Electrons in a ferromagnetic metal with a domain wall

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We present a theoretical description of conduction electrons interacting with a domain wall in ferromagnetic metals. The description takes into account the interaction between electrons. Within the semiclassical approximation we calculate the spin and charge distributions, particularly their modification by the domain wall. In the same approximation we calculate the local transport characteristics, including relaxation times as well as charge and spin conductivities. It is shown that these parameters are significantly modified near the wall and this modification depends on the electron-electron interaction. The spatial nonuniformity of the transport characteristics may give rise to new phenomena.

I. INTRODUCTION

It is generally believed that domain walls modify significantly all the transport properties of ferromagnetic metals. Early theoretical treatments of this phenomenon[1,2] were stimulated by magnetotransport measurements on single-crystal Fe wiskers. Recent progress in controlling the magnetic state of nanostructures enabled observation of a direct correlation between domain structure and transport properties.[3] For example, it is possible to extract the contribution to resistivity due to a single domain wall. In addition, the discovery of giant magnetoresistance (GMR) in magnetic multilayers, which is connected to the reorientation of the magnetic moments of neighboring magnetic layers from antiparallel to parallel alignments, renewed interest in domain wall resistivity. To some extent, the domain wall plays a similar role as the nonmagnetic layer separating two ferromagnetic films in a sandwich structure or in a multilayer, and therefore can be expected to lead to magnetoresistance effects similar to GMR. Indeed, there is growing experimental evidence of a large magnetoresistance due to a domain wall in ferromagnetic nanostructures.[3–7] This, in turn, led to growing interest in theoretical understanding of the behavior of electrons coupled to a ferromagnetic domain wall.[8–14] Moreover, progress in nanotechnology made it also possible to study electric current flowing through a narrow contact between two ferromagnetic metals (point contact), where a constrained domain wall is created in the antiparallel configuration. Such a domain wall[15] has a significant influence on the transport characteristics of the point contact.[16]

It has been shown experimentally[17] that the presence of a domain wall can either increase or decrease the electrical resistance of a system. This intriguing observation stimulated theoretical works aimed at understanding the role of a domain wall in transport properties. Levy and Zhang[10] developed a semiclassical model based on the mixing of spin-majority and spin-minority transport channels by the domain wall. This mixing results in an increase of the electric resis-

tance due to the presence of a wall. On the other hand, Tatara and Fukuyama[8] found a negative contribution, which is due to destruction of the weak localization corrections to conductivity by the domain wall. Another model which may lead to either a positive or negative contribution of a wall to resistivity was developed by van Gorkom et al.[13] The key point of this model is the fact that the wall can lead to a redistribution of the charge carriers between spin-majority and spin-minority channels. The domain wall contribution to resistivity depends then on the ratio of spin-majority and spin-minority relaxation times.

In this paper, we consider electrons in a ferromagnetic metal which interact with a domain wall. The description includes interaction between electrons, and therefore we use a self-consistent analysis to describe charge and spin distributions, as well as their modification by the domain wall. Using the Green's function technique, we calculate the electron relaxation times in a quasiclassical approximation. Apart from this, we also calculate the local charge and spin conductivities. These transport parameters are shown to be significantly modified near the domain wall, which may give rise to new effects.

The paper is organized as follows. In Sec. II we describe the model as well as the transformation used to replace the system with inhomogeneous magnetization by a system magnetized homogeneously. In Sec. III we present the transformed Hamiltonian, generalized by including self-consistent fields related to electrostatic and magnetic interactions. A semiclassical solution of the resulting Schrödinger equation for electrons is also presented there. Scattering from the wall in the Born approximation is calculated in Sec. IV. In Sec. V we calculate, within the quasiclassical approximation, both the spin and charge distributions in the vicinity of the domain wall, as well as the corresponding contributions generated by the wall. Local relaxation times are calculated in Sec. VI, whereas the local charge and spin conductivities are calculated respectively in Secs. VII and VIII. Final conclusions are provided in Sec. IX.

II. MODEL

Consider a general case of a ferromagnet with a nonuniform magnetization $\mathbf{M}(\mathbf{r})$. The one-particle Hamiltonian describing conduction electrons locally exchange coupled to the magnetization $\mathbf{M}(\mathbf{r})$ takes the form

$$H_0 = -\frac{1}{2m}\psi_\alpha^\dagger \frac{\partial^2}{\partial \mathbf{r}^2}\psi_\alpha - J\psi_\alpha^\dagger \boldsymbol{\sigma}_{\alpha\beta}\cdot\mathbf{M}(\mathbf{r})\psi_\beta, \qquad (1)$$

where J is the exchange parameter, ψ_α and $\psi_\alpha^\dagger$ are the spinor field operators of electrons, $\boldsymbol{\sigma}=(\sigma_x,\sigma_y,\sigma_z)$ are the Pauli matrices, and we use the units with $\hbar=1$.

The model Hamiltonian (1) will be used to describe electrons interacting with a domain wall in ferromagnetic metals or semiconductors. The domain wall will be modeled by a magnetization profile $\mathbf{M}(\mathbf{r})$. For the sake of simplicity we shall assume that $|\mathbf{M}(\mathbf{r})|=$ const. We can then write $J\mathbf{M}(\mathbf{r})=M\mathbf{n}(\mathbf{r})$, where $\mathbf{n}(\mathbf{r})$ is a unit vector field to be specified later, and M is measured in the energy units and includes the parameter J.

The first step of our analysis is to perform a local unitary transformation[8] $\psi\rightarrow T(\mathbf{r})\psi$, which removes the nonhomogeneity of $\mathbf{M}(\mathbf{r})$; that is, $T(\mathbf{r})$ transforms the second term in Eq. (1) as

$$\psi^\dagger \boldsymbol{\sigma}\cdot\mathbf{n}(\mathbf{r})\psi\rightarrow\psi^\dagger\sigma_z\psi. \qquad (2)$$

The transformation matrix $T(\mathbf{r})$ must then obey the condition

$$T^\dagger(\mathbf{r})\boldsymbol{\sigma}\cdot\mathbf{n}(\mathbf{r})T(\mathbf{r})=\sigma_z. \qquad (3)$$

Explicit form of $T(\mathbf{r})$ is given by[18]

$$T(\mathbf{r})=\frac{1}{\sqrt{2}}\left(\sqrt{1+n_z(\mathbf{r})}+i\frac{n_y(\mathbf{r})\sigma_x-n_x(\mathbf{r})\sigma_y}{\sqrt{1+n_z(\mathbf{r})}}\right). \qquad (4)$$

Applying the transformation (4) to the kinetic part of the Hamiltonian (1) one obtains

$$\psi^\dagger\frac{\partial^2}{\partial\mathbf{r}^2}\psi\rightarrow\psi^\dagger\left(\frac{\partial}{\partial\mathbf{r}}+\mathbf{A}(\mathbf{r})\right)^2\psi, \qquad (5)$$

where the non-Abelian gauge field $\mathbf{A}(\mathbf{r})$ is given by

$$\mathbf{A}(\mathbf{r})=T^\dagger(\mathbf{r})\frac{\partial}{\partial\mathbf{r}}T(\mathbf{r}). \qquad (6)$$

According to Eq. (4), the gauge field $\mathbf{A}(\mathbf{r})$ is a matrix in the spin space.

Let us consider now a more specific case of a domain wall in a bulk system. Assume that the wall is translationally invariant in the x-y plane: $\mathbf{M}(\mathbf{r})\rightarrow\mathbf{M}(z)$ and $\mathbf{n}(\mathbf{r})\rightarrow\mathbf{n}(z)$. For a simple domain wall with $\mathbf{M}(z)$ in the plane normal to the wall, one can parametrize the vector $\mathbf{n}(z)$ as

$$\mathbf{n}(z)=(\sin\varphi(z),\ 0,\ \cos\varphi(z)), \qquad (7)$$

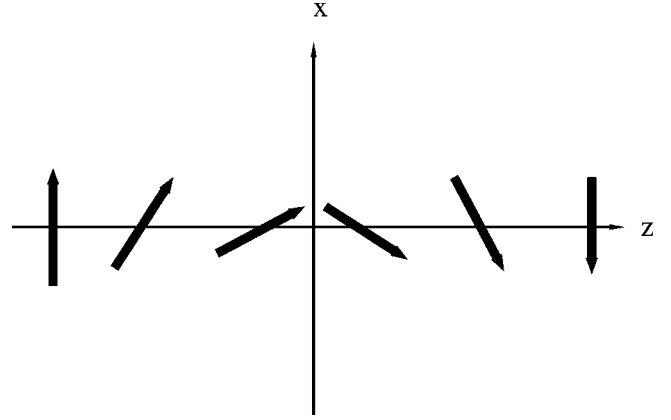where the phase $\varphi(z)$ determines the type of a domain wall. The transformation (4) is then reduced to

FIG. 1. Schematic picture of the magnetization orientations near the domain wall.

$$T(z)=\frac{1}{\sqrt{2}}\left(\sqrt{1+\cos\varphi(z)}-i\sigma_y\frac{\sin\varphi(z)}{\sqrt{1+\cos\varphi(z)}}\right), \qquad (8)$$

and the gauge field assumes a simple form

$$\mathbf{A}(z)=\left(0,0,-\frac{i}{2}\sigma_y\varphi'(z)\right), \qquad (9)$$

where $\varphi'(z)\equiv\partial\varphi(z)/\partial z$.

Taking into account Eqs. (5) and (9), one can write the transformed Hamiltonian in the form

$$H_0=-\frac{1}{2m}\frac{\partial^2}{\partial\mathbf{r}^2}-M\sigma_z+\frac{m\beta^2(z)}{2}$$
$$+i\sigma_y\frac{\beta'(z)}{2}+i\sigma_y\beta(z)\frac{\partial}{\partial z}, \qquad (10)$$

where

$$\beta(z)=\frac{\varphi'(z)}{2m}. \qquad (11)$$

When $k_F L\gg 1$, where k_F is the Fermi wave vector and L stands for the wall width, the perturbation due to the domain wall is weak and one may use the semiclassical approximation. In particular, the parameter $\beta(z)$ close to the center of the wall can be then treated as a constant. Such a model domain wall with a constant parameter β was analyzed in Ref. 12. Our following considerations will be restricted mainly to the semiclassical limit $k_F L\gg 1$. In that case, the last three terms on the right side of Eq. (10), which are due to the domain wall, will be treated as a small perturbation.

The description given above is quite general and may be used for various models of the domain wall. If we assume the domain wall in the form of a kink (Fig. 1), then

$$\varphi(z)=-\frac{\pi}{2}\tanh(z/L), \qquad (12)$$

and the parameter $\beta(z)$ is given by

$$\beta(z) = -\frac{\pi}{4mL\cosh^2(z/L)}. \qquad (13)$$

III. SEMICLASSICAL APPROXIMATION

In bulk magnetic metals like Fe, Ni, or Co, the width L of a magnetic domain wall is usually much larger then the electron Fermi wavelength λ_F. In such a case application of a semiclassical approximation is well justified.[1] The dominant perturbation from the domain wall is then described by the term with $\beta(\partial/\partial z)$ in Eq. (10), since it is of order of βk_F. The term proportional to β^2 is smaller, while the term including $\beta'(z)$ is of the order of β/L and therefore can be neglected.

For the sake of self-consistency, we will include now the Coulomb interaction of electrons, which allows a correct description of charge accumulated at the wall. The point is that the wall can give rise to some excess charge locally breaking electrical neutrality, as will be described in more detail later. This effect was not taken into account in a previous analysis.[8] On the other hand, the renormalization of the chemical potential forbidding the formation of excess charge[12] may be an overestimation of the Coulomb repulsion.

The Coulomb interaction will be taken into account via the coupling term

$$H_{int} = \frac{1}{2}\int d^3\mathbf{r}\, d^3\mathbf{r}'[\psi^\dagger(\mathbf{r},t)\psi(\mathbf{r},t) - n_0]V(\mathbf{r}-\mathbf{r}')$$
$$\times[\psi^\dagger(\mathbf{r}',t)\psi(\mathbf{r}',t) - n_0], \qquad (14)$$

where $V(\mathbf{r}-\mathbf{r}') = e^2/|\mathbf{r}-\mathbf{r}'|$ is the bare Coulomb interaction and n_0 is the mean electron density in the bulk. Using an auxiliary scalar field $\phi(z)$ we can incorporate the interaction by adding to the Hamiltonian the following term:

$$H_{int}^{(MF)} = -\int d^3\mathbf{r}\, \phi(z)\psi^\dagger\psi, \qquad (15)$$

where the field $\phi(z)$ is determined by the saddle-point equation

$$\frac{d^2\phi(z)}{dz^2} = 4\pi e^2(\langle\psi^\dagger\psi\rangle - n_0), \qquad (16)$$

with $\langle\cdots\rangle$ denoting the ground-state average. This makes the solution self-consistent, and the field $\phi(z)$ is the mean-field electrostatic potential in the presence of the wall. The use of the differential saddle-point equation for $\phi(z)$, Eq. (16), makes the problem more complicated due to the non-locality, but allows us to describe correctly the screening effects associated with a spatial distribution of charges in the vicinity of the domain wall.

To include the spin-dependent interaction, we introduce the contact interaction term in the form

$$H_{int}^s = -\frac{g_s^2}{2}\int d^3\mathbf{r}(\psi^\dagger\sigma_z\psi - s_0)^2, \qquad (17)$$

where g_s is the corresponding coupling constant. Microscopically, the Hamiltonian (17) and the phenomenological parameter g_s originate from the spin-dependent correlation terms, which in turn arrise from electron-electron interactions (similar to those giving rise to ferromagnetism of band electrons). Choosing s_0 as the spin density far from the wall guarantees that this interaction vanishes when there is no domain wall. This means that the effects due to magnetization of the conduction electrons in a system without a domain wall are included by the parameter M in the one-particle Hamiltonian. The effect of a domain wall is then to modify the internal magnetization, resulting from a redistribution of the spin density. The effects due to the interaction (17) can be taken into account by adding to the Hamiltonian the new term

$$H_{int}^{s(MF)} = \int d^3\mathbf{r}\, m_z(z)\psi^\dagger\sigma_z\psi, \qquad (18)$$

where the internal magnetization field $m_z(z)$ is determined by the saddle-point-like equation and is of the form

$$m_z(z) = -g_s^2(\langle\psi^\dagger\sigma_z\psi\rangle - s_0). \qquad (19)$$

Thus, the Schrödinger equation for electrons of energy ε in the fields $\phi(z)$ and $m_z(z)$ reads

$$\left(-\frac{1}{2m}\frac{\partial^2}{\partial\mathbf{r}^2} + \frac{m\beta^2(z)}{2} - [M - m_z(z)]\sigma_z\right.$$
$$\left. + i\sigma_y\beta(z)\frac{\partial}{\partial z} - \phi(z) - \varepsilon\right)\psi = 0, \qquad (20)$$

where the fields $\phi(z)$ and $m_z(z)$ have to be determined self-consistently via Eqs. (16) and (19). Equation (20) has the following semiclassical solutions ($i = 1,2$):

$$\psi_i(\boldsymbol{\rho},z) = \frac{\exp(\pm i\mathbf{q}\cdot\boldsymbol{\rho})}{[\varepsilon_i^2(z) + \beta^2(z)k_i^2(z)]^{1/2}k_i^{1/2}(z)}\begin{pmatrix}\mp i\beta k_i(z)\\ \varepsilon_i(z)\end{pmatrix}$$
$$\times\exp\left[\pm i\int_0^z k_i(z)dz\right], \qquad (21)$$

where $\boldsymbol{\rho} = (x,y)$, $\mathbf{q}$ is the momentum in the plane of the wall, the wave vector components normal to the wall (along the axis z) are given by

$$k_{1,2}^2(z) = \kappa^2(z) + m^2\beta^2(z) \pm 2m[M_r^2(z) + \beta^2(z)\kappa^2(z)]^{1/2}, \qquad (22)$$

$$\varepsilon_i(z) = \frac{k_i^2(z)}{2m} + \frac{m\beta^2(z)}{2} - M_r(z) - \frac{\kappa^2(z)}{2m}, \qquad (23)$$

and $\kappa(z)$ and $M_r(z)$ are defined as

$$\kappa^2(z) = 2m[\varepsilon + \phi(z)] - q^2, \qquad (24)$$

$$M_r(z) = M - m_z(z). \qquad (25)$$

For clarity of notation we omitted the subscript z of $k_{z;1,2}(z)$ $[k_{1,2}(z) \equiv k_{z;1,2}(z)]$.

There is no reflection from the wall in the semiclassical approximation. It should be noted, however, that for electrons moving nearly parallel to the wall (with a very small z component of the momentum), there is a reflection from the wall since for such electrons classical motion through the barrier is impossible. We do not consider here this effect since its contribution is very small.

IV. SCATTERING FROM THE WALL (BORN APPROXIMATION)

For the case of not too thin domain walls, the term proportional to $\beta(z)\partial/\partial z$ can be treated as a small perturbation and scattering from the wall can be evaluated within the Born approximation. The matrix elements of the $(k_z\uparrow)$ $\rightarrow(k_z'\downarrow)$ spin-flip scattering in the plane-wave basis are given by

$$V_{k_z k_z'}=\int_{-\infty}^{\infty}e^{-ik_z'z}\left(-\beta(z)\frac{d}{dz}\right)e^{ik_z z}dz. \quad (26)$$

Using Eq. (13), we obtain

$$V_{k_z k_z'}=\frac{i\pi k_z}{4mL}\int_{-\infty}^{\infty}\frac{\exp[-i(k_z'-k_z)z]dz}{\cosh^2(z/L)}. \quad (27)$$

After calculating the integral[19] we arrive at

$$V_{k_z k_z'}=\frac{i\pi^2 k_z(k_z'-k_z)L}{4m}\mathrm{csch}\left[\frac{\pi(k_z'-k_z)L}{2}\right]. \quad (28)$$

Correspondingly, the probability of backscattering ($k_z'=-k_z$) is

$$W_{back}\equiv 2\pi|V_{k_z,-k_z}|^2=\frac{\pi^5 k_z^4 L^2}{2m^2}\mathrm{csch}^2(\pi k_z L). \quad (29)$$

For $k_z L\gg 1$, from the last equation we find

$$W_{back}=\frac{2\pi^5 k_z^4 L^2}{m^2}e^{-2\pi k_z L}. \quad (30)$$

Thus, the probability of the backscattering with simultaneous spin flip vanishes exponentially in the limit of $k_F L\gg 1$.[1] Spin-conserving backscattering is determined by the term proportional to β^2 in the Hamiltonian (20). In the first approximation this term can be neglected as it is smaller than the term proportional to $\beta(z)\partial/\partial z$.

The question arises as to whether the Born approximation gives correct results in the problem under consideration. There are two general conditions for its applicability:[20]

$$|U(z)|\ll\frac{1}{mL^2}\ \text{ or }\ |U(z)|\ll\frac{k}{mL}, \quad (31)$$

where $U(z)$ is the scattering potential. In the first case the Born approximation is good for arbitrary electron energy, whereas in the second one it is good only for fast electrons. Therefore, if we choose the limit $k_F L\gg 1$, then $|U(z)|$ $\sim\beta k_z\sim(k_z/mL)$, and none of the conditions is satisfied. In the opposite case of a small domain-wall width $k_F L\ll 1$, we have $|U(z)|\sim 1/mL^2$ and the Born approximation is not justified again. Thus, the Born approximation can be used only for rough estimations. In the case under consideration, $k_F L$ $\gg 1$, it shows that the usual scattering from the wall is exponentially weak.

V. DISTRIBUTION OF SPIN AND CHARGE DENSITIES (SEMICLASSICAL APPROACH)

In the framework of the semiclassical approximation, one can calculate the local charge and spin densities in the vicinity of the wall, as well as the distribution of charge and spin currents. As follows from Sec. III, this can also be done taking into account the Coulomb interaction self-consistently.

The equation for the Green function with the term $\beta(z)$ weakly dependent on z,

$$\left(\varepsilon+\frac{1}{2m}\frac{\partial^2}{\partial\mathbf{r}^2}-\frac{m\beta^2(z)}{2}+\phi(z)+M_r(z)\sigma_z\right.$$
$$\left.-i\sigma_y\beta(z)\frac{\partial}{\partial z}+\mu\right)G_\varepsilon(\mathbf{r},\mathbf{r}')=\delta(\mathbf{r}-\mathbf{r}'), \quad (32)$$

has a quasiclassical solution ($k_z L\gg 1$)

$$G_\varepsilon(\mathbf{k})=\frac{\varepsilon-\varepsilon_\mathbf{k}-M_r(z)\sigma_z-k_z\beta(z)\sigma_y+\mu_r}{(\varepsilon-\varepsilon_{\mathbf{k}\uparrow}+\mu_r+i\delta\,\mathrm{sgn}\,\varepsilon)(\varepsilon-\varepsilon_{\mathbf{k}\downarrow}+\mu_r+i\delta\,\mathrm{sgn}\,\varepsilon)}, \quad (33)$$

where the following notation has been used:

$$\varepsilon_\mathbf{k}=\frac{q^2+k_z^2}{2m}, \quad (34)$$

$$\varepsilon_{\mathbf{k}\uparrow,\downarrow}=\varepsilon_\mathbf{k}\mp[M_r^2(z)+k_z^2\beta^2(z)]^{1/2}, \quad (35)$$

$$\mu_r=\mu-\frac{m\beta^2(z)}{2}+\phi(z), \quad (36)$$

and μ is the chemical potential. Equation (35) describes the energy spectrum in the spin-up and spin-down branches, where for the sake of notational simplicity we dropped the z dependence of $\varepsilon_{\mathbf{k}\uparrow,\downarrow}$ and μ_r. In what follows we also drop the z dependence of M_r and β.

Note that the square root in Eq. (35) contains contributions due to spin mixing caused by the perturbation $\sigma_y\beta(\partial/\partial z)$. Hence, what we call spin-up and spin-down branches of the spectrum [labeled as $\uparrow$ and $\downarrow$ in Eq. (35)] are in fact the eigenvalues corresponding to the wave functions with mixed up and down states. Correspondingly, the Green function (33) has poles at both Fermi surfaces with $k=k_{F\uparrow}$ and $k=k_{F\downarrow}$ in diagonal and nondiagonal components, where $k_{F\uparrow,\downarrow}$ are given by

$$k_{F\uparrow,\downarrow}^2=2m\mu_r+2m^2\beta^2\pm 2m(2m\mu_r\beta^2+m^2\beta^4+M_r^2)^{1/2}. \quad (37)$$

Using the Green function (33), one can calculate the spin density distribution in the presence of the wall. The real spin density distribution, i.e., transformed back to the original basis, is given by the formula

$$\mathbf{s}(z) = -i \, \mathrm{Tr} \int \frac{d\varepsilon}{2\pi} \frac{d^3\mathbf{k}}{(2\pi)^3} T^\dagger(z)\boldsymbol{\sigma}T(z)G_\varepsilon(\mathbf{k}). \qquad (38)$$

To obtain this expression one should use the inverse transformation, i.e., $G \to TGT^\dagger$. Using Eq. (3), one can rewrite Eq. (38) as

$$\mathbf{n}(z)\cdot\mathbf{s}(z) = -i \, \mathrm{Tr} \int \frac{d\varepsilon}{2\pi} \frac{d^3\mathbf{k}}{(2\pi)^3} \sigma_z G_\varepsilon(\mathbf{k}). \qquad (39)$$

Since the projection of $\mathbf{s}$ on the plane perpendicular to $\mathbf{n}$ vanishes, we can write the spin density as

$$\mathbf{s}(z) = -i\mathbf{n}(z)\mathrm{Tr} \int \frac{d\varepsilon}{2\pi} \frac{d^3\mathbf{k}}{(2\pi)^3} \sigma_z G_\varepsilon(\mathbf{k}). \qquad (40)$$

Substituting the Green function (33) into Eq. (40), we find

$$\mathbf{s}(z) = \mathbf{n}(z)\left(\int_{\varepsilon_{\mathbf{k}\uparrow}<\mu_r} - \int_{\varepsilon_{\mathbf{k}\downarrow}<\mu_r}\right)\frac{d^3\mathbf{k}}{(2\pi)^3}(1+k_z^2\beta^2/M_r^2)^{-1/2}. \qquad (41)$$

After evaluating these integrals, we find the spin density distribution

$$\mathbf{s}(z) = \frac{M_r\mathbf{n}(z)}{4\pi^2\beta}\left[-\frac{k_{F\uparrow}}{2\beta}(M_r^2+k_{F\uparrow}^2\beta^2)^{1/2}\right.$$
$$+\frac{k_{F\downarrow}}{2\beta}(M_r^2+k_{F\downarrow}^2\beta^2)^{1/2}+\left(2m\mu_r+\frac{M_r^2}{2\beta^2}\right)$$
$$\left.\times\left(\mathrm{arcsinh}\frac{k_{F\uparrow}\beta}{M_r}-\mathrm{arcsinh}\frac{k_{F\downarrow}\beta}{M_r}\right)+2m\beta(k_{F\uparrow}+k_{F\downarrow})\right]. \qquad (42)$$

The accumulation of the spin density at the domain wall is

$$\Delta\mathbf{s}(z) = \mathbf{s}(z) - \mathbf{s}_0, \qquad (43)$$

where $\mathbf{s}_0$ is the spin density in the limit of $\beta=0$. For small β, i.e., for very smooth magnetic wall and up to second order of β, this reads

$$\Delta\mathbf{s}(z) = -\frac{\mathbf{n}(z)\beta^2}{4\pi^2}\left[m^2(k_{F\uparrow}-k_{F\downarrow})\right.$$
$$\left.+\frac{m\mu}{3M_r^2}(k_{F\uparrow}^3-k_{F\downarrow}^3)-\frac{k_{F\uparrow}^5-k_{F\downarrow}^5}{10M_r^2}\right]. \qquad (44)$$

The sign of the factor in the square brackets of Eq. (44) is always positive.

The charge density distribution can be calculated in a similar way,

$$\rho(z) = -i \, \mathrm{Tr} \int \frac{d\varepsilon}{2\pi} \frac{d^3\mathbf{k}}{(2\pi)^3} G_\varepsilon(\mathbf{k}). \qquad (45)$$

After calculating the integral (45) we find

$$\rho(z) = \frac{1}{4\pi^2}\left[2m\mu_r(k_{F\uparrow}+k_{F\downarrow})-\frac{k_{F\uparrow}^3+k_{F\downarrow}^3}{3}\right.$$
$$+mk_{F\uparrow}(M_r^2+k_{F\uparrow}^2\beta^2)^{1/2}-mk_{F\downarrow}(M_r^2+k_{F\downarrow}^2\beta^2)^{1/2}$$
$$\left.+\frac{mM_r^2}{\beta}\mathrm{arcsinh}\frac{k_{F\uparrow}\beta}{M_r}-\frac{mM_r^2}{\beta}\mathrm{arcsinh}\frac{k_{F\downarrow}\beta}{M_r}\right]. \qquad (46)$$

Now we can use this expression in Eq. (16) to determine electrostatic potential $\langle\psi^\dagger\psi\rangle \equiv \rho(z)$.

We can linearize Eq. (16) in $\phi(z)$ assuming that the domain wall does not change significantly the electron density, i.e., for $\mu \gg |\phi(z)|$. Hence, after expanding $\rho(z)$ in $\phi(z)$ and Fourier transforming over z, we can write Eq. (16) as

$$(q_z^2+\kappa_0^2)\phi(q_z) = -4\pi e^2\Delta\tilde{\rho}(q_z), \qquad (47)$$

where $\kappa_0 = (4\pi e^2\nu_0)^{1/2}$ is the inverse screening length, $\nu_0 = \partial\rho/\partial\mu$ is the thermodynamic density of states, and $\Delta\tilde{\rho}(q_z)$ is the Fourier transform of

$$\Delta\tilde{\rho}(z) \equiv [\rho(z)-n_0]_{\phi(z)=0}. \qquad (48)$$

Using Eqs. (25), (35), (36), and (37), we find that for $\beta \to 0$ the accumulation of charge, $\Delta\tilde{\rho}(z) = \rho - \rho(\phi=0)$, is

$$\Delta\tilde{\rho}(z) = -\frac{m^2\beta^2}{4\pi^2}(k_{F\uparrow}+k_{F\downarrow})+\frac{m\beta^2}{12\pi^2M}(k_{F\uparrow}^3-k_{F\downarrow}^3). \qquad (49)$$

This value of $\Delta\tilde{\rho}(z)$ is the accumulated charge in the absence of Coulomb repulsion.

Due to Eq. (16), the real distribution of charge $\Delta\rho(z)$ is related to $\Delta\tilde{\rho}(z)$ by the relation which in Fourier space has the form

$$\Delta\rho(q_z) = \frac{q_z^2}{q_z^2+\kappa_0^2}\Delta\tilde{\rho}(q_z). \qquad (50)$$

Then, if the characteristic lengh of the domain wall is large, $\kappa_0 L \gg 1$, we obtain

$$\Delta\rho(z) = -\frac{1}{\kappa_0^2}\frac{d^2\Delta\tilde{\rho}(z)}{dz^2} \qquad (51)$$

and, finally, using Eq. (46), we find the distribution of charge:

$$\Delta\rho(z) = -\frac{m}{2\pi^2\kappa_0^2}\left[\beta(z)\frac{d^2\beta(z)}{dz^2}+\left(\frac{d\beta(z)}{dz}\right)^2\right]$$
$$\times\left[-m(k_{F\uparrow}+k_{F\downarrow})+\frac{1}{3M}(k_{F\uparrow}^3-k_{F\downarrow}^3)\right]. \qquad (52)$$
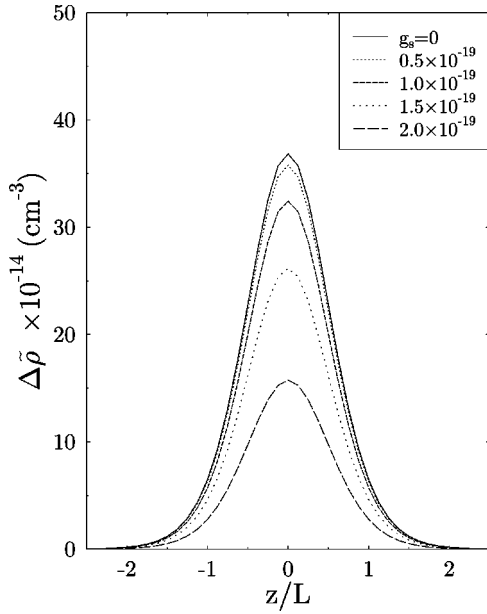
FIG. 2. Distribution of the excess charge for noninteracting electrons, $\Delta\tilde{\rho}(z)$, near the domain wall, calculated for different values of the spin coupling constant g_s. The coupling constant g_s is given in units of $\mathrm{erg}^{1/2}\,\mathrm{cm}^{3/2}$.

We performed numerical calculations of the charge $\Delta\tilde{\rho}(z)$ and excess spin density $\Delta s_l(z) \equiv \Delta\mathbf{s}(z)\cdot\mathbf{n}(z)$ using the set of equations (42), (46), (48), (25), (36), (37), and (19). The results are presented in Figs. 2 and 3 for different values of the spin coupling constant g_s. In the calculations we take the Fermi energies $\varepsilon_{F\uparrow}=3$ eV and $\varepsilon_{F\downarrow}=2.5$ eV in the bulk, and $m=4m_0$, where m_0 is the free electron mass. The figures demonstrate how the spin coupling constant g_s affects both the spin accumulation (Fig. 3) and charge accumulation (Fig.
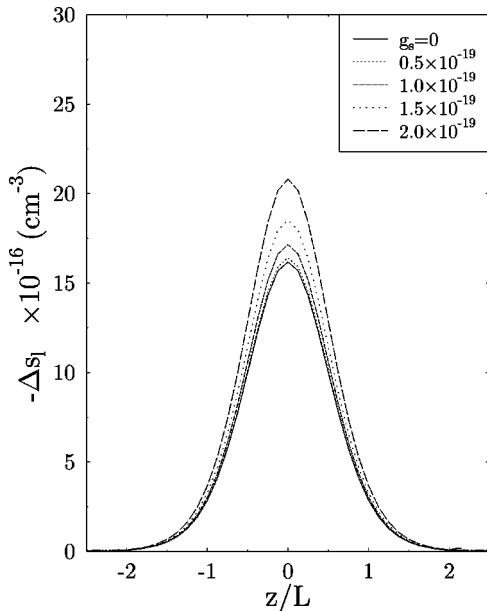

FIG. 3. Distribution of the excess spin density near the domain wall for different values of the spin coupling constant g_s.
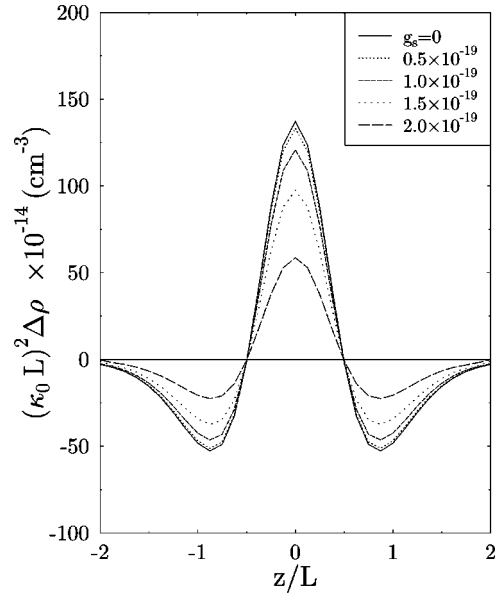

FIG. 4. Distribution of the charge density near the domain wall for interacting electrons, calculated for different values of the spin coupling constant g_s. Due to the screening effects and charge conservation, the integrated charge accumulated at the wall vanishes.

2). This effect is a result of self-consistency, because by controlling the spin density one modifies the magnetic wall, which in turn influences the electron density.

In view of Eq. (48), the function $\Delta\tilde{\rho}(z)$, presented in Fig. 2, is not the excess charge accumulated at the wall but an auxiliary function corresponding to the condition $\phi(z)=0$. The real distribution of accumulated charge, Eq. (51), is presented in Fig. 4 for different values of the coupling constant g_s. This figure demonstrates that the integral of $\Delta\rho(z)$ over z is zero due to the conservation of electric charge. The characteristic length of the charge distribution is determined by the characteristic thickness of the domain wall.

VI. IMPURITY SELF-ENERGY

In this section we shall take into account the scattering of electrons from impurities. The simplest choice are impurities with a short-range scattering potential, which scatter similarly both spin-up and spin-down electrons. Let the matrix element of the scattering potential of a defect be V_0. The self-energy operator in the Born approximation is

$$\Sigma(\varepsilon) = V_0^2 \int \frac{d^3\mathbf{k}}{(2\pi)^3} G_\varepsilon(\mathbf{k}). \tag{53}$$

After integrating the Green function given by Eq. (33), we get

$$\Sigma(\varepsilon) = -\frac{i\,\mathrm{sgn}\,\varepsilon}{2}\,\mathrm{diag}(1/\tau_\uparrow,\ 1/\tau_\downarrow), \tag{54}$$

where the momentum relaxation times for spin-up and spin-down electrons are

$$\frac{1}{\tau_\uparrow(z)} = \frac{mV_0^2}{2\pi}\left(k_{F\uparrow} + k_{F\downarrow} + \frac{M_r}{\beta}\text{arcsinh}\frac{k_{F\uparrow}\beta}{M_r}\right.$$

$$\left. - \frac{M_r}{\beta}\text{arcsinh}\frac{k_{F\downarrow}\beta}{M_r}\right), \tag{55}$$

$$\frac{1}{\tau_\downarrow(z)} = \frac{mV_0^2}{2\pi}\left(k_{F\uparrow} + k_{F\downarrow} - \frac{M_r}{\beta}\text{arcsinh}\frac{k_{F\uparrow}\beta}{M_r}\right.$$

$$\left. + \frac{M_r}{\beta}\text{arcsinh}\frac{k_{F\downarrow}\beta}{M_r}\right). \tag{56}$$

The difference in scattering times is due to a difference in the density of states at the Fermi level for spin-up and spin-down electrons. The formulas (55) and (56) take into account variation of scattering times near the domain wall. These correlations have been neglected in previous works.

VII. LOCAL CONDUCTIVITY

The general formula for local conductivity (without localization corrections), when an electrical field is applied along the axis z, has the following form:

$$\sigma_{zz} = \frac{e^2}{2\pi m^2}\text{Tr}\int\frac{d^3\mathbf{k}}{(2\pi)^3}(k_z - m\beta\sigma_y)G_\mathbf{k}^R(k_z - m\beta\sigma_y)G_\mathbf{k}^A, \tag{57}$$

where the gauge potential $\mathbf{A}(z)$, defined by Eq. (9), is taken into account, and the retarded (R) and advanced (A) Green functions are both evaluated at the Fermi level,

$$G_\mathbf{k}^{R,A} \equiv G_{\varepsilon=0}^{R,A}(\mathbf{k}) = \frac{-\varepsilon_\mathbf{k} - M_r\sigma_z - k_z\beta\sigma_y + \mu_r}{(-\varepsilon_{\mathbf{k}\uparrow} + \mu_r \pm i/2\tau_\uparrow)(-\varepsilon_{\mathbf{k}\downarrow} + \mu_r \pm i/2\tau_\downarrow)}. \tag{58}$$

Owing to the terms containing β in the Green functions and to the z dependence of $\varepsilon_{k\uparrow,\downarrow}$, μ_r, and M_r, the local conductivity σ_{zz} is a smoothly varying function of z. Given the $\sigma_{zz}(z)$, the resistivity of a sample with a domain wall can be found by (adding resistivities)

$$R \sim \int\frac{dz}{\sigma_{zz}(z)}. \tag{59}$$

Using Eqs. (35) and (36), we find the local conductivity in the form

$$\sigma_{zz} = \frac{e^2}{2\pi^2 m}\left[\tau_\uparrow\left(\frac{k_{F\uparrow}^3}{3} + m^2\beta^2 k_{F\uparrow} - m^2 M_r\beta\,\arctan\frac{k_{F\uparrow}\beta}{M_r}\right)\right.$$

$$\left. + \tau_\downarrow\left(\frac{k_{F\downarrow}^3}{3} + m^2\beta^2 k_{F\downarrow} - m^2 M_r\beta\,\arctan\frac{k_{F\downarrow}\beta}{M_r}\right)\right]. \tag{60}$$

One should note that the dependence on β enters here not only explicitly, but also through the parameters $\tau_\uparrow$, $\tau_\downarrow$, $k_{F\uparrow}$, and $k_{F\downarrow}$.

The description of the domain wall in terms of local conductivity is justified when $L \gg l$, where l is the electron mean free path. For such a smooth domain wall, there is no electron scattering from the wall but the local conductivity is changed. The system with a domain wall is macroscopically inhomogeneous, and thus the electric field in the vicinity of the domain wall is inhomogeneous when a bias voltage is applied.

VIII. SPIN CURRENTS AND LOCAL SPIN CONDUCTIVITY

The spin-current density in the untransformed basis has the form derived in the Appendix:

$$\mathbf{j}_{\uparrow,\downarrow} = -\frac{i}{2m}\text{Tr}\int\frac{d\varepsilon}{2\pi}\frac{d^3\mathbf{k}}{(2\pi)^3}[\mathbf{k} - i\mathbf{A} \pm T^\dagger\sigma_z T(\mathbf{k} - i\mathbf{A})]G_\varepsilon(\mathbf{k}). \tag{61}$$

Suppose the spin current is induced by an electromagnetic field with vector potential $\mathbf{A}_{em}$ acting on both up- and down-spin components. Then, using Eqs. (9), (11), and (61), we obtain for the up- and down-spin conductivity

$$\sigma_{zz}^{\uparrow,\downarrow} = \frac{e}{4\pi m^2}\text{Tr}\int\frac{d^3\mathbf{k}}{(2\pi)^3}[k_z - m\beta\sigma_y$$

$$\pm(n_z\sigma_z - n_x\sigma_x)(k_z - m\beta\sigma_y)]G_\mathbf{k}^R(k_z - m\beta\sigma_y)G_\mathbf{k}^A. \tag{62}$$

The result of calculation can be presented in the form

$$\sigma_{zz}^{\uparrow,\downarrow} = \frac{1}{2e}\sigma_{zz} + \frac{e}{4\pi^2 m}\left\{\tau_\downarrow\left[(m\beta^2 \mp M_r n_z)\left(mk_{F\downarrow} - \frac{mM_r}{\beta}\arctan\frac{k_{F\downarrow}\beta}{M_r}\right)\right.\right.$$

$$\left. + (2m\beta^2 \mp M_r n_z)\left(\frac{k_{F\downarrow}}{2\beta^2}\sqrt{M_r^2 + k_{F\downarrow}^2\beta^2} - \frac{M_r^2}{2\beta^2}\text{arcsinh}\frac{k_{F\downarrow}\beta}{M_r}\right)\right] + \tau_\uparrow\left[(m\beta^2 \mp M_r n_z)\left(mk_{F\uparrow} - \frac{mM_r}{\beta}\arctan\frac{k_{F\uparrow}\beta}{M_r}\right)\right.$$

$$\left.\left. - (2m\beta^2 \mp M_r n_z)\left(\frac{k_{F\uparrow}}{2\beta^2}\sqrt{M_r^2 + k_{F\uparrow}^2\beta^2} - \frac{M_r^2}{2\beta^2}\text{arcsinh}\frac{k_{F\uparrow}\beta}{M_r}\right)\right]\right\}. \tag{63}$$

In the limit of $\beta \to 0$ we obtain

$$\sigma_{zz}^{\uparrow,\downarrow} = \frac{1}{2e}\,\sigma_{zz} \pm \cos\varphi(z)\,\frac{e}{2m}\left(\frac{k_{F\uparrow}\tau_{\uparrow}}{6\pi^2} - \frac{k_{F\downarrow}\tau_{\downarrow}}{6\pi^2}\right). \quad (64)$$

The spin conductivity (63) and (64) describes a response in the form of up- and down-spin currents to the electric field, associated with the vector potential $\mathbf{A}_{em}$.

IX. SUMMARY AND CONCLUSIONS

We have described behavior of conduction electrons interacting with a magnetic domain wall in ferromagnetic metals. In the description we used a realistic model which includes the Coulomb interaction and screening effects. Within the semiclassical approximation we calculated self-consistently the equilibrium charge and spin distribution in the presence of a domain wall. We showed that this distribution is significantly modified by the wall. We have also calculated the local transport characteristics, like relaxation times and charge and spin conductivities.

Our approach applies to the linear response regime, and therefore such nonequilibrium phenomena like spin accumulation at the wall due to flowing current are not taken into account. In a recent paper Ebels et al.[21] observed large magnetoresistance due to a domain wall and attributed it to the spin accumulation. On the other hand, Simanek[22] showed that spin accumulation is partially suppressed by spin tracking and cannot explain such a large magnetoresistance.

The approach used in Ref. 22 is based on the kinetic equation for the Wigner function and takes into account nonlinear effects, particularly those due to spin accumulation. Such effects were not included in our description, since we analyzed the linear response regime only, which is determined by equilibrium characteristics. However, we took into account the interaction between electrons and showed that this interaction can singificaly modify the influence of the magnetic wall on transport properties. The local transport characteristics were described by few parameters characterizing the domain wall. Variation of the local conductivities at the wall may lead to several new effects. For instance, one may expect the Peltier effect at the domain wall. To our knowledge, such an effect has not been studied yet. Some other interesting phenomena may be related to the spin-dependent coupling, described by the parameter g_s.

ACKNOWLEDGMENTS

APPENDIX: SPIN CURRENT DENSITY

To find the expression for the spin current, we add to the Hamiltonian of Eq. (1) an auxiliary vector potential $\mathcal{A}_{em}(t)$ acting only on the spin-up states. It produces in the kinetic part of the Hamiltonian the following term (in the untransformed basis):

$$H_{kin} = -\frac{1}{2m}\,\psi^{\dagger}(\mathbf{r},t)\left(\frac{\partial}{\partial\mathbf{r}} - \frac{ie}{c}\frac{1+\sigma_z}{2}\mathcal{A}_{em}(t)\right)$$

$$\times\left(\frac{\partial}{\partial\mathbf{r}} - \frac{ie}{c}\frac{1+\sigma_z}{2}\mathcal{A}_{em}(t)\right)\psi(\mathbf{r},t). \quad (A1)$$

After expanding over $\mathcal{A}_{em}(t)$, we find the linear in $\mathcal{A}_{em}(t)$ term in the Lagrangian density

$$\Delta L = -H_{kin}$$

$$= -\frac{ie\mathcal{A}_{em}(t)}{2mc}\,\psi^{\dagger}(\mathbf{r},t)(1+\sigma_z)\frac{\partial}{\partial\mathbf{r}}\psi(\mathbf{r},t). \quad (A2)$$

The transformation (4) changes it to

$$\Delta L = -\frac{ie\mathcal{A}_{em}(t)}{2mc}\,\psi^{\dagger}(\mathbf{r},t)\left[\frac{\partial}{\partial\mathbf{r}} + \mathbf{A}(\mathbf{r})\right.$$

$$\left. + T^{\dagger}(\mathbf{r})\sigma_z T(\mathbf{r})\left(\frac{\partial}{\partial\mathbf{r}} + \mathbf{A}(\mathbf{r})\right)\right]\psi(\mathbf{r},t). \quad (A3)$$

The corresponding operator of the spin-current density can be found by variation

$$\mathbf{j}_{\uparrow} = \frac{c}{e}\frac{\delta L}{\delta\mathcal{A}_{em}(t)}, \quad (A4)$$

which gives us finally

$$\mathbf{j}_{\uparrow} = -\frac{i}{2m}\,\psi^{\dagger}(\mathbf{r},t)\left[\frac{\partial}{\partial\mathbf{r}} + \mathbf{A}(\mathbf{r})\right.$$

$$\left. + T^{\dagger}(\mathbf{r})\sigma_z T(\mathbf{r})\left(\frac{\partial}{\partial\mathbf{r}} + \mathbf{A}(\mathbf{r})\right)\right]\psi(\mathbf{r},t). \quad (A5)$$

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