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Spin exchange between ion probes and localized moments in ferromagnets as the origin of transient fields

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The transient field phenomenon has been ascribed to a polarization transfer between the electrons of the ionic projectiles and the surplus of majority spin electrons of the ferromagnetic host over the minority spin electrons. Earlier attempts to explain this crucial process failed to account for the order of magnitude of the experimentally observed transient field strengths. A recent model which proposes spin exchange scattering between bound projectile electrons and quasifree host electrons as the mechanism of polarization transfer arrives at the correct orders of magnitude but is in conflict with the weak velocity dependence of the experimental polarization, exhibiting a strongly decreasing behavior with increasing velocity. The new model presented here proposes spin exchange between the ionic shell and localized electrons of the ferromagnet as a more adequate approach to the problem. It is shown that calculations involving hydrogenlike ions explain the size of the experimentally observed polarization effects as well as their velocity dependence for various ion probes traversing thin iron foils.

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I. INTRODUCTION

Transient magnetic fields (TF) are observed at the nuclei of swift ions traversing ferromagnetic media [1,2]. Due to their extraordinary size in the 10 MG range the TF have made possible the experimental investigation of nuclear magnetic moments of extremely short-lived nuclei with lifetimes in the subpicosecond region [3–7]. Thus, using the TF, magnetic properties of high spin states have been explored [8] in nuclear spin precession measurements. The recent interest in magnetic moments in superdeformed bands, for instance of the isotope ^{194}Hg, has again focused the attention of nuclear spectroscopists strongly on the TF phenomenon [9]. Since no successful quantitative description of the TF from first principles has been given so far, g-factor measurements still depend on TF calibrations which are often hard to perform and also decrease the precision of the measured value of the g factor. Reliable predictions of the TF strength based on a theoretical explanation of the TF phenomenon could improve considerably the quality of nuclear moment studies which employ the TF method. Moreover, an analytic understanding of the TF would allow optimization of the experimental conditions in order to obtain a maximum TF strength corresponding to strongest nuclear spin precession effects.

Experimental measurements have been carried out in both heavy ions with a number of core states and complex valence configurations as well as highly charged ions in lithiumlike and hydrogenlike states. In the present work we concentrate on the hydrogenlike ions which makes the atomic physics associated with the problem simpler and thus allows one to attempt first-principle quantitative understanding of the important features involving the valence electrons which play a crucial role in the origin of the TF.

In the pioneering work on TF theory [10], the field was assumed to arise from the scattering of quasifree spin polarized electrons of the ferromagnet by the ion probe. The resulting polarization density enhancement at the ionic core was proposed to account for the high field strengths experimentally observed. While this work focused on the important role of the polarized electrons of the host for the first time, it led to an underestimation of the magnitudes of the TF.

The first experiments with hydrogenlike probe ions have clearly demonstrated [3], that the TF is produced by unpaired s electrons of the ion which are polarized by the interaction with the surplus number of majority electrons in the ferromagnet. Thus, the crucial problem in the understanding of the TF phenomenon consists in the explanation of the polarization transfer mechanism involved. As will be outlined in Sec. II, the use of ion probes in a hydrogenlike state allows for the determination of the degree of polarization acquired by the K-shell electrons of the projectiles as they pass through the ferromagnetic host. These experiments give the key to any theoretical treatment of the origin of the TF since a quantitative first-principles theory has to explain both the magnitude as well as trends of the ionic polarization with respect to the velocities and atomic numbers of the ion probes as well as the characteristics of the host material.

As a conceivable mechanism for the crucial polarization transfer process, the capture of polarized electrons of the ferromagnet into the inner s orbitals of the probe ion has been suggested [11]. This model, however, can readily be ruled out from energy matching considerations. Since the binding energies of 1s electrons in experimentally observed projectiles are much lower than those of the majority electrons of the ferromagnet, capture will mainly proceed from closed shells of the host atom. These are known to be polarized only to a very small degree [12], and thus cannot account for the sizable polarization effects measured.

A second model based on the finding that the TF is produced by unpaired electrons of the projectile ion considers polarization transfer by elastic spin-exchange scattering [13]. This process transfers preferentially the spin orientation of the majority electrons of the ferromagnet into the inner shells of the ion and therefore gives rise to spin polarization of these shells. Any closer examination of the effectiveness of this mechanism has to be based on numerical values of the spin exchange cross section σ^{sf}. This quantity has been evaluated before [13] following the formalism developed by Temkin and Lamkin [14] for the scattering of a free electron by a hydrogenlike target. The 1*s* polarizations deduced from this approach are found to be generally smaller than the experimental results by at least one order of magnitude. This calculation, however, neglects any cooperative phenomenon, especially the nonlinear response of the electron gas due to the high charge of the moving ion [15] which leads to host electron density enhancement near the ion core. Incorporation of this focusing effect does increase the degree of polarization to bring it to better agreement with the experimentally observed magnitudes [13]. However, some characteristic trends of the observed probe ion polarization cannot be explained in the framework of this model. Thus, the experimental finding is that the degree of 1*s* polarization stays constant over a sizable ion velocity range [16], while the theory outlined in Ref. [13] leads to the expectation of a strongly decreasing polarization as the ion velocity increases. The two processes which determine the effectiveness of polarization transfer according to the model discussed in Ref. [13], spin exchange between ion and target electron as well as host electron density enhancement at the ionic core, are both very markedly attenuated with increasing velocity.

To avoid these contradictions with experiment, one has to reinvestigate the spin-exchange approach. In the first place, the unrealistic assumption of a free electron representing the contribution of the host to the scattering process has to be replaced by a more appropriate description of the polarized electron states in the ferromagnet. As is well known, these states are localized to a very high degree, if not fully [17], in all ferromagnetic metals which have been used so far in TF experiments, these are Fe, Co, Ni, and Gd. It is thus necessary for theory to take the localized nature of these electrons properly into account.

The present work concentrates on the TF produced by the passage of light ions ranging from carbon ($Z=6$) to sulphur ($Z=16$) through Fe foils. The purpose of the research reported here is to demonstrate that the magnitude of the observed polarization effects is readily explained by elastic spin exchange scattering between bound projectile electrons and the localized electrons of the ferromagnet. The model introduced here is also shown to be in much better agreement with experimental trends than is the case for any of the foregoing theoretical attempts. In view of the very complex systems involved in the experiment, we have considered the situation in which the polarization transfer proceeds between a hydrogenlike ion probe and a Fe target atom whose 3*d* core is assumed to simulate the tightly bound 3*d* band electrons [12,17] in the ferromagnet. In Sec. II, we comment on the experimental observations related to our theory. A survey of available data for hydrogenlike ion probes in various ferromagnets is given. In Sec. III, our procedure is introduced. In Sec. IV, we compare experimental and theoretical findings. Section V adds some concluding remarks.

II. EXPERIMENTAL STUDY OF POLARIZATION TRANSFER TO HYDROGENLIKE IONS

The experimental determination of the degree of ion polarization is based on a microscopic description of the TF [18]:

$$B_{\mathrm{TF}}(v,Z,\mathrm{host})=\sum_{n} q_{ns}(v,Z,\mathrm{host})p_{ns}(v,Z,\mathrm{host})B_{ns}(Z) \ . \tag{1}$$

In this formula, $B_{ns}(Z)$ refers to the Fermi contact field produced by an unpaired electron in an *ns* orbital at the nuclear site of the ion. The "single electron factor" q_{ns} indicates the fraction of ions with half-filled *ns* orbital and p_{ns} their degree of polarization. Both quantities depend on the elementary parameters of the experiment, i.e., the ion's atomic number Z, its velocity v as well as on properties of the ferromagnetic host.

The expression (1) simplifies considerably when the TF is associated with H-like ions. In this case, the sum over all *ns* orbitals is reduced to the contribution from the K shell:

$$B_{\mathrm{TF}}(v,Z,\mathrm{host})=q_{1s}(v,Z,\mathrm{host})p_{1s}(v,Z,\mathrm{host})B_{1s}(Z) \ . \tag{2}$$

The Fermi contact field $B_{1s}(Z)$ can be evaluated analytically [19,20], and the single electron factor q_{1s} is known from measurements for a wide range of different ion sorts and ion velocities in Fe and Gd [21,22]. Thus, using Eq. (2), it is possible to extract the degree of polarization p_{1s} from the measured TF strength B_{TF}, the latter quantity being experimentally determined by observation of the nuclear spin precession angles of the probe ions as they traverse thin ferromagnetic layers [3,4]. The precession angle is measured using the technique of perturbed angular particle-gamma correlations [23]. Equation (2) is strictly valid only at high enough ion velocities $v \geq Zv_0$ (the "1*s* Bohr velocity"). In this velocity regime, the projectiles traverse the solid essentially in a hydrogenlike state or as bare nuclei which do not contribute to the field strength. The microscopic description of the TF given by formula (2) can still be applied in a situation of smaller ion velocities, corresponding to more complex electron configurations of the projectile, provided the single electron factors q_{ns} of higher ns orbitals are small as compared to q_{1s}. In this case, the contribution of the K shell to the TF strongly dominates the contributions of higher shells, as is evident from the marked decrease of the Fermi contact field B_{ns} with effective principal quantum number n_{eff} [19]:

$$B_{ns} = 16.7Z(Z - b_n)^2/n_{\text{eff}}^2 \ . \tag{3}$$

Here, b_n is a screening charge equal to the number of bound electrons with principal quantum number smaller than n. The formula (3) applies to B_{ns} quoted in the unit of tesla.

Figure 1 summarizes the results of a series of experiments where highly charged hydrogenlike ions ($6 \leq Z \leq 16$) were observed in Fe and Gd host. The ion probe K-shell polarization as obtained from Eq. (2) is shown versus the atomic number of the ion. From this systematic experimental study, three features emerge that any theoretical treatment of the polarization transfer problem would have to explain. (1) In both metals, high degrees of 1s polarization in the range of 10–30% are found. (2) There appears to be no significant difference between polarization data taken at $v \cong Zv_0$ and at $v \cong Zv_0/2$. (3) In both cases, the degree of 1s polarization seems to drop with increasing atomic number of the ion probe. This effect, however, is more pronounced in Gd than in Fe where a weakly decreasing tendency of the polarization with atomic number is accompanied by a marked oscillating behavior.

The apparent velocity independence of the polarization data poses a special challenge to theoretical explanation. Intuitively, one expects a decrease of polarization transfer efficiency as the ion velocity rises and, consequently, the ion-atom interaction time drops. In the following section, we give an interpretation of the data obtained for Fe host in the framework of a model which considers spin exchange scattering by localized moments of the host atoms as the critical polarization transfer mechanism.

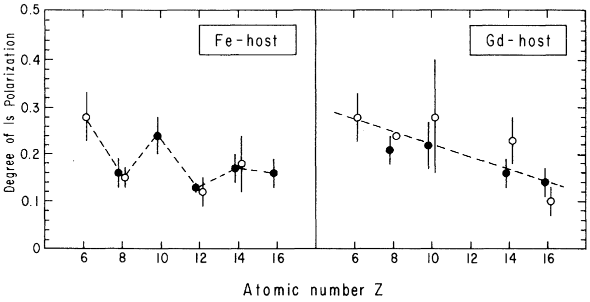

FIG. 1. Experimental degrees of 1s polarization for various ion probes traversing Fe and Gd hosts [16]. Open circles refer to high velocity data ($v \cong Zv_0$), closed circles to intermediate velocity data [$v \cong (Z/2)v_0$].

III. SPIN-EXCHANGE SCATTERING BETWEEN 1S IONS AND LOCALIZED MOMENTS IN FE

In this section, we first derive a general expression for the degree of 1s polarization of an ion ensemble which is predominantly in a hydrogenlike state. In a second step the spin exchange interaction between a 1s electron of a moving ion and a 3d electron of a target atom is described in detail.

A. Transfer of polarization to an ensemble of hydrogenlike ions: General formalism

As a hydrogenlike ion ensemble traverses a ferromagnetic medium, it acquires polarization via spin-exchange scattering between the electron bound by the ion nucleus and polarized host electrons. With the elapse of time, the ion population $P_1^{\downarrow}$ with the majority-spin orientation (electron spin "down") will increase over the ion population $P_1^{\uparrow}$ with minority-spin orientation (electron spin "up"). The surplus of majority over minority population, normalized to the overall fraction of hydrogenlike ions in the ensemble, yields the degree of polarization of the 1s electron on the hydrogenlike ion:

$$p_{1s}(t) = \frac{P_1^{\downarrow}(t) - P_1^{\uparrow}(t)}{P_1^{\downarrow}(t) + P_1^{\uparrow}(t)} \ . \tag{4}$$

The time-dependent behavior of the quantities $P_1^{\downarrow,\uparrow}$ and thus the degree of 1s polarization is governed by the interplay of two competing processes. The first refers to the production of polarization in the 1s orbitals of the ions by spin exchange. The second refers to spin quenching which arises from both loss of polarized electrons from the K shells of the ions and filling up the partially empty K shells by electron capture from host atoms. Obviously, the spin polarization of the ion is destroyed in both cases. After a time determined by the effectiveness of all mechanisms involved, the two opposing interactions will have balanced out and a constant equilibrium degree of 1s polarization will be reached.

The situation can be analyzed in a four state model where the ion ensemble is subdivided into the ion populations P_0, the fraction of ions with empty K shells (bare nuclei); P_2, the fraction of ions with completely filled K shells, and the hydrogenlike populations $P_1^{\downarrow,\uparrow}$ introduced above. The time evolution of the system is described by four coupled rate equations which can be expressed in compact matrix form:

$$\dot{\mathbf{P}}(\mathbf{t}) = \mathbf{M}\mathbf{P}(\mathbf{t}) \ , \tag{5}$$

where the vector $\mathbf{P} = (P_0, P_1^{\downarrow}, P_1^{\uparrow}, P_2)$ is introduced along with the 4×4 matrix $\mathbf{M}$:

$$\mathbf{M}=n_h v \begin{bmatrix} -\sigma^{\text{cap}} & \sigma^{\text{loss}} & \sigma^{\text{loss}} & 0 \\ \sigma^{\text{cap}} & -(n^{\uparrow}\sigma^{sf}+\sigma^{q}) & n^{\downarrow}\sigma^{sf} & \sigma^{\text{loss}} \\ \sigma^{\text{cap}} & n^{\uparrow}\sigma^{sf} & -(n^{\downarrow}\sigma^{sf}+\sigma^{q}) & \sigma^{\text{loss}} \\ 0 & \sigma^{\text{cap}} & \sigma^{\text{cap}} & -\sigma^{\text{loss}} \end{bmatrix} . \tag{6}$$

Here, σ^{cap} (σ^{loss}) are the electron-capture (electron-loss) cross sections of the K shells of the ion projectiles, σ^{sf} is the spin-exchange cross section.

The total spin quenching cross section σ^{q} is linked to σ^{cap} and σ^{loss} by

$$\sigma^{q}=\sigma^{\text{cap}}+\sigma^{\text{loss}} .$$

The quantity $n^{\downarrow}$ ($n^{\uparrow}$) denotes the number of majority (minority) electrons per host atom while n_h refers to the number of host atoms per cm^3. In Eq. (6), the assumption is made that the likelihood of double events like the simultaneous capture or loss of two electrons is negligibly small. By definition of the population vector **P**, the constraint

$$P_0+P_1^{\downarrow}+P_1^{\uparrow}+P_2=1 \tag{7}$$

holds for its components.

The ion ensemble described by the rate equation (5) tends towards both charge and spin equilibrium. The time scales characteristic for charge and spin exchange, however, are quite different. Whereas the ensemble acquires a stable average charge state in a time $T_q \leq 1$ fs, spin equilibrium is reached in a time $T_{sf} \leq 10$ fs [24]. Both times are small as compared to the effective interaction time between probe ions and ferromagnet [25]. In view of the relation $T_q \ll T_{sf}$, one might assume that charge equilibrium is reached instantaneously, so that the populations P_0 and P_2 can be treated as constants. It then follows, from (7)

$$\frac{dP_1^{\downarrow}}{dt}=-\frac{dP_1^{\uparrow}}{dt} . \tag{8}$$

In spin equilibrium conditions, the time derivatives of the components $P_1^{\downarrow,\uparrow}$ have to vanish. One then finds from (4) and (5) the following expression for the equilibrium degree of 1s polarization p_{1s}:

$$p_{1s}=\frac{n^{\downarrow}-n^{\uparrow}}{n^{\downarrow}+n^{\uparrow}}\left[1-\frac{1}{1+(n^{\downarrow}+n^{\uparrow})\sigma^{sf}/\sigma^{q}}\right] . \tag{9}$$

The numerical evaluation of this formula requires the knowledge of all contributing microscopic quantities: $n^{\downarrow}$, $n^{\uparrow}$, σ^{q}, and σ^{sf}.

The results which will be discussed in Sec. IV were obtained adopting for $n^{\downarrow,\uparrow}$ the average numbers of unpaired electron spins with down and up polarization, respectively, per Fe atom: $n^{\downarrow}=2.6$ and $n^{\downarrow}=0.4$, corresponding to the effective magnetization of $2.2\mu_B$ per atom [25]. These values refer to an undisturbed situation while the highly charged ion projectiles are likely to induce some ionization of a host target atom thus enhancing the total number of unpaired electron spins per atom, $n^{\downarrow}+n^{\uparrow}$. This quantity, however, has only a very slight influence on the equilibrium degree of 1s polarization as given by formula (9).

The spin quenching cross section of σ^{q} has been experimentally observed for the systems O in Fe [21] and for Si in Fe [22] at velocities close to $v=Zv_0$. In the remaining cases of C, Ne, Mg, and Si in Fe, where no experimental cross sections are available so far, a scaling procedure based on Oppenheimer-Brinkmann-Kramers and binary encounter approximations [13] has been employed to obtain realistic estimates of the capture and loss cross sections involved.

The spin exchange cross section σ^{sf} has been derived theoretically in the present work. In the remainder of this section, we want to give an account of the basic approach adopted in the evaluation of this quantity as well as computational details.

B. Spin exchange between ion probe and host atom: Microscopic description

Our treatment of the spin exchange process between the 1s projectile electron and a 3d electron of an Fe host atom follows the lines of the impact parameter approach [25]. In view of the high velocities involved, the probe ion can be assumed to move in a straight path with a well-defined impact parameter p and ion velocity v. Figure 2 indicates the scattering geometry adopted. Because

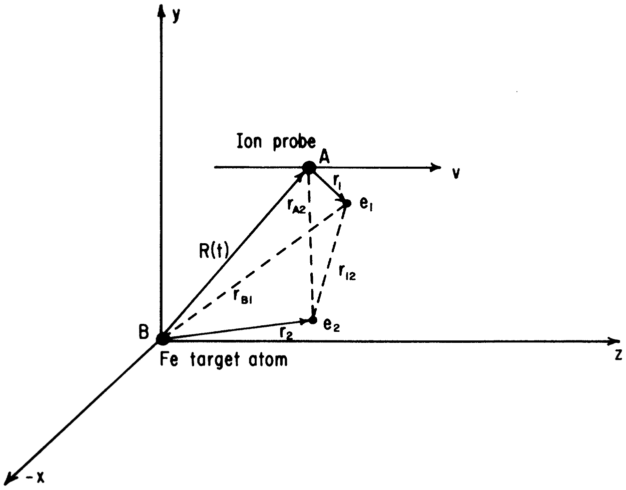

FIG. 2. Geometry of the two-center interaction between a hydrogenlike ion probe ("center A") and an Fe target atom ("center B"). The 1s electron of the ion probe and a 3d electron are indicated by e_1 and e_2, respectively.

of the dynamic character of the problem, involving high projectile charges and small interaction times, a molecular approach which allows for a rearrangement of the electron distributions over the host and the ion, whether employing the Hartree-Fock approach, or the local density approximation to it, is not suitable for an adequate description of the physical picture involved.

Instead, in the approach summarized below, one uses a spin-exchange process between the electrons of the host and the ion, employing a localized atomic 3*d* electron state to simulate the polarized state of the ferromagnetic host. The elementary exchange process is described as a two-center interaction of two electrons, one being attached to the probe ion and the other to a host atom core. The influence of the remaining host atom valence electrons on the 3*d* electron during the scattering process is neglected in the present context. With these simplifying constraints, the problem becomes tractable without demanding prohibitive computational efforts. This approach is used here to examine the potential of our model for a quantitative explanation of the TF phenomenon.

The system investigated consists of a 1*s* electron bound to a bare probe ion nucleus with charge Z as well as a 3*d* electron attached to an Fe atom core with effective charge $Z_{\mathrm{Fe}}^{\mathrm{eff}}$. The time evolution of this system is governed by the time-dependent Schrödinger equation:

$$\left[H_{\mathrm{el}} - i\frac{\partial}{\partial t} \right] \Psi_T(\mathbf{r}_1,\mathbf{r}_2,\mathbf{R},t) = 0 \ , \tag{10}$$

where the trial function Ψ_T depends on electron coordinates $\mathbf{r}_1$ and $\mathbf{r}_2$, while $\mathbf{R}$ is the vector of internuclear separation. The electronic Hamiltonian H_{el} is given by

$$H_{\mathrm{el}} = H_1 + H_2 + H_{\mathrm{int}} \ . \tag{11}$$

The operator H_1 represents the Hamiltonian of an electron of a free hydrogenlike ion (in atomic units):

$$H_1 = -\tfrac{1}{2}\nabla_1^2 - Z/r_1 \ . \tag{12}$$

H_2 describes the Hamiltonian of a 3*d* electron of the Fe atom:

$$H_2 = -\tfrac{1}{2}\nabla_2^2 - Z_{\mathrm{Fe}}^{\mathrm{eff}}/r_2 \ . \tag{13}$$

In this expression, the screening effect of all remaining electrons of the Fe shell is taken into account by the effective charge $Z_{\mathrm{Fe}}^{\mathrm{eff}}$. A value of $Z_{\mathrm{Fe}}^{\mathrm{eff}} = 6.25$ was adopted in accordance with the screening rules given by Slater [27].

The Hamiltonian H_{int} which describes the Coulomb interaction between target atom and probe ion is given by

$$H_{\mathrm{int}} = -\frac{Z}{r_{A2}} - \frac{Z_{\mathrm{Fe}}^{\mathrm{eff}}}{r_{B1}} + \frac{1}{r_{12}} + \frac{Z Z_{\mathrm{Fe}}^{\mathrm{eff}}}{R} \ . \tag{14}$$

The potentials Z/r_{A2} and $Z_{\mathrm{eff}}^{\mathrm{Fe}}/r_{B1}$ refer to the Coulomb attraction of the 3*d* target electron by the screened projectile ("center *A*") and of the 1*s* projectile electron by the core of the Fe atom ("center *B*"). As illustrated in Fig. 2, r_{A2} is the distance between the ion nucleus and the 3*d* electron attached to the Fe core, r_{B1} is defined correspondingly. The third term in (14) denotes the Coulomb interaction between the two electrons involved, their distance being given by r_{12}. The fourth term refers to the repulsion between the Fe core characterized by the effective charge $Z_{\mathrm{Fe}}^{\mathrm{eff}}$ and the nuclear charge of the ion Z.

As a trial function Ψ_T we choose

$$\Psi_T(\mathbf{r}_1,\mathbf{r}_2,\mathbf{R},t) = c_1(t)\Phi_{1s}^A(\mathbf{r}_1)\Phi_{3d}^B(\mathbf{r}_2) + c_2(t)\Phi_{1s}^A(\mathbf{r}_2)\Phi_{3d}^B(\mathbf{r}_1) \ . \tag{15}$$

This function is of the Heitler-London type [27], i.e., we neglect the "ionic solutions" which involve the capture of a 3*d* electron from the target atom into the 1*s* orbital of the projectile or vice versa. This choice is justified by the extremely small likelihood of the capture processes in question, the corresponding cross sections being in the order of $\sigma^{\mathrm{cap}} \cong 10^{-21}$ cm^2 and lower [28].

At large negative times, electron 1 is attached to the projectile, electron 2 to the target Fe atom. This defines the boundary conditions

$$|c_1(-\infty)|^2 = 1, \quad |c_2(-\infty)|^2 = 0 \ . \tag{16}$$

According to the outline given in Sec. III A, electron 2 which is initially bound to the Fe core has the majority spin orientation of the ferromagnet while electron 1 has the opposite spin orientation. Thus, the probability P^{sf} for the exchange process under examination is found from the second time evolution coefficient, $c_2(t)$. At some finite time t, this probability may be expressed as [26]:

$$P^{sf}(t) = |c_2(t)|^2 = \sin^2\left[\int_{-\infty}^{t} X(t')dt'\right] \tag{17}$$

with

$$X = \frac{\langle 1|H_{\mathrm{int}}|2\rangle - S^2\langle 1|H_{\mathrm{int}}|1\rangle}{1 - S^4} \ , \tag{18}$$

where

$$|1\rangle = \Phi_{1s}^A(\mathbf{r}_1)\Phi_{3d}^B(\mathbf{r}_2)$$

and

$$|2\rangle = \Phi_{1s}^A(\mathbf{r}_2)\Phi_{3d}^B(\mathbf{r}_1) \ . \tag{19}$$

It should be noted that the time dependence of the expression for X in Eq. (18) is due to the linear motion of the ion with respect to the Fe atom which is assumed to be static.

The overlap integral S^2 is given by the following expression:

$$S^2 = \int \Phi_{1s}^{A*}(\mathbf{r}_1)\Phi_{3d*}^{B}(\mathbf{r}_2)\Phi_{1s}^A(\mathbf{r}_2)\Phi_{3d}^B(\mathbf{r}_1)d\mathbf{r}_1 d\mathbf{r}_2 \ . \tag{20}$$

The exchange probability is calculated from (16) for the limiting case of large positive times:

$$P^{sf} = \sin^2\left[\int_{-\infty}^{+\infty} X(t)dt\right] \ . \tag{21}$$

The quantity X depends on both the projectile's impact parameter p and, via the relation $z = vt$, on the coordinate z of the projectile trajectory (see Fig. 2). Thus

$$P^{sf}(p,v)=\sin^2\left[\frac{1}{v}\int_{-\infty}^{+\infty}X(z)dz\right] . \qquad (22)$$

Finally, the exchange cross section σ^{sf} is obtained by an integration of $P^{sf}(p,v)$ over both the impact parameter and the azimuthal angle φ:

$$\sigma^{sf}=\int_0^{+\infty}dp\int_0^{2\pi}d\varphi\, pP^{sf}(p,v) . \qquad (23)$$

For the actual calculation of σ^{sf}, we expand the wave functions for the 1s and 3d electron states involved (assumed to be represented by Slater orbitals) in a basis of Gaussians [29]. This treatment has the advantage that all scalar products contained in (18) can be evaluated analytically. The wave functions were represented as

$$\Phi_{1s}^{A}=\sum_{j=1}^{j_{\max}}D_j\eta(\alpha_j,\mathbf{A},l_{\mathrm{A}}),\quad l_{\mathrm{A}}=0 ,$$

$$\Phi_{3d}^{B}=\sum_{j'=1}^{j'_{\max}}D_{j'}\eta(\alpha_{j'}\mathbf{B},l_{\mathrm{B}}),\quad l_{\mathrm{B}}=2 ,$$

where D_j and $D_{j'}$ denote expansion coefficients and the functions η are Gaussian primitives which depend on exponential factors α_j and $\alpha_{j'}$ as well as on particle positions **A** and **B** and on angular momenta l_{A} and l_{B} [29]. For the purpose of our work, STO-3G [29] representations ($j_{\max}=j'_{\max}=3$) which allow substantial economy in computing efforts were found to be sufficient. This computational economy is very helpful because of the integration over three variables involved in Eq. (23). The choice of STO-3G representation instead of more elaborate functions was justified by the observations that atomic orbital energies of both 3d functions of the Fe atom and 1s functions of various projectile ions could be reproduced with high precision using this type of expansion, and secondly that only small changes in the resulting cross sections were obtained when basis sets of higher complexity were employed. The latter statement is based on quantitative comparisons for the particular case of an O ion at $v=8v_0$, where bases consisting of 4, 5, and 6 Gaussians were used for the description of the two electronic states involved in the interaction.

Since there is no dependence on the magnetic quantum number m in the solid due to the quenching of angular momenta, we have averaged the exchange cross section [see Eq. (23)] over m to simulate the situation in the ferromagnet.

IV. RESULTS AND DISCUSSION

A comparison between measured and calculated degrees of 1s polarization for various ion species with $6\leq Z\leq 16$ in Fe is made in Table I. The theoretical values quoted refer to an ion velocity of $v=Zv_0$, i.e., the 1s Bohr velocity. At velocities $v\geq Zv_0$, the ion probes are predominantly in the hydrogenlike state. Since the spin-exchange formalism outlined in Sec. III is derived under the assumption of a hydrogenlike situation, it should apply best in the range of velocities equal to or greater than Zv_0. It must be noted, that a number of the experimental velocities indicated in Table I are somewhat lower than the 1s Bohr velocity, which can correspond to a more complex electron configuration of the probe ions than the hydrogenlike one. However, as already pointed out in Sec. II, no velocity dependence of polarization effects has been found empirically (see Fig. 1) in the region $(Z/2)v_0\leq v\leq Zv_0$ for ions traversing iron foils. This observation justifies a comparison between theoretical values referring to the 1s Bohr velocity and experimental data taken at velocities slightly lower than $v=Zv_0$.

A successful theory of the polarization exchange mechanism has to explain in the first place the order of magnitude of the observed polarization effects. Two other significant points of comparison between experimental and theoretical degrees of 1s polarization are their trends with ion velocity and atomic number.

Turning first to the magnitudes of calculated and measured values, one can notice in Table I that our calculations yield spin exchange cross sections in the order of $\sigma^{\mathrm{sf}}\approx 10^{-18}$ cm^2 which lead to degrees of polarization in the range of 15–30 %, i.e., the magnitude found in experiment. The observed size of polarization effects is thus well accounted for by the treatment presented here. The calculated degrees of polarization p_{1s}^{cal} are quoted with error limits, which stem from our use of measured capture and loss cross sections in the evaluation of p_{1s}^{cal}. The error limits of these latter quantities thus reflect typical uncertainties of experimental values of σ^{cap} and σ^{loss}. Within these uncertainties, there is an overlap of experimental and theoretical findings in a number of cases. For the heavier projectiles Mg, Si, and S, however, the calculation overestimates the experimental results by factors of 1.5–1.8. This feature might be ascribed to the high charges of the respective ion probes which cause excitation and ionization effects in the target atom and therefore could diminish the polarization transfer efficiency.

TABLE I. Comparison of experimental and calculated degrees of 1s polarization. The theoretical quantities are evaluated at an ion velocity $v=Z_0$.

Ion sort	$(v/v_0)^{\mathrm{exp}}$	σ^q (10^{-17} cm^2)	σ^{sf} (10^{-18} cm^2)	p_{1s}^{cal}	p_{1s}^{exp}
C	6	3.2(11)	2.51	0.14(6)	0.28(5)
O	6.9	2.8(6)	2.35	0.15(3)	0.14(2)
Ne	6.8	1.9(7)	1.79	0.17(7)	0.24(4)
Mg	8.7	0.8(3)	1.27	0.25(5)	0.12(3)
Si	10.8	0.4(1)	0.89	0.31(4)	0.18(6)
S	7.8	0.4(1)	0.62	0.24(3)	0.16(3)

A more refined model based on the approach presented in this work will have to examine the impact of these effects on the spin-exchange process.

As to the velocity dependence of the degree of 1s polarization, a direct comparison of our model with experimental data is difficult to make in the present state. The low velocity data indicated in Fig. 1 refer to velocities $v \approx (Z/2)v_0$, i.e., to a region where the model does not apply since the hydrogenlike electron configuration is not realized. The velocity dependence predicted for the region $v \approx Zv_0$ is plotted in Fig. 3 for the case of O and S ions. As can be seen from this figure, the calculated degrees of polarization pass through a minimum close to the 1s Bohr velocity. This observation is explained by the fact that for $v \leq Zv_0$, the polarization quenching cross section σ^q decreases more strongly with increasing velocity than the spin-exchange cross section σ^{sf} while, for $v \geq Zv_0$, σ^q decreases more rapidly than σ^{sf}. This velocity behavior is a particularly interesting aspect of the model discussed here since any theoretical approach proposed formerly to account for the polarization transfer implies a markedly decreasing trend with velocity, which is in contradiction to experiment. While all data obtained so far for ions traversing iron foils suggest velocity independence of the degree of 1s polarization, a rise of this quantity with velocity has been observed in Gd host (see Fig. 1). Especially, for Ne ions in Gd at $v = 12.5v_0$, measurement yielded a degree of polarization $p_{1s} = 0.32(13)$ [30] which is distinctly larger than the value $p_{1s} = 0.25(5)$ found experimentally at $v = 6.8v_0$. It would thus be interesting to test the validity of our present model by application to the computationally more complicated case of Gd as host material.

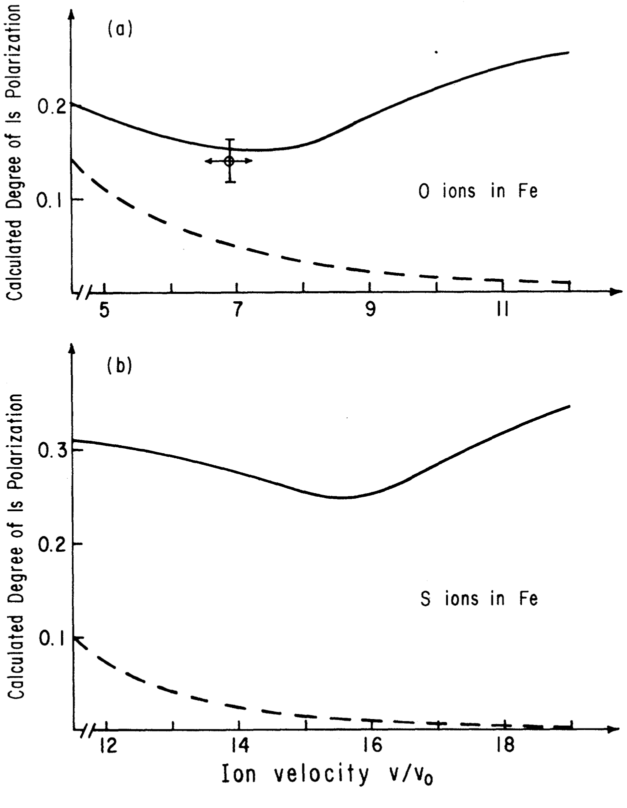

FIG. 3. Calculated degrees of 1s polarization for (a) O ions and (b) S ions both traversing Fe are shown as functions of ion velocity in the regime $v \approx Zv_0$. The solid lines display results based on the approach presented in this work. The dashed lines refer to calculations using the model introduced in Ref. [13]. An experimental degree of 1s polarization for fast O ions in Fe is also shown. The horizontal arrows indicate the velocity range of the ions in the host material.

Already, it can be said that the very moderate velocity dependence implied by the approach presented here seems to be much more compatible with the experimental observations than the strongly decreasing velocity dependence found in all foregoing models. In Fig. 3, comparison is made between calculations based on our present theory and values resulting from the approach introduced in Ref. [13], where spin exchange between bound projectile electrons and quasifree host electrons is proposed as the mechanism of polarization transfer. According to the prediction of this latter model, the 1s degree of polarization decreases monotonically as the velocity increases and attains extremely small values $p_{1s} < 0.01$ for $v > Zv_0$, as can be seen from the figure. Obviously, this behavior is not confirmed by trends and magnitudes of the experimental data.

The dependence of the theoretical degrees of polarization on the atomic number of the ion cannot be examined precisely at present since the results of our calculations presented in Table I refer to different ion velocities for the different projectile ions. This constraint is a necessity because we want to work in the region $v \geq Zv_0$ where the hydrogenlike character of the ions contributing to the TF is assured. The oscillating behavior of the experimental degrees of polarization as a function of Z (see Fig. 1) is not reflected in the theoretical findings. A more accurate statement about the Z dependence of our model, however, can only be made on the basis of a more comprehensive treatment of the polarization transfer problem. In particular, the effect of more complex projectile electron configurations than the hydrogenlike one, as well as target excitation and ionization effects caused by the impact of the high ionic charge, should be examined in detail.

V. CONCLUSION

It has been shown in this work that a model which considers spin exchange between a 1s electron and a localized electron of an Fe atom is able to predict a number of the observed polarization effects found in TF experiments. First, it yields the right order of magnitude for experimental degrees of polarization, as has been demonstrated by comparison of theoretical findings with results of measurements for various ions traversing iron foils. Secondly, the proposed theory is in agreement with the rather constant or even increasing trend of the experimental degrees of polarization with ion velocity whereas all former models lead to the expectation of a strong decrease of polarization as the velocity increases.

The marked rise in the degree of polarization calculated in the framework of our model for velocities $v > Zv_0$ makes its application on the case of Gd as ferromagnetic host particularly interesting, since polarizations observed in this medium exhibit a rising behavior for ions at velocities close to or higher than the 1*s* Bohr velocity. Thus, a calculation similar to the one reported here would be useful in making direct comparison with available experimental data in the velocity regime where the present theory is expected to be most valid. Correspondingly, it would be helpful to have experimental data in the future for ions traversing ferromagnetic iron foils for velocities $v > Zv_0$ to compare with our predictions in Sec. IV.

For a more detailed comparison with the data and especially for a more quantitative understanding of the trends they show as a function of the projectile atomic number and velocity, one has to generalize the theoretical approach introduced in Sec. III to apply also to the situation of velocities smaller than the 1*s* Bohr velocity. Thus, the model has to include the case of projectile electron configurations more complicated than the hydrogenlike one on which we have concentrated in this work. Also, a more refined treatment of the electronic structure of the host target atom will contribute to making our model more quantitative. In particular, the assumption made here that the exchange process involves on the side of the target atom a single electron which does not interact with other valence electrons of the atomic shell has to be replaced by a more accurate approach which takes the multiplet nature of the polarized electron states properly into account during the spin-exchange process. As a further step of generalization, one should examine to what extent the polarization transfer efficiency is influenced by target atom excitation and ionization due to the highly charged projectile.

Incorporation of these features into the presently existing theory will allow one to decide if the nature of the observed effects can all be explained satisfactorily on the basis of the ion-atom interaction model proposed here. To include the role of the solid in a more realistic fashion, it would be desirable to replace the atom simulating the ferromagnet by an atomic cluster which reflects the crucial electronic properties of the ferromagnetic systems iron and gadolnium. The present work has shown that an ion-atom scattering approach is able to explain essential qualitative and quantitative characteristics of the polarization transfer process as investigated experimentally. This encourages one to attempt the refinements listed in the preceding and present paragraphs and holds promise that such detailed investigations could lead to a thorough understanding of the transient field phenomenon in the future.

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