Elastic scattering of electrons by atoms with half-filled subshells

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A nonstandard theory of electron scattering by atoms with half-filled subshells is developed which is based on the formalism of the "spin-polarized" Hartree–Fock method. The results of calculations of various characteristics of electron elastic scattering by N ($1s^2 2s^2 2p^3$, ^4S) and Mn ($3d^5 4s^2$, ^6S) atoms are presented. The results are obtained in the present theory in the one-electron approximation and also by taking multi-electron effects into account. It is shown that the results are in accordance with the calculations by the "standard" methods of the theory of electron–atom scattering and with the available experimental data.

1. INTRODUCTION

Various approximations[1] have been developed for the purpose of calculating the probabilities of elastic $e^- + A$ scattering (e^- is the incident electron and A is the atomic scatterer), which, of course, have varying effects on the qualitative description and accuracy of the calculation of the corresponding characteristics of the process. Applied to the description of the scattering of electrons by atoms with unclosed shells, possessing nonzero total spin S_A, all of these methods, apart from their dependence on the specific approximations used in them, are based on the standard formalism. Specifically, the total wave function of the $e^- + A$ system is constructed in such a way that it is the exact eigenfunction of the squared total spin operator of this system. In the final analysis, this makes it possible to obtain an equation for the wave function of the scattered electron and to calculate the various characteristics of the $e^- + A$ scattering corresponding to the scattering channel with total spin $S = S_A + 1/2$ or $S = S_A - 1/2$. In what follows we will refer to all such methods for the calculation and description of the process of $e^- + A$ scattering as standard methods of the theory of electron–atom scattering.

In the present paper we develop a nonstandard theory of elastic scattering of electrons by atoms whose unclosed subshells are half-filled. It is based on the formalism of the "spin-polarized" Hartree–Fock method (SPHF),[2,3] which was originally developed for calculations of the features of a quantum structure only of the ground state of atoms (ions) with unclosed subshells, but which has relatively recently found successful application in the theory of the photoionization of atoms with half-filled subshells.[4–7] Here we extend SPHF to the description of the continuous spectrum of the $e^- + A$ system and apply it to the calculation of the characteristics of the elastic scattering of electrons by atoms with half-filled subsells.

In SPHF the radial functions of the incident electrons with opposite spin turn out to be different because of the presence or absence of the exchange interaction between these electrons and the electrons from the half-filled shell of the atom. This makes it possible by taking proper account only of the exchange interaction in the $e^- + A$ system to distinguish and describe the elastic scattering of electrons as a function of the spin state of the electron–atom system. The additional influence of multi-electron effects on the scattering process is taken into account within the framework of the simplified random-phase approximation with exchange, modified for these purposes to the case of atoms with half-filled subshells. On the basis of numerical calculations it is shown that the method developed in this paper makes it possible to obtain results which are in agreement with experimental data and with the results of the "standard" calculations of $e^- + A$ scattering.

2. THE SPHF METHOD IN PROBLEMS INVOLVING $e^- + A$ SCATTERING

Let us consider an atom possessing in its ground state a half-filled subshell, e.g., an atom of nitrogen N ($1s^2 2s^2 2p^3$, ^4S) whose $2p^3$ subshell is half-filled. According to Hund's rule, the spins of all the electrons in the half-filled subshell are all aligned. For definiteness, we will assume that the spins all point up. Electrons with this spin orientation we will denote as "$e^\uparrow$ electrons," and electrons with the spin pointing down, we will denote as "$e^\downarrow$ electrons." Let an electron beam consisting of both $e^\uparrow$ and $e^\downarrow$ electrons with orbital angular momentum l and energy ε be incident upon the atom. We note that there is no exchange interaction between electrons with opposite spins. Therefore the radial wave functions $p^\uparrow_{\varepsilon l}(r)$ and $p^\downarrow_{\varepsilon l}(r)$ of the incident $e^\uparrow$ and $e^\downarrow$ electrons, respectively, will be different as a result of the presence or absence of exchange between the incident electrons and the $e^\uparrow$ electrons of the half-filled subshell of the atom. Consequently, the scattering of the $e^\uparrow$ and $e^\downarrow$ electrons by the atom takes place with different probability, and the difference increases with the number of electrons in the half-filled subshell of the atom, i.e., with the total spin of the target atom.

To find the functions $p^\uparrow_{\varepsilon l}(r)$ and $p^\downarrow_{\varepsilon l}(r)$, let us begin in the following way. First, we will describe the ground state of the atom in SPHF. In this representation each atomic subshell, except for the half-filled one, is divided into two levels occupied only by either $e^\uparrow$ or $e^\downarrow$ electrons. This is a consequence of the presence or absence of the exchange interaction of these electrons with the $e^\uparrow$ electrons of the half-filled subshell of the atom. For example, the electronic configuration of the ground state of an atom of nitrogen in SPHF has the form N($1s\uparrow 1s\downarrow 2s\uparrow 2s\downarrow 2p^3\uparrow$). We assume that the wave functions $\varphi^\uparrow_j(r)$ and $\varphi^\downarrow_j(r)$ of the $e^\uparrow$ and $e^\downarrow$ electron levels, respectively, in the atom have already been found by solution of the SPHF equations for the ground state of the atom.[3,5,8,9] Second, in the description of the $e^- + A$ scatter-

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ing, we ignore the polarization of the atom by the incident electrons, and also spin-flip transitions of the electron spins. Then in analogy with ordinary Hartree–Fock theory it is easy to write the SPHF equations for the wave functions of the continuous spectrum of the $e^- + A$ system $\psi_{el\uparrow}(r)$ and $\psi_{el\downarrow}(r)$:

$$\left(-\frac{\Delta}{2}-\frac{z}{r}+\int\frac{\rho^{\uparrow}(\mathbf{r}')+\rho^{\downarrow}(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}d\mathbf{r}'\right)\psi_{el}^{\uparrow(\downarrow)}(\mathbf{r})$$
$$-\sum_{j\uparrow(j\downarrow)}\varphi_j^{\uparrow(\downarrow)}(\mathbf{r})\int\frac{\varphi_j^{\uparrow(\downarrow)}(\mathbf{r}')\psi_{el}^{\uparrow(\downarrow)}(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}d\mathbf{r}'=\varepsilon\psi_{el}^{\uparrow(\downarrow)}(\mathbf{r}). \quad (1)$$

Here the atomic system of units is used, the indices $\uparrow(\downarrow)$ correspond to the $e^{\uparrow}$ ($e^{\downarrow}$) electrons, $\rho\uparrow(\rho\downarrow)$ is the density of the distributions of the bound $e^{\uparrow}$ ($e^{\downarrow}$) electrons in the atom with nuclear charge z, and the wave functions both of the atoms and of the incident electrons can be represented in the form of a product of a radial and an angular part, e.g.,

$$\psi_{sl}^{\uparrow(\downarrow)}(\mathbf{r})=P_{el}^{\uparrow(\downarrow)}(r)\,Y_{lm_l}(\mathbf{r}/r) \quad (2)$$

Solving Eq. (1), we find the functions $p_{el}^{\uparrow\downarrow}(r)$. From their asymptotic behavior at $r\gg 1$ we determine the phases of the elastic scattering $\xi_l^{\uparrow}(\varepsilon)$ and $\xi_l^{\downarrow}(\varepsilon)$ of the $e^{\uparrow}$ and $e^{\downarrow}$ electrons, respectively, by the atom, from which we can then find the various characteristics of the $e^- + A$ scattering.

Figures 1 and 2 show the results of such calculations of the differential (in solid angle Ω) elastic scattering cross sections $d\sigma^{\uparrow}/s\Omega$ and $d\sigma^{\downarrow}/d\Omega$ of the $e^{\uparrow}$ and $e^{\downarrow}$ electrons with energy $\varepsilon = 20$ eV by atoms of $N(1s\uparrow 1s\downarrow 2s\uparrow 2s\downarrow 2p^3\uparrow)$ and $Mn(3d^5\uparrow 4s\uparrow 4s\downarrow)$. Also shown are the differential scattering cross sections averaged over the spin states of the $e^- + A$ system $\langle d\sigma^{\uparrow\downarrow}/d\Omega\rangle$:

$$\left\langle\frac{d\sigma^{\uparrow\downarrow}}{d\Omega}\right\rangle=A_{s_A+1/2}\frac{d\sigma^{\uparrow}}{d\Omega}+A_{s_A-1/2}\frac{d\sigma^{\downarrow}}{d\Omega}, \quad (3)$$

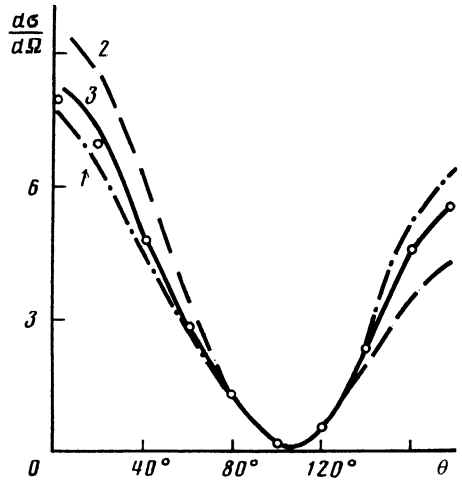

FIG. 1. Differential cross sections (in units of 10^{-16} cm$^2\cdot$sr^{-1}) of the elastic scattering of electrons by atomic nitrogen ($\varepsilon = 20$ eV): 1, 2, and 3) results of calculations respectively of $d\sigma^{\uparrow}/d\Omega$, $d\sigma^{\downarrow}/d\Omega$, and $\langle d\sigma^{\uparrow\downarrow}/d\Omega\rangle$, obtained using SPHF, taking into account the interference of the first five partial electron waves ($l = 0$–4). The points are the results of calculations using DWM[11] averaged over the spin states of the electron–atom system.

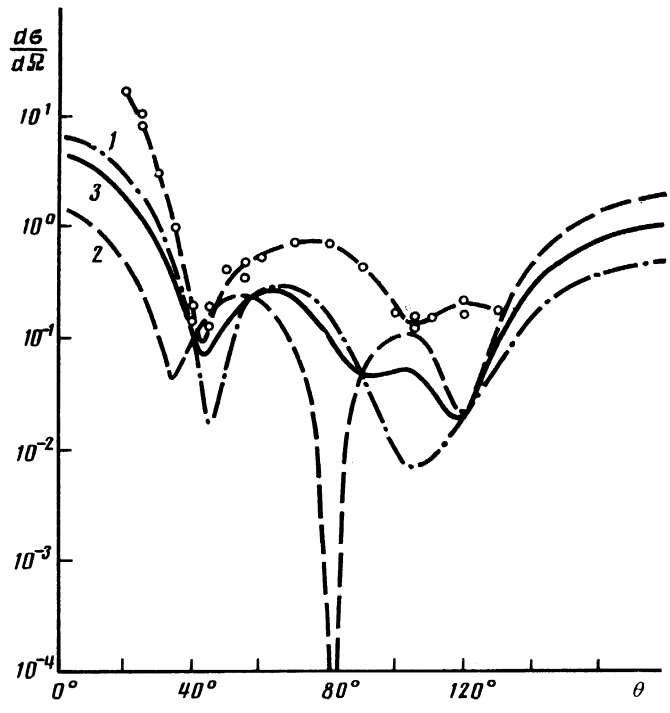

FIG. 2. Differential cross sections of the elastic scattering of electrons ($\varepsilon = 20$ eV) by atomic manganese: units and labeling of curves—the same as in Fig. 1. The points are the results of experiment[10] averaged over the spin states of the electron–atom system.

where

$$A_{s_A\pm 1/2}=\frac{2(S_A\pm s)+1}{(2S_A+1)(2s+1)}, \quad (4)$$

S_A is the spin of the atom and $s = 1/2$ is the electron spin. The results obtained for $\langle d\sigma^{\uparrow\downarrow}/d\Omega\rangle$ are compared with the corresponding experimental results for $e^- + Mn$ scattering[10] and with the results of calculations by the distorted wave method (DWM) for $e^- + N$ scattering.[11]

From Fig. 1 it can clearly be seen that the displayed results for $\langle d\sigma^{\uparrow\downarrow}/d\Omega\rangle$ in the case of $e^- + N$ scattering practically coincide with the corresponding data obtained from Ref. 11. The small discrepancy between them in the region of small scattering angles θ is due to polarization effects, which are ignored in SPHF but taken into account in DWM. Ignoring these effects here is completely appropriate in light of the small dipole polarization α of the nitrogen atom: $\alpha = 7.5\alpha_0^3$ (Ref. 12), where α_0 is the first Bohr radius of the hydrogen atom. As to the difference between $d\sigma^{\uparrow}/d\Omega$ and $d\sigma^{\downarrow}/d\Omega$, this also turns out to be small, as a consequence of the small number of electrons in the half-filled subshell $3p_{\uparrow}^3$ of the nitrogen atom. It is obvious that the differences between them should increase as one goes from the N atom to the Mn atom as a result of the increased role of the presence or absence of exchange of $e^{\uparrow}$ and $e^{\downarrow}$ electrons with the $e^{\uparrow}$ electrons of the many-electron $3d_{\uparrow}^5$ half-filled level of the Mn atom.

The results of the calculation of $e^- + Mn$ scattering are shown in Fig. 2. It can be seen that in fact $d\sigma^{\uparrow}/d\Omega$ and $d\sigma^{\downarrow}/d\Omega$ in the present case differ greatly from one another not only quantitatively, but also qualitatively in their dependence on the scattering angle θ. Consequently, the difference in the exchange interaction of the incident $e^{\uparrow}$ and $e^{\downarrow}$ electrons with the atomic electrons has a radical effect on the

character of their scattering by the atom. From Fig. 2 it can also be seen that the calculated reesults for $\langle d\sigma^{\uparrow\downarrow}/d\Omega\rangle$ faithfully reproduce the qualitative behavior of the corresponding experimental results of the dependence $\langle d\sigma/d\Omega\rangle$ on θ: both curves have a similar oscillatory character in their dependence on θ, as a result of which there are two maxima in the differential scattering cross section, one of which is weak. This qualitative agreement of the calculated and experimental results also with the results for $e^- + \mathrm{N}$ scattering allow one to assert that in its fundamentals this formalism is applicable to the description and calculation of elastic scattering of electrons by atoms with half-filled subshells. The quantitative discrepancies between the calculated and the measured values of $\langle d\sigma/d\Omega\rangle$ for $e^- + \mathrm{Mn}$ scattering are a completely natural result of neglecting the polarizability α of the Mn atom, which is large: $\alpha = 100a_0^3$ (Ref. 12). To obtain quantitatively accurate results, it is consequently necessary to develop a method which allows one to effectively take into account that part of the interelectron interaction in the $e^- + A$ system that is neglected in SPHF. The remainder of this paper is dedicated to this problem along with a discussion of specific results.

3. SIMPLIFIED RANDOM PHASE APPROXIMATION WITH EXCHANGE FOR SCATTERING OF ELECTRONS BY ATOMS WITH HALF-FILLED SUBSHELLS

In the SPHF formalism the atoms with half-filled subshells are similar to the atoms with closed subshells since it is not possible to add a single electron to any of the filled $e^\uparrow$ or $e^\downarrow$ levels of the atom. Therefore, to calculate that part of the interelectron interction in the $e^- + A$ system that is neglected in SPHF, it is possible, as was shown in Refs. 4–6, to make use in a relatively simple way of methods which are based on quantum many-body theory. For these purposes we will start from the very successful, previously so-called simplified random phase approximation with exchange (SRPAE),[6,9] modifying it here to the case of scattering of electrons by atoms with half-filled subshells.

Formally carrying over the SRPAE theory to the case of interest to us, we will assume that in the zeroth approximation—in SPHF—the scattering problem has already been solved, i.e., the one-electron scattering functions $p_{\varepsilon l}^{\uparrow(\downarrow)}(r)$ and the phase shifts in this approximation ${}^0\xi^{\uparrow(\downarrow)}(\varepsilon)$ have been found. Following SRPAE, we find the scattering phases $\xi_l^{\uparrow(\downarrow)}(\varepsilon)$ with the multi-electron corrections taken into account from the relation

$$\xi_l^{\uparrow(\downarrow)}(\varepsilon) = {}^0\xi_l^{\uparrow(\downarrow)}(\varepsilon) + \operatorname{arctg}\left(-\pi\langle P_{\varepsilon l}^{\uparrow(\downarrow)}|\tilde{\Sigma}_\varepsilon|P_{\varepsilon l}^{\uparrow(\downarrow)}\rangle\right). \quad (5)$$

Here $\tilde{\Sigma}_\varepsilon$ is the reduced proper energy part of the one-electron Green's function of the scattered electron, which satisfies an equation that in terms of the notation used in this paper is written as

$$\begin{aligned}\langle P_{\varepsilon l}^{\uparrow(\downarrow)}|\tilde{\Sigma}_\varepsilon|P_{\varepsilon' l}^{\uparrow(\downarrow)}\rangle &= \langle P_{\varepsilon l}^{\uparrow(\downarrow)}|\Sigma_\varepsilon|P_{\varepsilon' l}^{\uparrow(\downarrow)}\rangle \\ &+ \int_0^\infty \langle P_{\varepsilon l}^{\uparrow(\downarrow)}|\Sigma_\varepsilon|P_{\varepsilon'' l}^{\uparrow(\downarrow)}\rangle\langle P_{\varepsilon'' l}^{\uparrow(\downarrow)}|\tilde{\Sigma}_\varepsilon|P_{\varepsilon' l}^{\uparrow(\downarrow)}\rangle \frac{d\varepsilon''}{\varepsilon-\varepsilon''} \\ &+ \sum_{nl}\langle P_{\varepsilon l}^{\uparrow(\downarrow)}|\Sigma_\varepsilon|P_{nl}^{\uparrow(\downarrow)}\rangle\langle P_{nl}^{\uparrow(\downarrow)}|\tilde{\Sigma}_\varepsilon|P_{\varepsilon' l}^{\uparrow(\downarrow)}\rangle. \end{aligned} \quad (6)$$

Here Σ_ε is the unreduced proper energy part of the Green's function of the scattered electron, and the summation is carried out over all the allowed $e^\uparrow$ and $e^\downarrow$ hole states nl of the atom. As in Refs. 6 and 9, we will solve Eq. (6) in a simplified way, substituting in it the matrix elements of the operator Σ_ε, given to second order by the perturbation theory of the Coulomb interelectron interaction in the atom. The matrix elements of the operator Σ_ε, assigned in this way, are depicted in Fig. 3 with the help of diagrams from many-body theory.

In the case of atoms with closed subshells the matrix elements of the operator Σ_ε are always determined by all of the diagrams (a–d) depicted in Fig. 3. However, in the formalism we are developing here this is inadmissible. Indeed, let the atom scatter electrons of a given kind (say $e^\uparrow$ electrons) with the excited electrons in the atom being electrons of the other kind accordingly, $e^\downarrow$ electrons). Then diagrams b and d must be discarded since in the contrary case one would be taking account of spin-flip transitions of the electrons under the influence of the Coulomb interaction, which is impossible. For the same reason the summation over nl on the right side of Eq. (6) must be restricted to only those hole states whose spin orientation coincides with the spin orientation of the scattered electron. From what has been said, in particular, there follows an interesting conclusion, namely that the SRPAE corrections lead to additional differences in the scattering of the $e^\uparrow$ and the $e^\downarrow$ electrons by atoms with half-filled subshells. This should be especially strongly manifested in the interactions of the incident $e^\uparrow$ and $e^\downarrow$ electrons

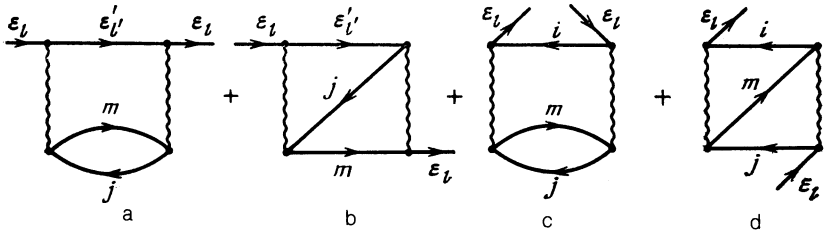

FIG. 3. Diagrammatic depiction of the matrix elements of the operator Σ_ε in the second-order perturbation theory of the interelectron interaction in the atom. The line with the arrow pointing right represents the electron ($|\varepsilon_l\rangle$ and $|\varepsilon'_{l'}\rangle$ are the initial and intermediate states of the incident electron, while $|m\rangle$ is the excited state of the atomic electron from the subshell j), the line with the arrow pointing left represents the hole in the atom, and the wavy line represents the Coulomb interaction .

with the half-filled subshell of an atom which contains only $e^{\downarrow}$ electrons.

The modification of ordinary SRPAE to atoms with half-filled subshells consists in the above peculiarities of the application of SRPAE to this class of atoms. To emphasize this, from now on we will call the SRPAE method modified here to allow its application to atoms with half-filled subshells the "spin-polarized" SRPAE method (SP-SRPAE).

4. RESULTS OF THE CALCULATION OF e^- + Mn SCATTERING IN SP-SRPAE

In Sec. 2 of the present paper it was observed that the quantitative discrepancies between the experimental results and those obtained with SPHF on the angular distribution of the elastically scattered electrons with $\varepsilon = 20$ eV in the case of scattering by Mn atoms are due to neglecting the effects of the polarizability of the atom. According to this, one should expect that taking such effects into account should substantially raise the theoretical curve for $d\sigma^{\uparrow(\downarrow)}/d\sigma$ (see Fig. 2) and cause its oscillations with respect to the θ axis to grow without thereby causing any qualitative change in its shape. This will also be demonstrated below by way of the results of detailed calculations of the differential scattering cross sections $d\sigma^{\downarrow}/d\Omega$ in the case of scattering of $e^{\downarrow}$ electrons with $\varepsilon = 20$ eV by Mn atoms.

To calculate $d\sigma^{\downarrow}/d\Omega$ it turns out to be sufficient to take into account the first five partial waves of the incident electrons $\varepsilon l\downarrow$ with $l = 0$-4, and to calculate the corresponding scattering phases in SP-SRPAE it turns out to be sufficient to take into account the monopole, and quadrupole excitations by the incident electrons of the outer ($3d^5_{\uparrow}$,$4s\uparrow$,$4s\downarrow$ and intermediate ($3p^3_{\uparrow}$,$3p^3_{\downarrow}$) subshells of the Mn atom. The main results of the calculation of the scattering phases $\xi^{\downarrow}_l$ are completely reflected in Table I. It can be seen that as a consequence of the large polarizability of the Mn atom the values of the scattering phases calculated in SP-SRPAE differ markedly from the corresponding one-electron values ${}^0\xi^{\downarrow}_l$. Figure 4 compares the results of calculations of $d\sigma^{\downarrow}/d\Omega$ in SPHF with the corresponding results of the calculations in SP-SRPAE. It is clear that taking account of the dynamic

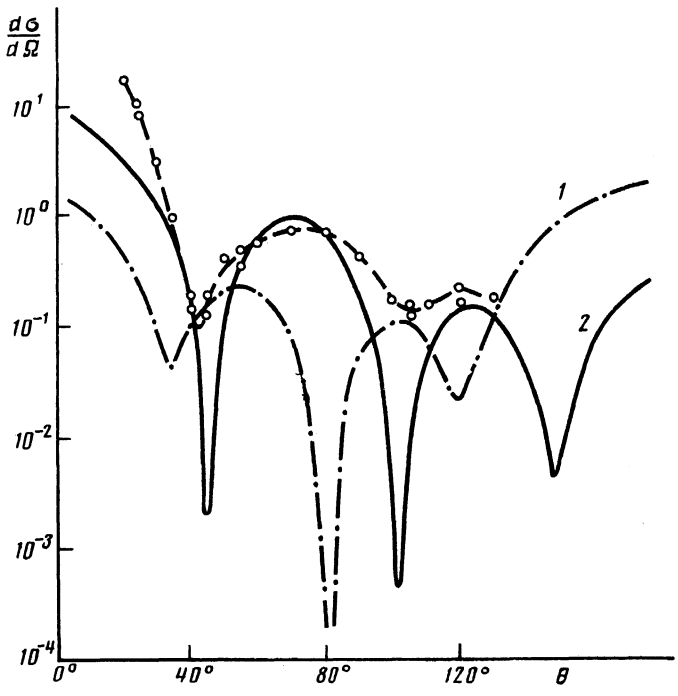

FIG. 4. Differential cross section of the elastic scattering (in units of 10^{-16} cm$^2\cdot$sr^{-1}) of electrons ($\varepsilon = 20$ eV) by atomic manganese: 1 and 2) $d\sigma^{\downarrow}/d\Omega$, calculated according to SPHF and SP-SRPAE, the points are the results of experiment[10] averaged over the spin-states of the electron–atom system.

TABLE I. Results of calculations of the phase shifts of elastic scattering by a Mn atom of the $e^{\downarrow}$ partial electron wave with energy 20 eV (in radians) in SPHF and SP-SRPAE.

l	ΔL	$\Delta\xi_l$					$\sum\Delta\xi_l$	$\xi^{\downarrow}_l$	${}^0\xi^{\downarrow}_l$
		$4s\uparrow$	$4s\downarrow$	$3d^5\uparrow$	$3p^3\downarrow$	$3p^3\uparrow$			
0	0	−0.0010	0.0033	0.0227	0.0019	0.0006			
	1	0.1626	0.0994	0.0658	0.0362	0.0006	0.4102	9.3878	8.9776
	2	0.0037	0.0014	0.0152	−0.0022	0			
1	0	−0.0016	0.0123	0.0198	0.0009	0.0001			
	1	−0.0409	−0.0060	−0.1140	0.0277	0.0031	−0.0573	6.4677	6.5250
	2	0.0190	0.0079	0.0098	0.0026	0			
2	0	0.0198	0.0338	0.4932	0.0411	0.0342			
	1	0.0105	0.0637	−0.0161	0.0096	0.0020	0.7223	3.6599	2.9376
	2	0.0131	0.0047	0.0121	0.0006	0			
3	0	0.0089	0.0080	0.0015	0.0001	0			
	1	0.0680	0.0846	0.0388	0.0080	0.0008	0.2458	0.5541	0.3091
	2	0.0082	0.0110	0.0072	0.0007	0			
4	0	0.0045	0.0023	0.0001	0	0			
	1	−0.0185	0.0129	−0.0590	0.0049	0	−0.0449	0.0698	0.1147
	2	−0.0052	0.0100	0.0029	0.0002	0			

Note: ${}^0\xi^{\downarrow}_l$ are the values of the scattering phase in SPHF; ξ_l are the SP-SRPAE corrections to ${}^0\xi^{\downarrow}_l$ due to the polarization of the corresponding atomic subshell ($3s\uparrow(\downarrow)$, $3p^3\uparrow(\downarrow)$, or $3d^5\uparrow$); $\Sigma\Delta\xi_l$ are the resulting SP-SRPAE corrections to the one-electron values of the scattering phases; $\xi^{\downarrow}_l$ are the values of the scattering phases in SP-SRPAE; l is the orbital angular momentum of the partial incident electron wave; ΔL is the multipolarity of the excitation of the atomic subshell.

reaction of the atom to the perturbation induced by the incident electron significantly raises the curve for $d\sigma^{\uparrow}/d\Omega$ and causes the osscillations to grow and shift along the θ axis, as was to be expected. It is interesting to note that, as a consequence, the positions of the first (strong) and second (weak) maxima in $d\sigma^{\uparrow}/d\Omega$ curve begin to coincide with the same for the spin-averaged experimental curve $\langle d\sigma/d\Omega\rangle$.

From a fundamental point of view the results obtained here serve as a support for the ideas developed here on the process of $e^- + A$ scattering. They are also of independent interest since the properties of electron scattering by high-spin, strongly polarized atoms have hardly been studied.

5. RESULTS OF CALCULATION OF e^- +N SCATTERING IN SP-SRPAE

For the case of $e^- + \mathrm{N}$ scattering, calculations of the scattering phases $\xi_l(\varepsilon)$ of the electrons in the range $\varepsilon = 0$–10 eV have been carried out using the "standard" method—the polarized orbital method (POM),[13] which takes into account the polarization of the atom by the incident electrons and the dependence of the scattering phases on the spin state of the electron–atom system. Therefore, to further verify and demonstrate the possibilities of SP-SRPAE, we have carried out the corresponding calculations of the phases $\xi_l^{\uparrow(\downarrow)}(\varepsilon)$ and partial cross sections $\sigma_l^{\uparrow(\downarrow)}(\varepsilon)$ of elastic scattering of $e^{\uparrow}$ and $e^{\downarrow}$ electrons by atomic nitrogen in the given energy region, which are compared in Figs. 5–7 with the results obtained within the POM framework.[13] We forego here a detailed discussion of the influence on $e^- + \mathrm{N}$ scattering of the coupling of the incident electrons with all the concrete channels of excitation of the atomic electrons. We note only that, as the calculations have shown, in the given case the coupling of the scattered electrons with the dipole excitations of the electrons of the $2p^3\uparrow$ and $2s\downarrow$ subshells of the atom absolutely dominates, and to a lesser extent that with the electrons of the $2s\uparrow$ subshell, whereas the contribution from the excitations of the electrons of the other subshells and of other multipolarity turns out to be negligibly small. Let us consider the results obtained.

Figure 5 presents the results of SPHF and SP-SRPAE calculations of the partial scattering cross sections of the $\varepsilon s\uparrow$ and $\varepsilon p\uparrow$ electron waves along with the results of the corresponding calculations using the polarized orbital method (POM) for the scattering channel with total spin of the $e^- + \mathrm{N}$ system $S = 2$. It can be seen that the effect of the dynamic reaction of the atom to the scattering process is quite substantial. This is especially characteristic of the $\varepsilon s\uparrow$ wave, where it qualitatively changes the behavior of the scattering cross section in comparison with the results of SPHF calculations in the region of small ε. Most importantly, the results of the SP-SRPAE and the POM calculations are found to be in good agreement with each other, which argues strongly in favor of the ideas on $e^- + A$ scattering developed in this paper and particularly in favor of SP-SRPAE.

Figure 6 displays values of the scattering phase and cross section of the $\varepsilon s\uparrow$ electron wave, calculated using SPHF and SP-SRPAE, as functions of ε and compares them with the corresponding results of the POM calculations for the scattering channel with total spin of the electron–atom system $S = 1$. From the comparison of the scattering phases $\xi_0^{S=1}(k)$ and $\xi_0^{\downarrow}(k)$, calculated respectively using POM and SP-SRPAE, it can be seen that in the region of incident

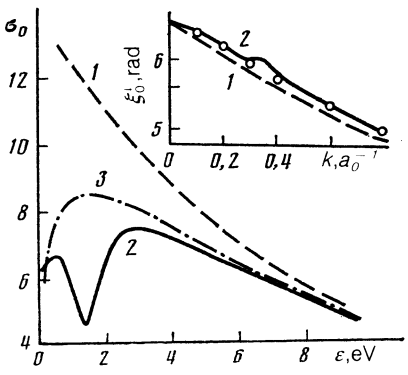

FIG. 6. Partial cross section of the elastic scattering $\sigma_0^{\downarrow}(\varepsilon)$ (in units of $10^{-16}\,\mathrm{cm}^2$) of $e^{\downarrow}$ electrons by atomic nitrogen: 1 and 2) results of calculations in SPHF and SP-SRPAE, respectively; 3) results of calculations within the POM framework, corresponding to the scattering channel with total spin of the electron–atom system $S = 1$ (Ref. 13). The insert shows the elastic scattering phase $\xi_0^{\downarrow}(k)$, calculated in SPHF (1) and SP-SRPAE (2); the points are the results of an POM calculation, k is the momentum of the incident electron.

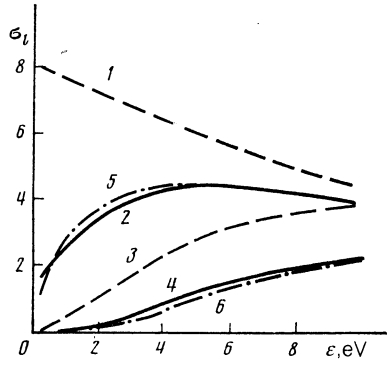

FIG. 5. Partial cross sections of the elastic scattering $\sigma_l^{\downarrow}(\varepsilon)$ (in units of $10^{-16}\,\mathrm{cm}^2$) of $e^{\downarrow}$ electrons by atomic nitrogen: 1 and 3) results of calculations of $\sigma_0^{\downarrow}(\varepsilon)$ and $\sigma_1^{\downarrow}(\varepsilon)$ in SPHF; 2 and 4) the corresponding results for SP-SRPAE; 5 and 6) the results of calculations of $\sigma_0^{S=2}(\varepsilon)$ and $\sigma_1^{S=2}(\varepsilon)$ within the POM framework, corresponding to the scattering channel with total spin of the electron–atom system $S = 2$ (Ref. 13).

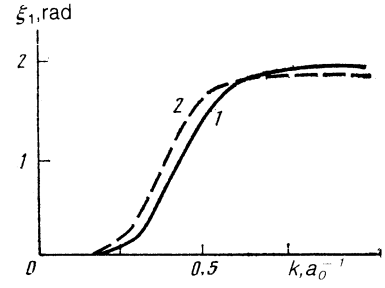

FIG. 7. Scattering phase $\xi_1^{\downarrow}(k)$ of the $\varepsilon p\downarrow$ electron wave as a function of the momentum of the scattered electron k: 1) results of calculation in SPHF, 2) results of calculation in the one-electron exchange approximation, corresponding to the scattering channel with total spin of the electron–atom system $S = 1$ (Ref. 13). In both calculations account is taken of only one ^4S term of the ground state of the atom.

electron momenta $k = (0.3\text{–}0.4)a_0^{-1}$ ($\varepsilon = 1.2\text{–}2.2$ eV) a small maximum is observed in $\xi_0^{\downarrow}(k)$ in contrast with $\xi_0^{S=1}(k)$, for which no such maximum is observed. This, in turn, leads to the appearance of a minimum in the scattering cross section of the $\varepsilon s\downarrow$ wave in the given energy region, in contrast with the results of the POM calculations.

On the subject of the discrepancies discovered here, it should be noted that in POM the dipole polarizability of the target atom and the resulting long-range potential are calculated rather accurately, in contrast with the short-range part of the potential, in the calculation of which certain arbitrary assumptions were implemented.[14] In addition, POM rests on the hypothesis of adiabaticity, according to which the energy of the incident electron does not vary in the process of deforming the electron subshells, even in the virtual states. The SP-SRPAE method is free of these shortcomings and limitations and, via the proper energy part of the Green's function of the scattered electron, in its basic form takes account of the atomic dynamic effects much more accurately than POM. This allows us to give preference to the results of the SP-SRPAE calculations of the $\varepsilon s\downarrow$ scattering cross section and to confirm to presence in it of a minimum in the region of incident electron energies 0.5–3 eV. Over the remainder of the energy region ε one can properly speak of agreement between the results of the POM and SP-SRPAE calculations, which gives additional support to the formalism developed in this paper to describe the scattering of electrons by atoms with half-filled subshells.

The question of the scattering of the $\varepsilon p\downarrow$ electron wave (the scattering channel with total spin of the $e^- + \mathrm{N}$ system $S = 1$) reauires separate discussion. A lively discussion has already been devoted to this question.[13,15–17] The calculations have been carried out in various approximations using various standard methods: in the one-electron exchange approximation[13] and taking polarization effects into account in POM,[13] and using the close-coupling method,[15] the R-matrix method,[16] and the matrix variational method.[17] It has been found that in the scattering cross section of this wave there is a low-energy narrow shape resonance with width $\Gamma = 0.013$ eV and position of the intensity peak in the incident electron energy $\varepsilon = 0.062$ eV.[16] It is found that an accurate calculation of the resonance parameters is a nontrivial problem which requires for its solution a very specific account of the dynamic reaction of the atom to the external perturbation along with an account of the coupling of the incident $\varepsilon p\downarrow$ wave with all the degenerate ^4S, ^2D, and ^2p terms of the ground-state $1s^2 2s^2 2p^3$ electronic configuration of the atom.[16,17]

Such a thorough investigation of this particular problem is not the goal of the present paper. It is rather aimed at a fundamental demonstration of the validity of the formalism developed here in its fundamentals. For this reason we have restricted the discussion to the one-electron calculation of $\varepsilon p\downarrow$ scattering using SPHF, and we will demonstrate here that it allows one to reproduce the main feature in $e^- + \mathrm{N}$ scattering—the presence of a shape resonance in the scattering cross section of the $\varepsilon p\downarrow$ wave. The results of the SPHF calculation of the scattering phase $\xi_1^{\downarrow}(k)$ of this wave as a function of k are shown in Fig. 7. It can be seen that as $k \to 0$ the scattering phase also tends to zero, passing on its way there through the value $\xi_1^{\downarrow}(k) = 1/2\pi$. Consequently, there is a shape resonance in the scattering cross section of the $\varepsilon p\downarrow$ wave, which is what we set out to show. The presence of this resonance in the scattering of the $\varepsilon p\downarrow$ wave and its absence in the scattering of the $\varepsilon p\downarrow$ wave are obvious from the point of view of the formalism developed here. Indeed, we note that the half-filled $2p^3_{\uparrow}$ subshell in the N atom is filled only with $e^{\uparrow}$ electrons and that this atom does not have a stable negative ion.[12] Therefore in the field of the neutral atom there are not—and cannot be—any coupled $np\downarrow$ states, and for this reason, according to Levinson's theorem,[18] the scattering phase satisfies $\xi_1^{\downarrow}(k) \to 0$ as $k \to 0$, in contrast with the scattering of the $\varepsilon p\uparrow$ wave, since according to this same theorem, we have $\xi_1^{\uparrow}(k) \to \pi$ as $k \to 0$. As a consequence, the scattering of the $\varepsilon p\uparrow$ and $\varepsilon p\downarrow$ waves in the small k region turns out to be substantially different and in the latter case in particular a shape resonance is formed.

Figure 7 compares the results of the SPHF calculation also with the corresponding results of the calculation of the scattering phase of the $\varepsilon p\downarrow$ wave in the standard one-electron exchange approximation.[13] The results of both calculations are in fair agreement with one another. This provides a basis for asserting that in scattering problems the SPHF method takes at least equal account of the same features of the effective one-electron potential in the system consisting of incident electron + atom with half-filled subshells as do the standard one-electron methods.

6. CONCLUSION

On the basis of the results presented here of the calculations of elastic $e^- + \mathrm{Mn}$ and $e^- + \mathrm{N}$ scattering we have shown that the method for calculating the characteristics of electron scattering by atoms with half-filled subshells developed in the present paper and based on SPHF concepts allows one to obtain results in agreement with experiment and with the results of calculations by the standard methods. Consequently, this method can be seen as an alternative method in the theory of $e^- + A$ scattering that makes it possible by taking proper account only of the exchange interaction in the $e^- + A$ system to distinguish and to describe the characteristics of electron scattering by atoms with half-filled subshells as a function of the spin state of the electron–atom system. From this point of view it is simpler than the standard methods used for such purposes and makes it possible when constructing the scattering equations to avoid the use of procedures that require the construction of the exact wave functions of the squared total spin operator of the $e^- + A$ system without at the same time decreasing the accuracy of the calculation of the characteristics of the electron scattering. In addition, it provides a framework in which the differences and peculiarities in the scattering by an atom of electrons with opposite spin orientation becomes physically transparent, as was demonstrated by the example of the interpretation of the shape resonance in the scattering of the $\varepsilon p\downarrow$ electron wave by atomic nitrogen. Finally, the advantage of the concept of the $e^{\uparrow}$–$e^{\downarrow}$ formalism in electron scattering proposed in the present paper consists in the fact that it makes it possible in a natural and relatively simple way to use the reliable apparatus of quantum many-body theory to obtain an accurate account of multi-electron effects in the scattering of electrons by atoms with half-filled levels, which other methods achieve in a more complicated way. As a result, within the framework of the developed method we have discovered the presence of a minimum in the partial scatter-

ing cross section of the $\varepsilon s\downarrow$ electron wave of the nitrogen atom. The results presented here give reason to hope that the formalism developed here will find successful application in the description and calculation of the characteristics of electron scattering by atoms with half-filled subshells.

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