On $e^- + \mathrm{Mn}$ elastic scattering at $\varepsilon = 20$ eV impact energy

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Synopsis Current situation relating to 20-eV electron elastic scattering off Mn is discussed and complemented by the author's calculation. Noticeable discrepancies between available calculated and experimental data for large scattering angles are highlighted. Existing understanding of electron scattering off Mn is, thus, inconclusive. Further probes into the matter are urged.

$e^- + \mathrm{Mn}$ elastic scattering is an interesting and important case study in view of both the high spin of $\mathrm{Mn}(3d^54s^2,{}^6S)$ and its open $3d^5$ subshell. To date, however, conclusive agreement exists neither between experiment [1] (absolute scale) and [2] (relative scale), nor between experiments and available theoretical data [2, 3, 4, 5, 6] relating to the total $\sigma_{\mathrm{tot}}(\varepsilon)$ and differential $d\sigma/d\Omega$ elastic scattering cross sections at the electron energy of $\varepsilon = 20$ eV. Corresponding R-matrix results [2] are inconclusive because, first, they do not agree well with experiment and, second, more complete 83-state R-matrix calculated data are in worse agreement with experiment than a only 5-states calculation. Calculated data [3, 4, 5] (spin-polarized RPAE) are incomplete and, thus, inconclusive because of accounting for too few (for $\varepsilon = 20$ eV) electronic ℓ-partial waves, up to only $\ell_{\max} = 5$, for a reason. Some of calculated data of work [6] (spin-polarized LDA) agree somewhat with experiment [1] until about $\theta \approx 50^{\circ}$, but sharply fall considerably below experiment at larger θs, and calculated $\sigma_{\mathrm{tot}} \approx 11 \cdot 10^{-16}$ cm^2 [6] makes it only one-half of experiment [1]. Clearly, another study of $e^- + \mathrm{Mn}$ elastic scattering is in order. This constitutes the aim of the present work.

To meet the goal, the author embeds a semiempirical polarization potential $V_{\mathrm{p}}(r)$ into spin-polarized Hartree-Fock equations [3, 5], rather than into spin-polarized LDA equations used by the authors of work [6], to account for the polarization impact on $e^- + \mathrm{Mn}$ scattering. The potential $V_{\mathrm{p}}(r)$ is approximated by a static dipole polarization potential in the form of $V_{\mathrm{p}} = -\alpha/(r^2 + \bar{r}^2)^2$, for a reason. Here, α and $\bar{r}$ are the static dipole polarizability and mean radius of an atom, respectively. This is a well detailed potential used broadly in atomic physics since 1930th [7]. Excellent agreement between thus calculated $\sigma_{\mathrm{tot}} \approx 21 \cdot 10^{-16}$ cm^2 and experimental $\sigma_{\mathrm{tot}} = 22 \cdot 10^{-16}$ cm^2 [1] is obtained. Present calculated data for $d\sigma/d\Omega$ are depicted in Fig. 1 along with experiments [1, 2] and theories [2, 6]. Excellent agreement between present theory and experiment [1] persists up to $\theta \approx 65^{\circ}$. At larger angles, theory falls noticeably below experiment; this is in line with predictions by other theories [2, 6]. Thus, either there exists an important part of the interaction that affects electron scattering at large angles, which either of the reviewed theories fails to underpin, or experiment is incorrect. Hence, knowledge of $e^- + \mathrm{Mn}$ elastic scattering is incomplete. The author urges the renewing of corresponding experimental and theoretical studies of $e^- + \mathrm{Mn}$ elastic scattering, to dot the i's and cross the t's concerning this important case study.

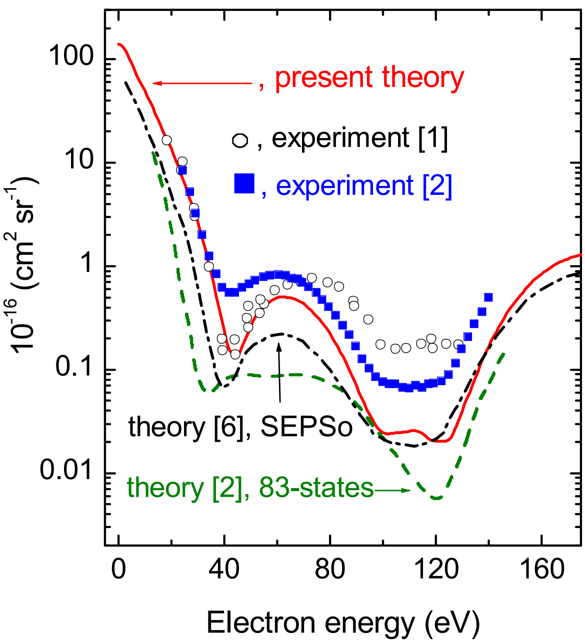

Figure 1. $d\sigma/d\Omega$ for $e^- + \mathrm{Mn}$ elastic scattering at $\varepsilon = 20$ eV. Parameters of theory used in the present calculation: $\alpha \approx 100$, $\bar{r} \approx 3.6$ a.u. and $\ell_{\max} = 40$.

References

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