using Mn and similar targets may be ‘...due to the inherent difficulty associated with producing a useful atomic beam of open-shell atoms...’ [17]. Since experimentalists have succeeded both in studying electron scattering [15, 16] from Mn and photoionization of semifilled-shell Mn and Cr and their ions [18–21] (and references therein), there is no doubt that positron scattering cross section on these targets can be experimentally addressed as well, if desired.

In this paper, in order to fill the gap in knowledge about the scattering of positrons by a multielectron atom with a semifilled shell, we choose Mn as a case-study-atom. The choice is not accidental. It is dictated by our experience and success in studying multielectron processes involving semifilled-shell atoms and their ions. Our theoretical studies of photoionization of Mn, Mn$^+$, Mn$^{2+}$ and a similar Cr atom and its ion (see, for example [22–26],) led to fairly good agreement with existing and/or subsequently initiated experimental and other theoretical studies. The reader is referred to, e.g., topical review and original papers [18–21] (and references therein) where our results are reviewed along with the results by other methods and experiments. Furthermore, previously [27–29], we have generalized a theoretical formalism based on the Feynman diagrammatic technique and Green’s function of the electron to scattering of electrons by semifilled-shell atoms and provided the insight into elastic electron scattering by the Mn and Cr atoms. The latter studies will give us a basis for a direct elucidation of the similarities and differences between the scattering of positrons and electrons by Mn.

Positron scattering off a 3$d$-transition-metal atom like Mn involves a number of important elements of novelty. Indeed, the 3$d$ subshell of Mn has a kind of dual nature. On the one hand, it is an inner subshell, because it is collapsed into an inner region of the atom (its averaged radius is about 1.12 a.u.). On the other hand, this is a valence subshell in energy, because its ionization potential (approximately 14 eV) is close to the 8 eV ionization potential of the outermost 4$s^2$ subshell. Previously [26], the duplicity of the ‘inner-valence’ 3$d$ subshell was proven to be the key to the understanding of some differences between the 3$p$-photoabsorption spectra of Mn, Mn$^+$, and Mn$^{2+}$. However, how such duplicity of the 3$d$ orbital can affect positron scattering through a virtual Ps formation with a virtually excited 3$d$-electron is not known. This presents an interesting novel topic for study. Furthermore, there are two distinctly different routes for the excitation of the 4$s^2$ subshell of Mn(...3$d^5$4$s^2$, 6$S$). One of them makes the ionic core of the excited Mn be a 4$s^{-1}$5$S$ state, whereas the other one results in a 4$s^{-1}$6$S$ state. The differences between the scattering of positrons during the formation of virtual Ps in different channels are unknown. Thus, clarifying these differences is another interesting topic for study. In addition, it is not clear apriori how the formation of a virtual Ps during the $e^+ + Mn$ scattering is affected by the interference between the two virtually excited channels of the 4$s$ electrons, and how such ‘interference-formed’ Ps does affect the scattering process itself. Neither is clear how both the formation of a virtual Ps and the scattering process are influenced by the interference between the virtually excited channels of the 4$s^2$ subshell and the ‘inner-out’ 3$d^5$ subshell of Mn.

Thus, certainly, the study of elastic positron scattering by high-spin semifilled-shell atoms is a topic of novelty and significance at least from a viewpoint of basic science. In the present paper, we unravel how the perturbation of various atomic subshells of Mn by a scattering positron affects the scattering process both quantitatively and qualitatively, how this process is affected by the formation of virtual Ps in individual and coupled virtual states of the $e^+ + Mn$ system, and we reveal the similarities and differences between elastic $e^+ + Mn$ and $e^- + Mn$ scattering.

The correlated response of the $e^+ + Mn$ system to the scattering process is taken into account in the framework of the self-energy part of the incident positron’s Green function, which represents the polarization interaction, as in our studies of the electron scattering by the semifilled-shell Mn and Cr atoms [27–29].

To account for the virtual Ps formation upon $e^+ + A$ scattering is a difficult task overall. It requires to take into consideration the bound, exited and continuous states in the presence of the $e^+ + e^-$ pair in the field of the atom. The incident positron during the collision $e^+ + A$ is located relatively far from the target atom due to its repulsion by the nucleus. It is for this reason that the $e^+ + e^-$ interaction becomes important even far from the atom, which leads to the temporary
formation of a bound state e⁺ + e⁻, which we refer to as ‘virtual Ps’. The desire to theoretically accurately explain this effect leads to the need to deal at least with the three-body problem, namely, with the need to take into account the interaction between e⁺ and e⁻ under the action of the static potential of the residual ion. This is not a simple task at all. Different types of approximations based on first principles have been suggested to solve the problem. However, not in all of them the virtual Ps formation is taken into account in a physically transparent manner. This is particularly typical for a close-coupling approximation (see, e.g. [9]). In the latter case, the Ps formation is to some extent taken into account by a proper choice of a number of configurations taken into account in the calculations usually guided not by theoretical arguments but by desire to reach a reasonable agreement with experiment. However, the physical role of the phenomenon itself—the formation of Ps upon e⁺ + A scattering—is not visible in this approximation. In contrast, in our work we are committed to using a physically transparent approach to a solution to this problem. The most physically transparent theories, in our opinion, are the theories based on a combination of the Feynman diagram technique and the Dyson equation for the Green function of a scattering particle, such as methods developed, e.g., in [1, 4, 6, 10]. Among these methods, works [4, 6], particularly work [10], suggest significantly more complicated and complete methods than the method suggested in [1] and developed in [6, 7]. Specifically, e.g., the approximation developed in [4] assumes that the relative motion of the e⁺ + e⁻ pair is determined by the real wavefunction of the ground-state Ps, whereas the motion of the center-of-mass of the pair in a virtual state is considered unaffected by the atomic field; this is a drastic approximation to the real very complicated problem. As for work [10], it provides a well-developed, complete theoretical formalism, in which the electron–positron integral equation for Feynman ladder diagrams is converted into linear algebra equations by discretizing the electron and positron continuum states using a square-integrable basis of B-spline functions. However, one should recognize that the exact solution of this problem is not possible without subsequent approximations. In contrast, works [1, 6] suggest a simpler approximation to the scattering problem. There, the formation of virtual Ps in e⁺ + A scattering is accounted by reducing the virtual excitation energies of the atom by the magnitude of the actual Ps binding energy, Iₚₛ ≈ 6.8 eV. Despite such simplification is crude, it was proven to be a viable approximation. For instance, in figure 1, we depicted calculated data for e⁺ + Xe elastic scattering, obtained in [6], in a more strict work [10] and corresponding experimental data [30, 31].

A reasonably good agreement between the calculated results of work [6] and experiment is obvious, thereby indicating the viability of the method suggested in [1, 6]. Interestingly, though, in this case of e⁺ + Xe scattering, the simple method [6] leads to a better agreement with experimental data better than the sophisticated theory [10] (the difference between experiment and theory [10] becomes particularly striking at the positron’s energy E < 1 eV).

To meet the goals of the present study, we used the simplified approximation [1, 6], since it turns to be a viable one, rather than to carry out the most sophisticated detailed calculation of the process. Thus, our research provides only the initial insight into the spectrum of effects that can be characteristic of the e⁺ + Mn elastic (non-resonant) scattering and differ from its analog—scattering of electrons by Mn.

The results obtained may be of interest to related sciences. For example, to astrophysics, since Mn is found in astrophysical objects, see, e.g. [32]. Therefore, knowledge of the collision of a positron with Mn can be useful for understanding astrophysical phenomena. All in all, the Mn atom itself is one of the important elements of our environment. All this requires a detailed knowledge of its properties, and the collision of a positron with Mn serves as an auxiliary sensitive tool for obtaining such knowledge.

2. Main points of theory

The present study is based on the principles that were detailed in our previous calculations of the structure, photoionization of, and elastic electron scattering by, semifilled shell atoms [22, 23, 27–29, 33] (and references therein). Therefore, in the present paper, we only highlight the main provisions of the theory.

As the zeroth-order approximation, we choose the spin-polarized Hartree–Fock (SPHF) approximation [22, 33, 34]. In SPHF; an atom with a semifilled subshell in the ground state is considered as consisting of two different kinds of electrons—the ‘spin-up’ (↑) electrons (a z-component of their spin is sₗ = 1/2) and the ‘spin-down’ (↓) electrons (sₗ = −1/2). There is no exchange interaction between the spin-up and spin-down electrons. Therefore, they occupy states with different energies: Eₗ↑ and Eₗ↓, respectively. As a result, a semifilled-subshell atom can be viewed as an atom with fully occupied subshells (the ‘closed’ subshells) which, however, are either completely spin-up or spin-down subshells. Thus, e.g., the ground-state configuration of the Mn atom in SPHF is as follows: Mn(...3p³↑³↑↑↓↑↓↓↓↓↓↓↑↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓→
The reducible self-energy part \( \bar{\Sigma}^{(2)}(\ell) \) of the Green function of a scattered electron as defined in the SP RPAE theory in the second-order approximation in the Coulomb interaction. Here, a line with a right arrow denotes an electron, a line with a left arrow denotes a vacancy (‘hole’) in the atom, and a wavy line marks the Coulomb interelectron interaction, \( V \). The notations like \( \epsilon, \epsilon_{s}, \) and \( n\ell \) present corresponding states \( |\epsilon, \epsilon_{s}, n\ell\rangle \) of the electrons and ‘holes’, arrows \( \uparrow \) and \( \downarrow \) denote the spin-up or spin-down states, respectively. Designation \( \langle \uparrow + \downarrow \rangle \) means that the contributions of the corresponding spin-up and spin-down states must be summed up in the calculation.

2.1. \( e^{-} + A \) Scattering

We define the scattering phases of spin-up and spin-down electrons upon their collision with a semifilled shell atom as follows \cite{33, 35}:

\[
\delta^{(1)}_{e} = \delta^{(0)(1)}_{e} + \Delta \delta^{(1)}_{e},
\]

where \( \delta^{(0)(1)}_{e} \) are calculated SPHF scattering phases of the spin-up and spin-down electrons, whereas \( \Delta \delta^{(1)}_{e} \) is the correlation (polarization) correction to \( \delta^{(0)(1)}_{e} \):

\[
e^{i\Delta \delta^{(1)}_{e}(\epsilon)} \sin \Delta \delta^{(1)}_{e}(\epsilon) = \langle \epsilon \ell_{T(1)} | \bar{\Sigma}^{(2)}(\ell) | \epsilon \ell_{T(1)} \rangle.
\]

In the above equation, \( \bar{\Sigma}^{(2)}(\ell) \) is the operator of the reducible self-energy components of the Green-function operator for the incoming electron.

2.1.1. SPRPAE theory in the second-order approximation in the Coulomb interaction \( (\bar{\Sigma}^{(2)}, \text{approximation}) \). In the \( \bar{\Sigma}^{(2)} \)-approximation, the \( \bar{\Sigma}^{(2)}_{\ell_{T}(1)}(\epsilon) \) operator is denoted as \( \bar{\Sigma}^{(2)}_{\ell_{T}(1)}(\epsilon) \) and presented using the Feynman diagrams in figure 2.

Correspondingly, the correlation (polarization) correction, \( \Delta \delta^{(1)}_{e} \), is determined as

\[
\Delta \delta^{(1)}_{e}(\epsilon) = \langle \epsilon \ell_{T(1)} | \bar{\Sigma}^{(2)}_{\ell_{T}(1)} | \epsilon \ell_{T(1)} \rangle.
\]

2.1.2. A fuller \( \Sigma \)-approximation. If the contribution of the four terms in figure 2 is not small, then a fuller account of correlation is in order. Correspondingly, in the fuller SPRPAE approximation, called the \( \Sigma \)-approximation in the present paper, the \( \langle \epsilon \ell_{T(1)} | \bar{\Sigma}_{\ell_{T}(1)}(\epsilon) | \epsilon \ell_{T(1)} \rangle \) matrix element is the solution of the Dyson integral equation with the kernel \( \langle \epsilon \ell_{T(1)} | \bar{\Sigma}_{\ell_{T}(1)}(\epsilon) | \epsilon \ell_{T(1)} \rangle \) \cite{33, 35}:

\[
\langle \epsilon \ell_{T(1)} | \bar{\Sigma}_{\ell_{T}(1)}^{(1)}(\epsilon) | \epsilon \ell_{T(1)} \rangle = \langle \epsilon \ell_{T(1)} | \bar{\Sigma}^{(1)}_{\ell_{T}(1)}(\epsilon) | \epsilon \ell_{T(1)} \rangle
\]

\[
+ \sum_{\epsilon'} \frac{\langle \epsilon \ell_{T(1)} | \bar{\Sigma}^{(1)}_{\ell_{T}(1)}(\epsilon') | \epsilon \ell_{T(1)} \rangle \langle \epsilon' \ell_{T(1)} | \bar{\Sigma}^{(1)}_{\ell_{T}(1)}(\epsilon) | \epsilon \ell_{T(1)} \rangle}{\epsilon_1 - \epsilon' + i\delta}.
\]

Here, the label of summation over the intermediate energy, \( \epsilon' \), also assumes integration over the continuous values of \( \epsilon' \). Consequently, when the energy of the incident electron, \( \epsilon \), exceeds the ionization potential of the perturbed atomic subshell of the atom-scatterer, \( \epsilon_{1} \), the scattering phases become complex: \( \delta^{(1)}_{e} = \delta^{(1)}_{e}^{(R)} + i\delta^{(1)}_{e}^{(I)} \). Here, \( \delta^{(1)}_{e}^{(R)} \) and \( \delta^{(1)}_{e}^{(I)} \) denote the real and imaginary parts of the scattering phases, respectively.

2.2. \( e^{+} + A \) scattering

Similar to the case of \( e^{-} + A \) scattering, the positron scattering phases, \( \delta^{+}_{e} \), are defined as

\[
\delta^{+}_{e} = \delta^{(0)+}_{e} + \Delta \delta^{+}_{e}.
\]
Here, \( \delta^{(0)+} \) are SPHF scattering phases of the positron and \( \Delta^{+} \) is the correlation (polarization) correction to \( \delta^{(0)+} \):

\[
e^{-\frac{\Delta^{+}(\epsilon)}{}\sin \Delta^{+}(\epsilon)} = \langle \vec{e} \vec{f} | \Sigma^{+}_{a}(\vec{\epsilon}) | \vec{e} \vec{f} \rangle.
\]

Here, the tilde sign denotes the positron energy and states and \( \Sigma^{+}_{a}(\vec{\epsilon}) \) is the operator of the positron Green function. Similar to \( e^+ + A \) scattering, we consider \( \Sigma^{+}_{a}(\vec{\epsilon}) \) in different approximations. They are listed and explained below.

### 2.2.1. The \( \Sigma^{(0)}_{00} \) and \( \Sigma^{00} \) approximations.

These approximations do not take into account the formation of a virtual Ps in \( e^+ + A \) scattering. Furthermore, in the \( \Sigma^{(0)}_{00} \)-approximation, the Green-function operator, \( \Sigma^{(0)}_{00}(\epsilon) \), is determined only by the diagram shown in figure 2(a), where the upper electronic lines must be replaced with the positron lines. In contrast, the \( \Sigma^{00} \)-approximation is equivalent to the fuller SPRPAE approximation (the \( \Sigma \)-approximation) for electron scattering, equation (4). There, of course, all electron scattering states \( (\epsilon, \ell, \text{ etc}) \) and energies \( (\epsilon, \text{ etc}) \) must be replaced with the positron scattering states and energies, and the electron \( \Sigma^{(2)}_{00}(\epsilon) \) operator must be replaced by the positron \( \Sigma^{(2)}_{00}(\epsilon) \) operator.

### 2.2.2. The \( \Sigma^{(2)}_{ps} \)-approximation.

This approximation does take into account the formation of a virtual Ps during the scattering process. The limitation imposed on this approximation is that the Green-function operator, to be denoted as \( \Sigma^{(2)}_{ps}(\epsilon) \), is break presented only by the diagram shown in figure 3, where the shaded oval denotes the interaction of a \( e^+ + e^+ \) virtual pair with other electrons of the atomic core.

As mentioned in the introduction, the interaction between \( e^+ \) and a virtually excited atomic electron cannot be neglected. Their mutual attraction is decisively important. Taking it into account requires going far beyond the limits of the lowest order of the perturbation theory in the Coulomb interaction. Accordingly, the entire infinite sequence of so-called ‘ladder’ Feynman diagrams must be added to the diagrams depicted in figure 2(a) to accurately account for the formation of a temporary bound state of the \( e^+ + e^+ \) pair called ‘virtual Ps’. This infinite series of ladder diagrams, ‘explaining’ the formation of ‘virtual Ps’, is implicitly present (hidden) in the shaded oval block in figure 3. This modifies both the wavefunction of the \( e^+ + e^+ \) pair and the energy denominator in the expression for the matrix element associated with the diagram in figure 2(a).

It is difficult to accurately take into account all these changes. Instead, as stated in the introduction, in the present paper we adopt a much simpler theory developed and proven to be viable in [1, 6]. Namely, in order to account for the formation of the virtual \( e^+ + e^+ \) pair and its interaction with the atomic core, we subtract the binding energy of free Ps, \( E_{\text{Ps}} \approx 6.8 \text{ eV} \), from the energy denominator of the matrix element shown in figure 2(a). Correspondingly, the irreducible matrix element of the \( \Sigma^{(2)}_{ps}(\epsilon) \) operator is calculated as

\[
\langle \vec{e} \vec{f} || \Sigma^{(2)}_{ps}(\epsilon) || \vec{e} \vec{f} \rangle = \frac{1}{2L + 1} \sum_{\ell \in F, \ell_{min} > F, (\ell, \ell)} \int_{0}^{\infty} \int_{0}^{\infty} \langle \vec{e} \vec{f}, (\epsilon, \ell, \ell') | V_{L} | \vec{e} \vec{f}, (\epsilon', \ell', \ell') \rangle \langle \vec{e} \vec{f}, (\epsilon', \ell', \ell') | V_{L} | \vec{e} \vec{f}, (\epsilon, \ell, \ell') \rangle \ d\epsilon d\epsilon',
\]

for \( \ell \geq F \) notation marks the occupied electronic states in the atom, the \( \ell > F \) label denotes the excited discrete and continuous atomic states, and the ‘tilde’ sign denotes positron states.

### 2.2.3. The \( \Sigma_{ps} \)-approximation.

In essence, this approximation is similar to a fuller \( \Sigma^{00} \)-approximation, but with the important correction: it takes into account the formation of a virtual Ps upon \( e^+ + A \) scattering. Correspondingly, in the \( \Sigma_{ps} \)-approximation, the matrix element \( \langle \vec{e} \vec{f} || \Sigma^{(2)}_{ps}(\epsilon) || \vec{e} \vec{f} \rangle \) in equation (6) is the solution of the following Dyson integral equation:

\[
\langle \vec{e} \vec{f} || \Sigma^{(2)}_{ps}(\epsilon_{1}) || \vec{e} \vec{f} \rangle = \langle \vec{e} \vec{f} || \Sigma^{(0)}_{ps}(\epsilon_{1}) || \vec{e} \vec{f} \rangle + \sum_{\epsilon'} \frac{1}{\epsilon_{1} - \epsilon' + i P_{\text{Ps}} + i \delta} \langle \vec{e} \vec{f} || \Sigma^{(2)}_{ps}(\epsilon_{1}) || \vec{e} \vec{f} \rangle \langle \vec{e} \vec{f} || \Sigma^{(0)}_{ps}(\epsilon_{1}) || \vec{e} \vec{f} \rangle.
\]

### 2.2.4. Concluding remarks.

In conclusion, the basic principle of a strictly consistent application of the diagrammatic technique to atomic processes requires the use of one-electron wave functions, \( P_{\text{nl}}(r) \), and the bound energies, \( E_{\text{nl}} \), of the atomic \( \text{nl} \)-orbitals, which are calculated in the same independent-particle approximation—in our case, the SPHF approximation. Only the replacement of \( E_{\text{nl}} \) with an experimental (or other) value is inadmissible, because it leads to uncontrolled accounting of electron correlation in addition to what seems to be taken into account in such calculations. This can uncontrollably worsen or improve calculated data relative to the corresponding experimental data. Speaking of the \( e^+ + \text{Mn} \) scattering, no corresponding experimental data are available to date. Therefore, in the present work, for the sake of its strict consistency, we use (we must use) the calculated SPHF values for the energies of its spin-up and spin-down orbitals. They are as follows: \( E_{4t^1} = -7.44 \text{ eV}, \quad E_{4t^1} = -6.15 \text{ eV} \) and \( E_{3d^1} = -17.43 \text{ eV} \) [22].
E

The above means that the threshold value of the positron energy, at which the imaginary part of the phase shift begins to grow from zero to a non-zero value, is approximately (7.4–6.8 ≈ 0.6) eV for the scattering process taking into account the polarization of the 4s ↑-subshell and approximately (17.4–6.8 ≈ 10.6) eV for the case of the 3d ↑ polarization (6.8 eV is the approximate binding energy of the Ps, E\textsubscript{Ps}). This will be clearly seen on the inserts in the figures 4 and 5 below in the manuscript (note: our figures start with the positron energy of only about 0.23 eV).

For polarization of the 4s ↓-subshell by the positron the situation is more intriguing. This is because |E\textsubscript{SPHF} \approx 6.15 eV < |E\textsubscript{Ps}|. Hence, the threshold value of the positron energy at which the imaginary part of the phase shift begins to grow from zero to a non-zero value is 0 eV (again, note that our figures start with a positron energy of about only 0.23 eV). Moreover, since |E\textsubscript{4s}| < |E\textsubscript{Ps}|, the energy denominator in (5) and (6) changes sign and becomes negative in the region of positron energies close to zero, when the formation of virtual Ps is considered. This implies that the polarization potential ‘felt’ by the positron due to polarization of the 4s ↓-subshell becomes attractive. This must force the scattering of the positron on the 4s ↓-subshell to prevail over the scattering on the 4s ↑-subshell, near threshold. This is in a complete analogy with the explanation given in [35], in the similar terms as above, for the observed notioned near-threshold differences between the large e \textsuperscript{+} + Li scattering section (P\textsubscript{3f} \approx |E\textsubscript{Ps}|) and small for its nearest neighbor, the He atom (P\textsubscript{3s} \gg |E\textsubscript{Ps}|).

The situation when the ionization threshold of the polarized subshell of the atom is less than the binding energy of Ps is, thus, not new and not unique in atomic physics. In addition to reference [35], we would like to refer the reader to similar (in the spirit of the used diagrammatic technique and discussion) works [4, 8] (and references therein), which also discuss the cases of I\textsubscript{ps} < |E\textsubscript{Ps}|. As it was underlined in [8], ‘atoms with I < 6.8 eV ... differ in ... important aspect: the Ps-formation channel (A \textsuperscript{+} + e \textsuperscript{+} \rightarrow A\textsuperscript{+} + Ps) is open at all positron energies for them’.

Atomic units (a.u.) are used throughout the paper unless specified otherwise.

3. Results and discussion

In the carried out study of e \textsuperscript{+} + Mn elastic scattering, we accounted for monopole, dipole, quadrupole, and octupole virtual excitations of the three outer subshells of Mn: the 4s \textsuperscript{↑}, 4s \textsuperscript{↓}, and 3d \textsuperscript{↑} subshells. The contributions of the higher-order multipolar terms and deeper atomic subshells are negligible compared to those indicated above.

3.1. Impact of the positron-perturbed 4s \textsuperscript{↑} and 4s \textsuperscript{↓} subshells on e \textsuperscript{+} + Mn elastic scattering

Corresponding calculated results for the elastic scattering phase shifts of the s, p, d and f partial positronic waves in the case of e \textsuperscript{+} + Mn scattering, obtained in various approximations, are depicted in figure 4.

One can see that calculated results, obtained without (‘\Sigma\textsubscript{00,4s^{-}}-line’) and with (‘\Sigma\textsubscript{Ps,4s^{-}}-line’) taking into account the formation of a virtual Ps in the calculations of \delta \textsubscript{8}, differ from each other dramatically. Thus, the influence of the formation of a virtual Ps on the scattering process is so great that it cannot be excluded from the study. This is understandable. Indeed, the polarization potential of an easily polarizable semifilled subshell of Mn is itself large. In addition, including I\textsubscript{Ps} in the energy denominator of (8) significantly reduces the denominator. This makes the matrix element (8) even larger, which leads to a large difference between the scattering phases calculated within the \Sigma\textsubscript{00,4s^{-}}, and \Sigma\textsubscript{Ps,4s^{-}} approximations, respectively.

Next, note how the impact of electron correlation on scattering phases depends on a utilized approximation. Specifically, the \Sigma\textsubscript{00,4s^{-}}-approximation predicts a very strong effect of electron correlation in the entire energy region (cf the ‘SPHF’ and ‘\Sigma\textsubscript{00,4s^{-}}-line’ lines in figure 4). However, the more complete \Sigma\textsubscript{Ps,4s^{-}}-approximation, which takes into account the formation of a virtual Ps in the scattering process, shows that the correlation effect is strong only up to about 10 eV of the positron energy (cf the ‘SPHF’ and \Sigma\textsubscript{Ps,4s^{-}}-line in the figure). This is because the term I\textsubscript{Ps} = 6.8 eV becomes less and less essential with the increasing incident energy beyond about 10 eV.

Now, let us discuss, on a relative scale, the individual and aggregated impacts, exerted by the perturbed 4s \textsuperscript{↑} and 4s \textsuperscript{↓} subshells, on the scattering phases. To do this, intercompare graphs \Sigma\textsubscript{Ps,4s^{-}} (dash), \Sigma\textsubscript{Ps,4s^{-}} (dash-dot), and \Sigma\textsubscript{Ps,4s^{-}} (solid) in figure 4. It is seen that the individual effects of these subshells on scattering phases (cf the \Sigma\textsubscript{Ps,4s^{-}}- and \Sigma\textsubscript{Ps,4s^{-}}-lines) differ from each other. It was expected, of course. However, the relative difference between them is not strong, except, perhaps, for the difference between the imaginary parts of the scattering phases of the s-positron-wave at low incident energies. More interesting and important is that the energy dependence of the real parts of the phase shifts, calculated with taking into account only the individual impact of the 4s \textsuperscript{↑} or 4s \textsuperscript{↓} subshell on scattering phases, is close to a monotonic energy dependence, with insignificant exceptions, which are most noticeable for the f-wave. In contrast, the aggregated influence of these subshells on scattering phases results in a pronouncedly non-monotonic energy dependence of the phases in the energy region up to about 10 eV. This reveals strong interference between the individual impacts of the 4s \textsuperscript{↑} or 4s \textsuperscript{↓} subshell on the scattering phases.

Finally, we note that the influence of both electron correlation and the formation of a virtual Ps on the scattering phases...
Figure 4. Real ($\delta'$) and imaginary ($\delta''$) parts of the elastic scattering phase shifts, $\delta_\ell$ ($\ell = s, p, d$ and $f$), in the case of $e^+ + Mn$ collision, as marked. The corresponding calculations took into account the individual responses of the Mn 4s $\uparrow$-subshell (dash, ($\Sigma_{Ps,4s}^\uparrow$)) and the 4s $\downarrow$-subshell (dash-dot, ($\Sigma_{Ps,4s}^\downarrow$)), the collective response of the 4s $\uparrow$ + 4s $\downarrow$ subshells (solid, ($\Sigma_{Ps,4s}$)) all being calculated in the $\Sigma_{Ps}$-approximation, as well as the collective response of the 4s $\uparrow$ + 4s $\downarrow$ subshells calculated both in the $\Sigma_{00}$-approximation (dots, ($\Sigma_{00,4s}$)) and SPHF (dash-dot-dot).

turns out to be especially significant, both quantitatively and qualitatively, at low scattering energies.

3.2. Impact of the positron-perturbed 3d$^5$ $\uparrow$ subshell on $e^+ + Mn$ elastic scattering

Corresponding calculated results for the scattering phases for the s, p, d, and f partial positron waves, obtained in the SPHF, $\Sigma_{00,3d}$, and $\Sigma_{Ps,3d}$ approximations, are depicted in figure 5.

One can see that the relative difference between the real parts of the scattering phases, calculated in the $\Sigma_{00,3d}$ and $\Sigma_{Ps,3d}$ approximations, is not strong. In other words, the effect of the formation of a virtual Ps on the scattering phases in this case is relatively weak, in comparison with this effect in the case of the aggregated impact of the 4s $\uparrow$ and 4s $\downarrow$ subshells on the scattering phases (figure 4). In our opinion, this is due to the ‘inner-orbital’-side of the 3d$^5$ $\uparrow$ subshell whose mean radius is about only 1 a.u.

Neither is strong the effect of electron correlation on the scattering phases (cf graphs ‘$\Sigma_{00,3d}$’, ‘$\Sigma_{Ps,3d}$’, and ‘SPHF’ in figure 5) in comparison to that owing to the combined influence of the 4s $\uparrow$ + 4s $\downarrow$ subshells on the scattering phases. Nevertheless, the electron correlation influence of the 3d$^5$ $\uparrow$-subshell on the scattering phases is stronger than the influence of the formation of a virtual Ps in the excited spectrum of this subshell on the scattering process. We attribute the stronger role of electron correlation in this case to the ‘valence-orbital’-side of the 3d$^5$ $\uparrow$-subshell nature which is reflected in its weak binding energy and large dynamical polarizability.
It is interesting to note that all of the above is in sharp contrast to a much stronger influence of both the electron correlation and formation of a virtual Ps on the scattering phases in the case of the combined impact of the 4s ↑ and 4s ↓ subshells on the scattering process.

3.3. Combined effect of the 4s ↑, 4s ↓ and 3d⁵ ↑ subshells on e⁺ + Mn elastic scattering

The combined correlated influence of the positron-perturbed 4s ↑, 4s ↓, and 3d⁵ ↑ subshells on the scattering phases was calculated in two approximations, namely, without taking into account the formation of a virtual Ps in the scattering process (the Σ₀0,4s approximation) and with this formation taken into account (the Σ Ps,4s + 3d approximation). The calculated data, together with the scattering phases calculated in the Σ₀0,4s and Σ Ps,4s approximations (see figure 4), are shown in figure 6.

Intercomparison of the presented results reveals a significant feature. Indeed, let us recall that the individual influence of the positron-perturbed 3d⁵ ↑ semifilled subshell of Mn on scattering phases is relatively small both on an absolute scale (figure 5) and in comparison with the effect associated only with the 4s ↑ and 4s ↓ subshells (see figure 4). However, when perturbation of all three subshells—4s ↑, 4s ↓, and 3d⁵ ↑—by the incoming positron is taken into account, the results obtained (graphs 'Σ Ps,4s + 3d' in figure 6) differ drastically from the results obtained in the Σ Ps,4s approximation alone (graphs 'Σ Ps,4s' in figure 6). The differences, both quantitative and qualitative, are particularly spectacular between the real parts of the scattering phases calculated in the Σ Ps,4s + 3d and Σ Ps,4s approximations. We attribute the discovered peculiarity in the scattering phases calculated in the Σ Ps,4s + 3d approximation to the ‘valence-orbital’-side of the 3d⁵ ↑-subshell nature. Namely, because its binding energy (≈14 eV) is relatively close to the binding energies of the 4s ↑ and 4s ↓ subshells (≈8 eV), it is as easily perturbed by the incoming positron as the single-electron 4s ↑ and 4s ↓ subshells. However, its oscillator strength significantly exceeds...
Figure 6. Real ($\delta'$) and imaginary ($\delta''$) parts of the elastic scattering phases, $\delta$, calculated in various approximations for the case of $e^+ +$ Mn scattering. Dots, SPHF. Dash, $\Sigma_{00,4s+3d}$ (see text). Solid, $\Sigma_{Ps,4s+3d}$ (see text). Dash-dot-dot, $\Sigma_{00,4s}$ (see figure 4). Dash-dot, $\Sigma_{4s}$ (see figure 4).

the oscillator strengths of the 4s $\uparrow$ and 4s $\downarrow$ subshells. Correspondingly, the excitation channels of the 4s $\uparrow$ and 4s $\downarrow$ subshells are strongly influenced by the excitation channels of the 3d$^5$ $\uparrow$ subshell due to interchannel coupling. Therefore, the combined impact of the 4s $\uparrow$, 4s $\downarrow$, and 3d$^5$ $\uparrow$ subshells on the scattering of the positron by the atom turns out to be stronger than the combined influence of only the 4s $\uparrow$ and 4s $\downarrow$ subshells. This happens even though the individual influence of the 3d$^5$ $\uparrow$ subshell alone on the scattering process is by itself relatively weak.

In the next, we discuss the $e^+ +$ Mn total elastic scattering cross section, calculated by taking into account the combined influence of, (a), only the positron-perturbed 4s $\uparrow$ and 4s $\downarrow$ subshells in the $\Sigma_{Ps,4s}$ and $\Sigma_{Ps,4s}$ approximations and, (b), the positron-perturbed 4s $\uparrow$, 4s $\downarrow$, and 3d$^5$ $\uparrow$ subshells in the $\Sigma_{Ps,4s+3d}$ and $\Sigma_{Ps,4s+3d}$ approximations. The corresponding calculated data are plotted in figure 7.

Perhaps, the most unusual result is that the inclusion of the influence of the ‘inner-valence’ 3d$^5$ $\uparrow$ subshell in addition to that of the two outer 4s $\uparrow$ and 4s $\downarrow$ subshells radically changes the numerical value of the scattering cross section with decreasing energy of the incident positron in comparison with the results obtained in the $\Sigma_{Ps,4s}$ and $\Sigma_{Ps,4s}$ approximations. It is also interesting to note that calculated data obtained in the two latter approximations differ significantly from each other at low positron energies, whereas the calculated results obtained in the $\Sigma_{Ps,4s+3d}$ and $\Sigma_{Ps,4s+3d}$ approximations stay close to each other in the entire energy domain. Such a large cross section for elastic scattering near the threshold, $E = 0$, can be a manifestation of a certain type of scattering resonance or the existence of a very low energy bound state of the
Figure 7. The total elastic scattering cross section in the case of the $e^+ + \text{Mn}$ collision calculated in SPHF and other approximations by taking into account the combined influence of only two $4s$↑ and $4s$↓ subshells on the scattering process (the $\Sigma_{Ps,4s}^{(2)}$ and $\Sigma_{Ps,4s}$ approximations) as well as the combined impact of the three $4s$↑, $4s$↓, and $3d^5$↑ subshells (the $\Sigma_{Ps,4s+3d}$ and $\Sigma_{Ps,4s+3d}$ approximations), as marked in the figure.

3.4. $e^+ + \text{Mn}$ scattering versus $e^- + \text{Mn}$

Finally, in figure 8 we demonstrate the differences between the calculated $e^+ + \text{Mn}$ elastic scattering cross section, $\sigma^+$, and our earlier calculated [28] spin-averaged $e^- + \text{Mn}$ elastic scattering cross section, $\sigma^-$, obtained in the framework of the identical formalism.

Calculated data show significant quantitative and qualitative differences between $\sigma^+$ and $\sigma^-$ at low projectile energies regardless of the approximation used. For instance, the energy dependence of $\sigma^+$ and $\sigma^-$, calculated in the corresponding $\Sigma$-approximations, is seen to be taking qualitatively opposite routes when the projectile energy falls below about 2 eV. Moreover, $\sigma^+$ begins to absolutely dominate $\sigma^-$ with decreasing energy. We believe that we have uncovered the situation which does not exist for low-polarizable noble gas atoms. Namely, we found a situation where scattering of a positron by an atom predominates over scattering of an electron by an atom to an extent that was not observed in any earlier studies of $e^+ + A$ and $e^- + A$ scattering processes.

Taking the opportunity presented by figure 8, we emphasize once again the importance of accounting for the formation of a virtual Ps during the $e^+ + \text{Mn}$ scattering process (the $\Sigma_{Ps,4s+3d}$ approximation) that hugely alters the cross section calculated without this formation taken into account (the $\Sigma_{00,4s+3d}$ approximation).

4. Conclusion

In conclusion, we have provided the initial insight into elastic scattering of positrons by an atom with a multielectron semifilled subshell—the Mn(\ldots3d^54s^26s) atom.

One particularly surprising finding is that, although the individual influence of the ‘inner-out’ $3d^5$↑ semifilled subshell of Mn on $e^+ + \text{Mn}$ scattering is not strong, but, when its virtual excitation is combined with virtual excitations of the $4s$↑ and $4s$↓ subshells, the net effect on the scattering process...
turns out to be significantly stronger than the effect caused by the 4s ↑ and 4s ↓ subshells alone.

Another spectacular finding is that the effect of electron correlation on e− + Mn scattering, with decreasing energy of an incident particle, takes the opposite route compared to the case of e+ + Mn scattering. On the whole, the e+ + Mn elastic scattering cross section proves to be dominant over the e− + Mn elastic scattering cross section at low energies up to a degree not previously observed in the studies of the scattering of positrons and electrons by alkali metals and noble atoms. The rise of the e+ + Mn scattering cross section suggests the existence of a weakly bound positron state or a resonance near a zero energy. This could be because, as discussed in subsection 2.2.4 of section 2, the polarization potential ‘felt’ by the positron due to polarization of the 4s ↓-subshell becomes attractive in the region of positron energies close to zero, when the formation of virtual Ps is considered. On the other hand, it is known that Mn cannot form a negative ion, so that no near-zero bound states of an electron in the field of Mn can exist. As a result, one could expect the formation of near-threshold resonances, or very weakly bound states, upon elastic scattering of positrons off Mn in contrast to the case of the electron-Mn scattering. Our study has clearly identified the actual existence of such qualitative difference between e+ + Mn and e− + Mn scattering. Correspondingly, the elastic scattering cross section takes an opposite route for e+ + Mn scattering compared to e− + Mn at a near-zero energy. And, of course, it has been undoubtedly demonstrated in the present paper that taking into account both the electron correlation and the formation of a virtual Ps in the calculation of e+ + Mn elastic scattering is crucial for (initial) understanding of the scattering process.

Of interest, of course, remains to learn about the importance (or unimportance) of the higher-order effects omitted in the present work. For instance, to study a resonant positron scattering off Mn as it was done, e.g., for alkali atoms [2], to perform a study with a better account for Ps formation and positron annihilation upon scattering, as it was done, e.g., in [10] for noble gases, etc. In this regard, the present work provides researchers with useful background research to initiate future studies aimed at clarifying the significance of the effects beyond those that were taken into account in the present work. We hope that our study will serve as an impetus for both more complete/sophisticated future theoretical studies along with experimental investigations of the scattering of positrons by atoms with multielectron semifilled shells.

Data availability statement

All data that support the findings of this study are included within the article (and any supplementary files).

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