Featured trends in $e^- + \text{Mn}$ electron elastic scattering

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The impacts of both exchange interaction and electron correlation, as well as their combined impact, on electron elastic scattering off a semifilled shell Mn(...3d$^4$4s$^2$, 6S) atom are theoretically studied in the electron energy range of $\epsilon = 0 - 25$ eV. Corresponding elastic scattering phase shifts $\delta_\uparrow(\epsilon)$ as well as partial $\sigma_\uparrow(\epsilon)$ and total $\sigma(\epsilon)$ cross sections are found to be subject to a strong correlation impact. The latter is shown to be drastically different for oppositely spin-polarized scattered electrons, in some cases, thereby bringing significant differences in corresponding $\delta_\uparrow(\epsilon)$s, $\sigma_\uparrow(\epsilon)$s, and $\sigma(\epsilon)$s between said electrons. This is proven to be an inherent features of electron scattering off a semifilled shell atom in general. Electron correlation is accounted for in the framework of the self-energy part $\Sigma$ of the Green function of a scattered electron concept. The latter is calculated in the second-order perturbation theory in the Coulomb interelectron interaction as well as beyond it by solving the Dyson equation for $\Sigma$. The significance of the “Dyson” correlation corrections in electron energy range of 0 to 10 eV. The performed calculations, following the work [12], utilized a concept of the reducible self-energy part $\tilde{\Sigma}(\epsilon)$ of the Green function $G$ of an incoming electron. The calculations are carried out in three consecutively growing levels of sophistication. First, this is a one-electron “spin-polarized” Hartree-Fock (SPHF) approxi-

I. INTRODUCTION

The 3d$^5$ semifilled shell Mn(...3d$^4$4s$^2$, 6S) atom has long served as the bridge to, and touchstone for, a better understanding of the interaction of transition metal atoms with X-ray and Vacuum-Ultraviolet radiations from early days (see, e.g., works by Connerade et. al. [1], Davis and Feldkamp [2], Amusia et. al. [3] to now (see review papers by Somntag and Zimmermann [4], Martin et. al. [5], as well as some of the most recent papers by Frolov et. al. [6], Osawa et. al. [7], Hirsch et. al. [8] and references therein). The structure and spectra of the Mn atom are of self-interest as well, in view of the found abundance of unique features associated with its semifilled 3d$^5$ subshell.

In contrast, studies of another process of the basic and applied significance - electron scattering off the Mn atom - are too scarce. The Mn atom presents a special interest for studying electron scattering processes. This is because it belongs to a class of atoms with the highest spin multiplicity. The latter is owing to co-directed spins of all five electrons in the Mn 3d$^5$ subshell, due to Hund’s rule. As of today, understanding of electron scattering off Mn is rudimentary. The only available experimental data relate to corresponding $e^- + \text{Mn}$ differential scattering cross sections (DSC) measured at a single value of the electron energy $\epsilon = 20$ eV by Williams et. al. [9] and Meintrup et. al. [10]. The same stands for theoretical studies as well. Thus, to understand and interpret experiment, Amusia and Dolmatov [11] calculated the 20 eV $e^- + \text{Mn}$ elastic DCS in the framework of a multielectron simplified “spin-polarized” random phase approximation with exchange (SPRPAE) [12], Meintrup et. al. [10] did it in a R-matrix framework, and recently Remeta and Kelemen [13] performed their calculations of said DCS in the framework of a local spin density approximation, but, again, only at discrete values of the electron energies of 10 and 20 eV.

Whatever interesting effects were found in the above cited works they provide only a limited insight into a problem, since things might work quite differently at other, especially lower electron energies but just 10 and 20 eV energies. Clearly, studying the scattering process through a continuum spectrum of electron energies is a way toward a deeper understanding of, as well as discovering new trends in, $e^- + \text{Mn}$ elastic scattering, in particular, and $e^- + \text{any semifilled shell atom}$, in general. However, no such study has been performed to date, to the best of these authors’ knowledge. Its performance is, thus, not merely a wish but necessity.

It is the ultimate aim of the present paper to study $e^- + \text{Mn}$ elastic scattering through a continuum spectrum of electron energies, to fill in an important gap in the current knowledge on said process. To meet this end, we focus on calculations of $e^- + \text{Mn}$ elastic scattering phase shifts $\delta_\uparrow(\epsilon)$ and corresponding total cross section $\sigma(\epsilon)$ in the electron energy range of 0 - 25 eV.

The performed calculations, following the work [12], utilize a concept of the reducible self-energy part $\tilde{\Sigma}(\epsilon)$ of the Green function $G$ of an incoming electron. The calculations are carried out in three consecutively growing levels of sophistication. First, this is a one-electron “spin-polarized” Hartree-Fock (SPHF) approxi-
A convenient starting approximation to study the structure and spectra of semifilled shell atoms is a “spin-polarized” Hartree-Fock (SPHF) approximation \[14\]. Over the years, SPHF has been extensively and successfully exploited by the authors of this paper and their colleagues (see, e.g., Refs. \[3, 15–18\]) by using it directly, or utilizing it as the zero-order approximation for a multi-electron random phase approximation with exchange \[12\], to study photoionization of said atoms and their ions. As noted earlier, SPHF was also used successfully by Amusia and Dolmatov \[11\] to provide the wavefunctions of spin-up and spin-down electrons in the ground, excited, or scattering state of the atom. For the continuum energy spectrum of scattered electrons, \(P_{\ell \lambda}^{\uparrow}(r)\) have the well-known for a central field asymptotic behavior at large \(r \gg 1\):

\[
P_{\ell \lambda}^{\uparrow}(r) \approx \frac{1}{\sqrt{\pi k}} \sin \left( k r - \frac{\pi \ell}{2} + \delta_{\ell}^{(0)\uparrow}(\epsilon) \right). \tag{1}
\]

Here, \(k\), \(\ell\), \(\epsilon\), and \(\delta_{\ell}^{\text{SPHF}\uparrow}(\epsilon)\) are the momentum, orbital momentum, energy, and the phase shift of a scattered electron, respectively. The total electron elastic scattering cross sections of spin-up (\(\sigma^{\uparrow}\)) and spin-down (\(\sigma^{\downarrow}\)) electrons are determined as

\[
\sigma^{\lambda}(k) = \frac{4\pi}{k^2} \sum_{\ell=0}^{\infty} (2\ell + 1) \sin^2 \delta_{\ell}^{\text{SPHF}\lambda}(k). \tag{2}
\]

B. SPRPAE1

A simplified random phase approximation with exchange, version-1 (SPRPAE1), accounts for electron correlation in a \(\text{e}^{-} + A\) system in the second-order perturbation theory in the Coulomb interelectron interaction \(V\) between the incoming and atomic electrons \[12\]. The approximation exploits the concept of the reducible self-energy part of the one-electron Green function \(\Sigma(\epsilon)\) of a spin-up, \(\Sigma^{\uparrow}(\epsilon)\), or spin-down, \(\Sigma^{\downarrow}(\epsilon)\), scattered electron. In the framework of SPRPAE1, \(\Sigma^{\lambda}(\epsilon)\) is illustrated with the help of Feynman diagrams in Fig. \[4\].

In Fig. \[4\] diagrams (a) and (c) are called “direct” diagrams, in contrast to “exchange” diagrams (b) and (d). The latter two are due to exchange interaction in a \(\text{e}^{-} + A\) system. Basically, the diagrams in Fig. \[4\] illustrate how an incoming electron “\(\epsilon_{\sigma}\)” polarizes a \(j\)-subshell in the atom by causing actual or virtual excitations \(j \rightarrow m\) from the subshell, and couples with these excited states itself via the Coulomb interaction. Note, exchange diagrams (b) and (d) in Fig. \[4\] vanish whenever spin directions of an incoming electron and polarized subshell of the atom are opposite, due to orthogonality of electron spin-functions. We do not account for spin-flip effects since they are negligible in \(\text{e}^{-} + \text{Mn}\) scattering \[10\], at the energies of interest.
Once $\Sigma^{\uparrow}(\omega)$ is calculated, the elastic electron scattering phase shifts of spin-up and spin-down electrons are determined as [12]

$$\delta^{\uparrow}(\omega) = \delta^{\rm SPHF\uparrow}(\omega) + \Delta \delta^{\uparrow}(\omega). \quad (3)$$

Here, $\Delta \delta^{\uparrow}(\omega)$ is the correlation correction term to the SPHF calculated phase shift $\delta^{\rm SPHF\uparrow}(\omega)$:

$$\Delta \delta^{\uparrow}(\omega) = \tan^{-1}\left( -\pi \langle \ell^{\uparrow}(\omega) | \hat{\Sigma}^{\uparrow}(\omega) | \ell^{\uparrow}(\omega) \rangle \right). \quad (4)$$

A mathematical expression for the matrix element $\langle \ell^{\uparrow}(\omega) | \hat{\Sigma}^{\uparrow}(\omega) | \ell^{\uparrow}(\omega) \rangle$ is obtained with the help of the many-body correspondence rules [12]: we refer the reader for details to Ref. [12].

When the energy of a scattered electron exceeds the ionization threshold of the atom-scatterer, the term $\Delta \delta^{\uparrow}(\omega)$ and, thus, the phase shift $\delta^{\uparrow}(\omega)$ itself become complex [12]. Correspondingly,

$$\delta^{\uparrow}(\omega) = \lambda^{\uparrow}(\omega) + i \mu^{\uparrow}(\omega). \quad (5)$$

Here, $\lambda^{\uparrow}(\omega)$ and $\mu^{\uparrow}(\omega)$ are the real and imaginary parts of $\delta^{\uparrow}(\omega)$, respectively:

$$\lambda^{\uparrow}(\omega) = \delta^{\rm SPHF\uparrow}(\omega) + \Re \Delta \delta^{\uparrow}(\omega), \quad \mu^{\uparrow}(\omega) = \Im \Delta \delta^{\uparrow}(\omega). \quad (6)$$

The total electron elastic scattering cross section is then determined [12] by

$$\sigma = \frac{2m}{k^2} \sum_{\ell=0}^{\infty} (2\ell + 1) (\cosh 2\mu - \cos 2\lambda) e^{-2\mu}. \quad (7)$$

In the context of the present paper, $\sigma \equiv \sigma^{\uparrow}(\omega)$, $\mu \equiv \mu^{\uparrow}(\omega)$, and $\lambda \equiv \lambda^{\uparrow}(\omega)$.

### C. SPRPAE2

A version-2 of the simplified random phase approximation with exchange (SPRPAE2) provides a fuller account for electron correlation. There, the reducible self-energy part of the one-electron Green function of a scattered electron is sought as the solution of corresponding Dyson equation [12]. The latter, in an operator form, in terms of spin-up and spin-down electrons, is

$$\hat{\Sigma}^{\uparrow}(\omega) = \hat{\Sigma}^{\uparrow}(\omega) - \hat{G}^{\rm SPHF\uparrow}(\omega) \hat{G}^{\rm SPHF\uparrow}(\omega) \hat{\Sigma}^{\uparrow}(\omega). \quad (8)$$

Here, $\hat{\Sigma}^{\uparrow}(\omega)$ and $\hat{\Sigma}^{\uparrow}(\omega)$ are the operators of the irreducible and reducible self-energy components of the Green-function operator for an incoming electron, respectively, and $\hat{G}^{\rm SPHF\uparrow}(\omega)$ is the operator of the Green function in the framework of SPHF: $\hat{G}^{\rm SPHF\uparrow}(\omega) = (\hat{H}^{\rm SPHF\uparrow}(\omega) - \epsilon)^{-1}$, where $\hat{H}^{\rm SPHF\uparrow}(\omega)$ is the SPHF Hamiltonian operator of the system.

In SPRPAE2, to avoid tremendous calculation difficulties, the general Dyson equation, Eq. (8), is simplified [12]. This is achieved by replacing the operator of the irreducible self-energy component of the Green function $\hat{\Sigma}^{\uparrow}(\omega)$ by $\hat{\Sigma}^{\rm SPRPAE1\uparrow}(\omega)$ (see Fig. 1), to a good approximation. As in SPRPAE1, corresponding SPRPAE2 phase shifts $\delta^{\uparrow}(\omega)$ and total cross sections $\sigma^{\uparrow}(\omega)$ are determined by Eqs. (3)-(7).

### III. RESULTS AND DISCUSSION

#### A. Elastic scattering phase shifts

In the present paper, $e^- + \text{Mn}$ elastic electron scattering is investigated in the electron energy range between approximately 0 and 25 eV, as a case study. This is because core-polarization effects in $e^- + \text{Mn}$ elastic electron scattering are expected to be particularly strong at low electron energies. A trial calculation showed that, at the given energies, accounting for contributions of only $s$, $p$, $d$, and $f$ partial waves to the total elastic scattering cross section, as well as accounting for only monopole, dipole, quadrupole, and octupole excitations of the atomic core in calculations of $\hat{\Sigma}^{\uparrow}(\omega)$ is an excellent approximation. SPHF, SPRPAE1, and SPRPAE2 calculated data for real ($\lambda^{\uparrow}$) and imaginary ($\mu^{\uparrow}$) parts of elastic scattering phase shifts $\delta^{\uparrow}(\omega)$ of spin-down electronic waves are depicted in Figs. 2 and 3 and those for $\lambda^{\uparrow}$ and $\mu^{\uparrow}$ of $\delta^{\uparrow}$ for spin-up electronic waves - in Figs. 4 and 5.

The depicted data unravel important trends in low energy $e^- + \text{Mn}$ elastic scattering which are detailed below.

#### 1. The effects of electron correlation in $e^- + \text{Mn}$ elastic scattering

First, one can see from Figs. 2-5 that both SPRPAE1 and SPRPAE2 correlation affects strongly all phase shifts quantitatively and in a number of cases - for $p$, $d$, and $f$ partial waves - even qualitatively, compared to SPHF calculated data. Thus, the utter importance of electron cor-
FIG. 2. (Color online) SPHF (dashed line), SPRPAE1 (dotted line) and SPRPAE2 (solid line) calculated data for real ($\lambda_s^\downarrow$) and imaginary ($\mu_s^\downarrow$) parts of the e$^-\text{Mn}$ elastic scattering phase shifts $\delta_s^\downarrow(\epsilon) = \lambda_s^\downarrow(\epsilon) + i\mu_s^\downarrow(\epsilon)$ of $s$ and $p$ spin-down electronic waves versus the electron energy $\epsilon$.

FIG. 3. (Color online) SPHF (dashed line), SPRPAE1 (dotted line) and SPRPAE2 (solid line) calculated data for real ($\lambda_d^\downarrow$) and imaginary ($\mu_d^\downarrow$) parts of the e$^-\text{Mn}$ elastic scattering phase shifts $\delta_d^\downarrow(\epsilon)$ of $d$ and $f$ spin-down electronic waves.

FIG. 4. (Color online) SPHF (dashed line), SPRPAE1 (dotted line) and SPRPAE2 (solid line) calculated data for real ($\lambda_s^\uparrow$) and imaginary ($\mu_s^\uparrow$) parts of the e$^-\text{Mn}$ elastic scattering phase shifts $\delta_s^\uparrow(\epsilon)$ of $s$ and $p$ spin-up electronic waves.

FIG. 5. (Color online) SPHF (dashed line), SPRPAE1 (dotted line) and SPRPAE2 (solid line) calculated data for real ($\lambda_d^\uparrow$) and imaginary ($\mu_d^\uparrow$) parts of the e$^-\text{Mn}$ elastic scattering phase shifts $\delta_d^\uparrow(\epsilon)$ of $d$ and $f$ spin-up electronic waves.
relation in the $e^-+\text{Mn}$ low energy elastic electron scattering is revealed.

Second, notice how SPRPAE2 calculated data for low energy $\delta_d^\uparrow(\epsilon)$ phase shifts differ drastically from calculated data obtained in the framework of SPRPAE1. Indeed, the SPRPAE2 calculated phase shift $\delta_d^\uparrow(\epsilon)$ (Fig. 3) drops abruptly, with decreasing electron energy, from $\delta_d^\uparrow(\epsilon) \approx 3.5$ to $\delta_d^\uparrow(\epsilon) \approx 0.5$ rad between 8 to 7 eV, then develops a maximum at yet lower energies, after which it approaches its final value of $\delta_d^\uparrow(\epsilon) \approx 0$ at $\epsilon = 0$. Clearly, the described behavior of SPRPAE2 calculated $\delta_d^\uparrow(\epsilon)$ has little in common with that obtained in the framework of SPRPAE1. Strong quantitative differences take place between SPRPAE1 and SRPAR2 calculated data for $\delta_d^\uparrow(\epsilon)$ as well, see Fig. 5. Also, notice abrupt changes in SPRPAE2 calculated phase shifts $\delta_d^\uparrow(\epsilon)$ between approximately 0 and 2 eV, in opposition to those calculated in SPRPAE1. The unraveled drastic differences between SPRPAE2 and SPRPAE1 calculated phase shifts is a novel result; it was not observed in previous similar calculations performed for other atoms. Thus, the present work reveals, and generally proves, the necessity for a fuller account (as in SPRPAE2) of correlation beyond the second-order approximation (SPRPAE1) for an adequate understanding of $e^-+\text{Mn}$ scattering.

Third, which is of significant importance, notice differences between phases of scattered electronic waves with the same $f$s but opposite spin orientations, $\delta_d^\uparrow$ versus $\delta_d^\downarrow$. Said differences are drastic for $cd$ as well as $ef$ spin-up and spin-down waves in all three SPHF, SPRPAE1, and SPRPAE2 approximations (cp. Figs. 3 and 5). For other spin-up and spin-down waves the differences in question are less spectacular, but, nevertheless, exist as well. Thus, it is revealed in the present study that, generally, scattering of oppositely spin-polarized electrons off the Mn atom take different routes.

Below, we provide reasons for the unraveled trends in the $e^-+\text{Mn}$ electron scattering phase shifts.

2. The origin of the zero-order (SPHF) difference between scattering of spin-up and spin-down electrons off Mn

In SPHF, the dependence of $e^-+\text{Mn}$ scattering phase shifts on a spin-orientation of a scattered electron is a straightforward effect. It is due to the presence/absence of exchange interaction between, respectively, $\epsilon f^\uparrow/\epsilon f^\downarrow$ incoming electrons and primarily five $3d^\uparrow$ electrons in the semifilled $3d^\uparrow$ subshell in the atom. This is a characteristic feature of elastic electron scattering off any semifilled shell atom, for an obvious reason.

Next, since no stable negative Mn ion exists with the ground-state atomic core configuration [19], the number $q_{d\uparrow}$ of bound $d^\uparrow$ states in the atom is $q_{d\uparrow} = 1$ (due to the presence of $3d^\uparrow$ subshell in the atom), whereas corresponding $q_{d\downarrow} = 0$. Consequently, in accordance with the generalized Levinson’s theorem $[\delta_f(\epsilon) \rightarrow (n_f + q_f)\pi$ as $\epsilon \rightarrow 0$, $n_f$ being the number of bound states with given $\ell$ in the field of an atom and $q_f$ being the number of occupied $\ell$ states in the atom itself] $20$, $\delta_d^{\text{SPHF}}(\epsilon) \rightarrow \pi$, whereas $\delta_d^{\text{SPHF}}(\epsilon) \rightarrow 0$ as $\epsilon \rightarrow 0$. This translates into the initial drastic quantitative and qualitative differences between SPHF calculated phase shifts $\delta_d^{\text{SPHF}}(\epsilon)$ (Fig. 3 dashed line) and $\delta_d^{\text{SPHF}}(\epsilon)$ (Fig. 5 dashed line).

3. The origin of the second-order (SPRPAE1) difference between scattering of spin-up and spin-down electrons off Mn

In SPRPAE1, compared to SPHF, differences between $\delta_d^\uparrow$ and $\delta_d^\downarrow$ scattering phases become even more spectacular. Indeed, one can see (Fig. 3, dotted line) that the SPRPAE1 calculated real part $\lambda_f^\uparrow$ of $\delta_d^\uparrow$ is a monotonic function of $\epsilon$ in the interval of 8 to 0 eV, but the real part $\lambda_f^\downarrow$ of $\delta_d^\downarrow$ (Fig. 5 dotted line) is not. The latter now has a well developed minimum followed by an appreciable maximum with decreasing energy $8 \rightarrow 0$ eV. This results, partly, in an additional, compared to SPHF, quantitative as well as qualitative difference between $\delta_d^\uparrow$ and $\delta_d^\downarrow$, due to the effects of electron correlation.

Next, when SPRPAE1 correlation is accounted for, no lesser spectacular differences also emerge between the calculated $\delta_d^\uparrow$ and $\delta_d^\downarrow$ scattering phases. Indeed, SPRPAE1 correlation is seen to induce strong differences between the real parts $\lambda_f^\uparrow$ (Fig. 4, dotted line) and $\lambda_f^\downarrow$ (Fig. 5 dotted line) of phase shifts $\delta_f^\uparrow$ and $\delta_f^\downarrow$: $\lambda_f^{\text{SPRPAE1}}$ turns into an oscillating function of $\epsilon$ whereas $\lambda_f^{\text{SPRPAE1}}$ does not.

A trial calculation showed that the SPRPAE1 correlation induced differences between $\lambda_f^{\text{SPRPAE1}}$ and $\lambda_f^{\text{SPRPAE1}}$ are due primarily to polarization of the $3d^\uparrow$ subshell by an incoming $\epsilon$ electron. Thus, when the incoming electron is a spin-up electron, exchange diagrams (b) and (d) with $j = 3d^\uparrow\uparrow$ in Fig. 6 contribute to phase shifts, whereas their contributions vanish for a spin-down incoming electron, as was explained earlier in text.

4. The higher-order (SPRPAE2) correlation difference between scattering of spin-up and spin-down electrons off Mn

Higher order SPRPAE2 correlation corrections, compared to SPRPAE1, induce additional significant changes, primarily in $\delta_d^\uparrow$ and $\delta_d^\downarrow$ scattering phases. While the impact of said corrections on a real part $\lambda_f^\uparrow(\epsilon)$ of $\delta_d^\uparrow$ (Fig. 5 solid line) results mostly in its quantitative change compared to corresponding SPRPAE1 data, it (the impact) makes a real part $\lambda_f^\downarrow(\epsilon)$ of $\delta_d^\downarrow$ to become both quantitatively and qualitatively different than $\lambda_d^{\text{SPRPAE1}}$, Fig. 5 solid line.

The unraveled different impact of SPRPAE2 correlation on $\delta_d^\uparrow$ compared to $\delta_d^\downarrow$ is because the SPRPAE2 equation for the reducible self-energy part of the Green-
function, Eq. (8), contains many cross-product terms between terms associated with each of the diagrams depicted in Fig. 1. Note, there are no cross-products terms in the framework of SPRPAE1 at all. Since the number of $3d$ electrons in the Mn atom is a 100% unbalanced in favor of $3d^\uparrow$ electrons, many SPRPAE2 cross-product terms, involving various excitations of $3d^\uparrow$ electrons, vanish for an incoming spin-down electron but remain for a spin-up scattered electron. This aggravates the difference between the SPRPAE2 correlation impact on scattering of spin-up compared to spin-down electrons off the atom compared to the difference emerging in SPRPAE1 calculations. For $ed$ incoming electrons, this difference is huge, as was illustrated above.

Thus, the carried out study reveals that the lower-order SPRPAE1 approximation is clearly insufficient for a proper understanding of electron scattering off a semi-filled shell atom. This is an important finding.

Note, the demonstrated fast variation of the SPRPAE2 $\delta_d^\downarrow$ phase with energy in a quite narrow energy region near 8 eV can be interpreted as a prominent time-delay of the partial $ed\downarrow$ wave while crossing the atomic region. Indeed, long ago, Wigner [21] connected the time of quantum mechanical reaction procedure $\tau_c$ with the derivative on the phase over energy. In the considered case of up and down electrons, one has

$$\tau_c^{\uparrow(\downarrow)} = \frac{d\delta_c^{\uparrow(\downarrow)}}{dc}$$

(9)

With the help of this expression, one can estimate not only the time duration of the scattering process of a given $\ell\ell$ wave, but also the time duration difference $\Delta\tau_c^{\uparrow\downarrow}$ for up and down partial waves $\ell$. For the $ed\uparrow$ and $ed\downarrow$ waves in $e^-\+Mn$ scattering near $\epsilon \approx 8$ eV, we find that $\Delta\tau_c^{\uparrow\downarrow} \approx 2 \times 10^{-13}$ s, in the framework of SPRPAE2.

### B. Total $e^-\+Mn$ elastic scattering cross section

To get insight into both the individual correlation and exchange interaction impacts, as well as their combined effect, on observable elastic electron scattering characteristics, we calculated the $e^-\+Mn$ total spin-up $\sigma^\uparrow$ and spin-down $\sigma^\downarrow$ elastic scattering cross sections in the framework of SPHF, SPRPAE1, and SPRPAE2. The performed calculations utilized the above presented data for phase shifts. The thus calculated $\sigma^\uparrow$ and $\sigma^\downarrow$ are depicted in Fig. 6.

The depicted results are self-illustrating in the demonstration of the found significance of correlation impacts on $e^-\+Mn$ elastic electron scattering cross sections of spin-up and spin-down electrons. Clearly, a fuller account of correlation, secured by the SPRPAE2 approximation, is seen to be decisive.

Of significant interest is unraveling of the existence of a narrow resonance in $\sigma^\downarrow$ near $\epsilon \approx 8$ eV in the framework of SPRPAE2 (see the middle and bottom panels in Fig. 6). This resonance has an interesting nature which is associated both with a semi-filled shell structure of, and electron correlation in, the Mn atom.

Indeed, as was discussed and demonstrated above, Fig. 3 it is because of the semi-filled shell structure of the Mn atom that the elastic scattering phase shift $\delta_d^{\downarrow}$ as well as real parts $\lambda_d^{\downarrow}$ of both $\delta_d^{\downarrow}$ of both $\delta_d^{\downarrow}$ of both $\delta_{\text{SPRPAE1}}^{\downarrow}$ and $\delta_{\text{SPRPAE2}}^{\downarrow}$ phases drop to a zero at $\epsilon = 0$. On the way to a zero, $\delta_d^{\downarrow}$ as well as $\lambda_d^{\downarrow}$ pass through the value of $\delta_d^{\downarrow}(\lambda_d^{\downarrow}) = \pi/2$, at certain values of the electron energy. Correspondingly, at such energy, a resonance emerges in a partial $\sigma_d^{\downarrow}$ elastic scattering cross section both in SPHF, where $\sigma_d^{\downarrow} \propto \sin^2 \delta_d^{\downarrow}$, Eq. (2), and SPRPAE1 or SPRPAE2, where $\sigma_d^{\downarrow}$ depends on $\cos 2\lambda_d^{\downarrow}$, Eq. (4). Naturally, the existence of this resonance in partial $\sigma_d^{\downarrow}$ translates into its emergence in the total elastic scattering cross $\sigma^\downarrow$ section at the same electron energy as well. Indeed, as seen in Fig. 6 the resonance in question is present in $\sigma_{\text{SPRPAE1}}^{\downarrow}$ and $\sigma_{\text{SPRPAE2}}^{\downarrow}$ at $\epsilon \approx 8$ eV, as well as in $\sigma_{\text{SPRPAE1}}^{\downarrow}$ at $\epsilon \approx 5$ eV. The resonance is broad and weakly developed both in the SPHF and SPRPAE1 calculated cross sections. In contrast, it is sharp and well developed in $\sigma_{\text{SPRPAE2}}^{\downarrow}$. SPRPAE2, without doubt, is a more complete approximation than either of the SPHF or SPRPAE1 approximations. Prediction based on the basis of SPRPAE2 should,
thus, match reality better than those in the framework of SPHF or SPRPAE1. The SPRPAE2 calculated results in question, thus, allow us to claim the discovery of the actual existence of the 8 eV sharp resonance in the e\(^{-}\)+Mn total elastic electron scattering cross section. Furthermore, as follows from the discussion, the resonance in question can exist neither without the semifilled shell nature of the Mn atom nor without accounting for electron correlation in the e\(^{-}\)+Mn scattering process. This permits us to speak about the discovery of a novel type of a resonance in electron-atom scattering which we name the semifilled-shell-correlation resonance, to stress its uniqueness.

Note, the semifilled-shell-correlation resonance shows up not only in the total elastic electron scattering cross section \(\sigma\) of spin-down electrons but in corresponding spin-averaged total cross section \(\sigma_{avrg}\) as well, see inset in bottom panel of Fig.6. The latter - \(\sigma_{avrg}\) - was calculated as

\[
\sigma_{avrg}(\epsilon) = A_{S_A+s} \sigma_{\uparrow}(\epsilon) + A_{S_A-s} \sigma_{\downarrow}(\epsilon),
\]

where

\[
A_{S_A\pm s} = \frac{2(S_A \pm s) + 1}{(2S_A + 1)(2s + 1)},
\]

\(S_A\) being the spin of the atom \((S_A = 5/2\) for the Mn atom\) and \(s = 1/2\) being the electron spin.

\[\text{IV. CONCLUSION}\]

In summary, it is unraveled in the present paper that (a) SPRPAE1 and SPRPAE2 electron correlation affects significantly e\(^{-}\)+Mn electron elastic scattering phase shifts and cross sections, (b) correlation may affect, and in the case of the Mn atom does affect, drastically differently scattering phase shifts of electrons with opposite spin-orientations, (c) a fuller account of correlation (as in SPRPAE2) beyond the second-order approximation of perturbation theory in the Coulomb interelectron interaction (SPRPAE1) may be, and in the case of e\(^{-}\)+Mn scattering is, crucial for an adequate understanding of the spectrum of corresponding phase shifts and cross sections versus the electron energy, and (d) a combined impact of the semifilled shell nature of the Mn atom and electron correlation results in the emergence of a novel type of the resonance - the semifilled-shell-correlation resonance - in the e\(^{-}\)+Mn total elastic scattering cross section. We urge experimentalists and other theorists to verify the made predictions.

Furthermore, the unraveled physics behind the discovered effects in e\(^{-}\)+Mn scattering is so clear that the present authors have little doubts that most of the effects are inherent features of electron elastic scattering off any multielectron semifilled shell atom in general, not just off the Mn atom. The predicted effects should even be stronger for atoms-scatterers with a higher spin multiplicity (than that of Mn), such as the Cr(...3d\(^{10}\)4s\(^{1}\)\uparrow, \(\uparrow\uparrow\uparrow\), \(\uparrow\uparrow\uparrow\)) or Eu(...4f\(^{7}\)6s\(^{1}\)6s\(^{1}\)\downarrow, \(\downarrow\downarrow\downarrow\)) atoms, or similar. We are currently undertaking such study.

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