

Nonlinear spin transport in a rectifying ferromagnet/semiconductor Schottky contact

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The electrical creation and detection of spin accumulation in ferromagnet/semiconductor Schottky contacts that exhibit highly nonlinear and rectifying electrical transport is evaluated. If the spin accumulation in the semiconductor is small, the expression for the spin voltage is identical to that of linear transport. However, if the spin accumulation is comparable to the characteristic energy scale that governs the degree of nonlinearity, the spin detection sensitivity and the spin voltage are notably reduced. Moreover, the nonlinearity enhances the backflow of spins into the ferromagnet and its detrimental effect on the injected spin current, and the contact resistance required to avoid backflow is larger than for linear transport. It is also shown that by virtue of the nonlinearity, a nonmagnetic metal contact can be used to electrically detect spin accumulation in a semiconductor.

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I. INTRODUCTION

The development of electronic devices and circuits that use spin to encode digital information is an attractive alternative to charge-based computing, particularly if the unique attributes of semiconductors (amplification and gating) and ferromagnets (nonvolatility) can be combined into a unified and energy-efficient computing technology. Much progress has recently been made in developing the basic building blocks of such a semiconductor spintronics technology [1–5]. Since mainstream semiconductors such as silicon and GaAs are nonmagnetic and do not possess any spin polarization in equilibrium, contacts between a ferromagnet (FM) and a semiconductor (SC) are key components. On the one hand, such junctions enable the transfer of spins from the ferromagnetic reservoir into the semiconductor and thereby the creation of a sizable (nonequilibrium) spin polarization of the carriers in the semiconductor. Equally important, a ferromagnetic contact can probe the spin polarization in a semiconductor and convert it into a detectable signal.

In order to efficiently inject spins from a ferromagnetic metal into a semiconductor, an interfacial energy barrier with a sufficiently large resistance times area (RA) product is needed. This interface barrier limits the backflow of the accumulated spins from the semiconductor into the ferromagnetic source and avoids the so-called conductivity mismatch that prevents spin injection from contacts with vanishingly small RA product [5,6]. Therefore, ferromagnetic contacts on semiconductors are either FM/I/SC structures, where I is a thin tunnel insulator, or direct FM/SC contacts in which the Schottky barrier formed at the metal/SC interface provides the energy barrier. In the latter case one normally employs a semiconductor with a heavily doped surface region [7] or a δ -doping layer [8] near the surface in order to obtain a Schottky barrier with a narrow depletion region and an appropriate RA product.

Hitherto, it has been common practice to compare the experimental spin signals for such structures to the theory previously developed for spin injection from a ferromagnetic metal into a nonmagnetic metal [9–13], which starts from a linear current-voltage relation. While this is appropriate for metallic junctions, it does not capture the features that are specific for semiconductor junctions. These include the

energy band profile in the semiconductor and the associated energy barrier (Schottky barrier), the localized states formed at the I/SC interface, as well as nonlinear, rectifying, and/or thermally activated transport. To better describe the experimental results for magnetic tunnel devices on semiconductors, some of these aspects have been examined [14–21]. Notably, for FM/SC Schottky contacts it was described [14] how spin transport is changed due to the subsurface potential well that is formed in the semiconductor due to the doping profile (heavily doped surface layer on a substrate with lower doping density). For FM/I/SC junctions, the presence of two barriers (tunnel insulator and Schottky barrier) was shown to alter the spin detection efficiency when transport across the Schottky barrier is by thermionic emission [15]. Subsequently, spin injection by two-step tunneling via interface states near the semiconductor surface was modeled and it was elucidated that this transport process can modify spin signals in a profound way [16]. Important additions to and refinements of the latter model have also been reported [17–19].

Here we focus on the effect of nonlinearity. In most semiconductor-based devices studied so far, the transport does exhibit some degree of rectification and nonlinearity, and in some cases it is rather strong. Although the bulk of the experimental data is obtained on devices with heavily doped semiconductors (doping density in the 10^{19} cm⁻³ range) for which tunneling is expected to dominate, nonlinearity is nevertheless commonly observed. A representative result can be found in Ref. [22] for Fe/MgO/Si contacts that reveal rectification as well as a significant nonlinearity, particularly at low temperature (with the resistance changing by several orders of magnitude as the bias voltage is increased). For contacts on semiconductors with lower doping density, which are not as frequently used, transport is clearly rectifying, thermally activated, and highly nonlinear. Examples are recent experiments [23] with direct Mn₅Ge₃ Schottky contacts on moderately doped Ge (doping density of 1×10^{18} cm⁻³), and experiments with magnetic tunnel contacts on Si and Ge with even lower doping density [24,25] including the nondegenerate regime (doping density down to 10^{15} – 10^{16} cm⁻³). Since it is common practice to compare the spin signal magnitude to that predicted by models that assume perfectly linear transport, it is important to establish whether or not this is justified and under which conditions. It has been argued recently that

experimentally there is a connection between the nonlinearity of the transport and the magnitude of the spin signals and that nonlinearity produces an enhancement of the detected spin signal [22,26].

Thus, we evaluate spin transport in a direct Schottky contact between a ferromagnetic metal and a semiconductor with a homogeneous doping density. In order to examine the role of the nonlinearity of electrical transport across the interface, we choose the extreme case of transport by thermionic emission, which is highly nonlinear and produces rectifying (diode-like) current-voltage characteristics. Although it may not be the source of nonlinearity in the experiments described above, which also include contacts with an oxide insulator, thermionic emission serves as an extreme case of nonlinearity that can readily be analyzed. We present a theory to describe the electrical creation of a spin accumulation and its electrical detection via the Hanle effect. It is shown, by explicit evaluation starting from spin-dependent nonlinear transport equations, that for a rectifying Schottky diode the expressions for the spin current, spin-detection sensitivity, and detectable spin voltage signal are essentially the same as those of linear models, provided that the spin splitting $\Delta\mu$ in the SC is small compared to the energy scale E_0 that governs the degree of nonlinearity of the transport across the interface. When $\Delta\mu$ is larger and comparable to E_0 , the nonlinearity causes a reduction in the spin detection sensitivity of the contact as well as a significant enhancement of the backflow of spins into the ferromagnetic electrode as compared to linear transport. Importantly, the nonlinearity does not produce any enhancement of the detectable spin signal. We discuss our results in light of previous descriptions of the effect of the contact nonlinearity on the spin signals [22,26,27] in which the essential ratio of $\Delta\mu$ and E_0 does not appear. Finally, it is shown that the nonlinearity enables a means to electrically detect an (externally generated) spin accumulation in a semiconductor, namely by using a *rectifying* contact with a *nonmagnetic* metal electrode.

II. SUMMARY OF LINEAR SPIN TRANSPORT THEORY

Let us first briefly summarize the results of the theory previously developed for spin injection from a ferromagnetic metal into a nonmagnetic metal, which starts from a linear current-voltage relation [9–13]. The voltage across such a contact is the sum of the regular resistive contribution ($R_0 J$, with J the current density and R_0 the RA product of the contact in the absence of spin accumulation) and an additional contribution, the spin voltage, given by $P_G \Delta\mu/2$. Here P_G is the conductance spin polarization of the contact and $\Delta\mu = \mu^\uparrow - \mu^\downarrow$ is the induced spin accumulation, represented by a spin splitting between the electrochemical potentials μ^\uparrow and μ^\downarrow of the electrons with spin pointing up or down, respectively. The magnitude of $\Delta\mu$ is proportional to the density of injected spin current J_s and to the so-called spin resistance r_s of the nonmagnetic material (i.e., $\Delta\mu = 2 J_s r_s$). Experimentally, the spin voltage can be detected [4] via a measurement of the Hanle effect, in which the spin accumulation is reduced to zero by spin precession in an external transverse magnetic field. Keeping the current constant, this results in a change in the voltage across the contact equal to the spin voltage.

III. THEORY OF SPIN TRANSPORT IN A RECTIFYING CONTACT

The model we introduce to describe nonlinear spin transport starts from the expressions for electronic transport across a direct metal-semiconductor contact by thermionic emission [28]. The basic parameters are the bias voltage V , the temperature T , and the height Φ_B of the Schottky barrier. Including the spin splitting $\Delta\mu$ of the electrochemical potential in the semiconductor, the currents of majority and minority spin electrons, J^\uparrow and J^\downarrow , respectively, are

$$J^\uparrow = -J_0^\uparrow \left[\exp\left(\frac{-q(V - \frac{\Delta\mu}{2})}{E_0}\right) - 1 \right], \quad (1)$$

$$J^\downarrow = -J_0^\downarrow \left[\exp\left(\frac{-q(V + \frac{\Delta\mu}{2})}{E_0}\right) - 1 \right]. \quad (2)$$

Here, q is the electronic charge and the voltage is defined as $V = V_{sc} - V_{fm}$, with V_{fm} the potential of the ferromagnetic electrode and V_{sc} the spin-averaged potential of the semiconductor. The forward bias condition (see Fig. 1) of the contact thus corresponds to negative voltage and current density. The spin-dependent conductance of a Schottky contact with a ferromagnetic metal is included via the prefactors

$$J_0^\uparrow = \left(\frac{1 + P_G}{2}\right) A^{**} T^2 \exp\left(\frac{-q\Phi_B}{E_0}\right), \quad (3)$$

$$J_0^\downarrow = \left(\frac{1 - P_G}{2}\right) A^{**} T^2 \exp\left(\frac{-q\Phi_B}{E_0}\right). \quad (4)$$

The A^{**} is the modified Richardson's constant [28] that incorporates the finite probability of reflection at the semiconductor-ferromagnet interface, which also produces the nonzero spin polarization $P_G = (J_0^\uparrow - J_0^\downarrow)/(J_0^\uparrow + J_0^\downarrow)$ of the conductance across the contact. The parameter E_0 is a characteristic energy scale that controls the degree of nonlinearity. For pure

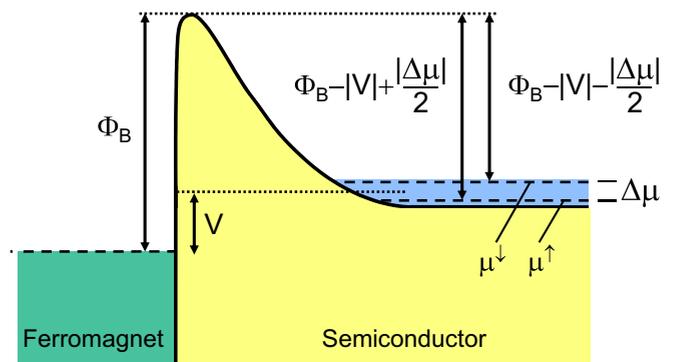


FIG. 1. (Color online) Energy band diagram for a Schottky contact of a ferromagnetic metal on a semiconductor under forward bias ($V < 0$), corresponding to extraction of spins from the semiconductor. This produces a negative spin accumulation ($\Delta\mu = \mu^\uparrow - \mu^\downarrow < 0$) in the semiconductor, as indicated, assuming that the spin polarization P_G of the conductance across the interface is positive. The energy barriers for thermionic emission from the ferromagnet to the semiconductor (Φ_B) and from the semiconductor to the ferromagnet for each spin ($\Phi_B - |V| + |\Delta\mu|/2$ and $\Phi_B - |V| - |\Delta\mu|/2$, respectively) are indicated.

thermionic emission $E_0 = kT$, with k the Boltzmann constant. When transport is nonideal, for instance, when there is also a contribution from tunneling through the Schottky barrier, the expressions have the same form, but the prefactor is different and the energy scale is changed to $E_0 = nkT$, where n is the so-called ideality factor [28]. Since $n \geq 1$ this reduces the nonlinearity. Note that a parameter E_0 that describes the degree of nonlinearity can be defined for any type of contact and transport mechanism. For transport by tunneling it is not governed by kT but expressed in terms of tunneling parameters such as the tunnel barrier height. When transport is by strictly linear tunneling, E_0 goes to infinity.

At small enough bias ($|qV| \ll E_0$) the transport approaches the linear regime without rectification. Since spin transport in the linear regime has been described previously, we shall focus here on the nonlinear regime and consider a sufficiently large forward bias such that $\exp(-qV/E_0) \gg 1$. The total charge current $J = J^\uparrow + J^\downarrow$ and the spin current $J_s = J^\uparrow - J^\downarrow$ across the contact are then

$$J = -\exp\left(\frac{-qV}{E_0}\right) \left[J_0^\uparrow \exp\left(\frac{+q\Delta\mu}{2E_0}\right) + J_0^\downarrow \exp\left(\frac{-q\Delta\mu}{2E_0}\right) \right], \quad (5)$$

$$J_s = -\exp\left(\frac{-qV}{E_0}\right) \left[J_0^\uparrow \exp\left(\frac{+q\Delta\mu}{2E_0}\right) - J_0^\downarrow \exp\left(\frac{-q\Delta\mu}{2E_0}\right) \right]. \quad (6)$$

The way the spin accumulation is incorporated into the expressions for thermionic emission deserves some attention. First, it is noted that the presence of the spin accumulation in the semiconductor does not affect the current due to thermal emission of electrons over the Schottky barrier in the direction from the ferromagnet to the semiconductor. The emission barrier height is given by the energy difference between the maximum of the barrier and the electrochemical potential of the metal, both of which do not depend on shifts of the electrochemical potential in the semiconductor (see also Fig. 1). Hence, $\Delta\mu$ does not appear in the second term between brackets in Eqs. (1) and (2), just as the voltage does not appear, for the same reasons [28]. In principle there is also a spin accumulation in the ferromagnetic metal, but it is negligibly small owing to the very fast spin relaxation in ferromagnets. Second, in the theory of thermionic emission transport [28] only the height of the Schottky barrier is relevant, not its shape. Therefore, shifts of the electrochemical potential by a spin accumulation or by a voltage are equivalent [29] and have the same effect on the thermionic emission current of electrons from the semiconductor to the ferromagnet. The corresponding barrier heights for spin up and spin down electrons under forward bias ($V < 0$ and $\Delta\mu < 0$; see also Fig. 1) are thus given by $\Phi_B + V - \Delta\mu/2$ and $\Phi_B + V + \Delta\mu/2$, respectively [first term between brackets in Eqs. (1) and (2)].

A. Spin detection sensitivity and spin current

The existence of a spin accumulation can be detected electrically because the contact resistance for forward bias

depends on the value of $\Delta\mu$ [see Eq. (5)]. The spin voltage signal $\Delta V_{\text{spin}} = V(\Delta\mu) - V(\Delta\mu = 0)$, obtained under the usual experimental condition (Hanle effect measurement with the current kept constant [4]), is given by

$$\Delta V_{\text{spin}} = \frac{E_0}{q} \ln \left[\left(\frac{1 + P_G}{2} \right) \exp\left(\frac{+q\Delta\mu}{2E_0}\right) + \left(\frac{1 - P_G}{2} \right) \exp\left(\frac{-q\Delta\mu}{2E_0}\right) \right]. \quad (7)$$

This result captures the effect of the nonlinearity: the spin voltage is not simply given by $P_G \Delta\mu/2$ and depends in a nontrivial manner on the magnitude of the spin accumulation.

In the particular regime for which $|q\Delta\mu| \ll 2E_0$ we have $\Delta V_{\text{spin}} = (E_0/q) \ln[1 + P_G(q\Delta\mu/2E_0)]$, which, using $\ln(1+x) = x$ when $|x| \ll 1$, reduces to $\Delta V_{\text{spin}} = P_G \Delta\mu/2$. This is exactly the same result as for the case of linear current-voltage characteristics. Hence, even for highly nonlinear and rectifying transport across a Schottky diode by thermionic emission, the spin detection sensitivity of the contact ($\Delta V_{\text{spin}}/\Delta\mu$) is given by the linear response result, as long as the magnitude of the induced spin splitting remains small compared to the characteristic energy scale E_0 that parametrizes the degree of nonlinearity (i.e., if $|q\Delta\mu| \ll 2E_0$). The spin detection sensitivity as a function of $|q\Delta\mu|/E_0$ is depicted in the bottom panel of Fig. 2. Indeed, for small $\Delta\mu$, the spin detection sensitivity is given by $P_G/2$. However, the spin detection sensitivity decays when the value of the spin splitting becomes large and approaches E_0 , and it even changes sign if the spin splitting becomes much larger than E_0 . These two features are not obtained in linear transport models, for which the spin detection sensitivity does not depend on the magnitude of the spin accumulation. We emphasize that the change of the spin detection sensitivity is a consequence of the nonlinearity of the transport; i.e., it is not related to the backflow of spins into the ferromagnet (see below). The nonlinearity will also cause the Hanle line shape to deviate from the typical Lorentzian variation as a function of magnetic field, because the spin detection sensitivity changes as the spin accumulation is reduced. This aspect is not explored any further here. It is also noteworthy that for reverse bias ($V > 0$), the spin detection sensitivity goes to zero, since the reverse bias current is dominated by emission from the ferromagnet to the semiconductor, which does not depend on $\Delta\mu$, as already mentioned.

Next, we evaluate the spin current density. From Eqs. (5) and (6) we obtain

$$J_s = J \left[\frac{J_0^\uparrow \exp\left(\frac{+q\Delta\mu}{2E_0}\right) - J_0^\downarrow \exp\left(\frac{-q\Delta\mu}{2E_0}\right)}{J_0^\uparrow \exp\left(\frac{+q\Delta\mu}{2E_0}\right) + J_0^\downarrow \exp\left(\frac{-q\Delta\mu}{2E_0}\right)} \right]. \quad (8)$$

In the limit $|q\Delta\mu| \ll 2E_0$ the spin current becomes

$$J_s = J \left[\frac{P_G + \left(\frac{q\Delta\mu}{2E_0}\right)}{1 + P_G \left(\frac{q\Delta\mu}{2E_0}\right)} \right]. \quad (9)$$

The spin current is shown as a function of $|q\Delta\mu|/E_0$ in the top panel of Fig. 2. If the spin accumulation is small, the injected spin current is simply given by $P_G J$. When the spin

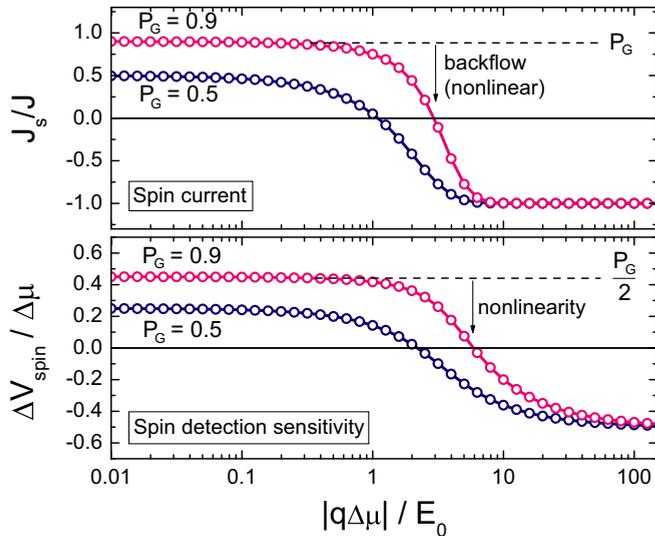


FIG. 2. (Color online) Spin current (J_s/J , top panel) and spin detection sensitivity ($\Delta V_{\text{spin}}/\Delta\mu$, bottom panel) calculated for a rectifying Schottky contact of a ferromagnetic metal and a semiconductor under sufficiently large forward bias [i.e., $\exp(-qV/E_0) \gg 1$]. Results are shown as a function of the spin splitting $q\Delta\mu$ relative to E_0 , for two different values of the conductance spin polarization P_G . Since forward bias corresponds to the extraction of spin-polarized electrons from the semiconductor and P_G was taken to be positive, the induced spin accumulation is negative, so the calculation was performed using negative values of $\Delta\mu$. The regime for which the spin current is positive is relevant when the spin accumulation is created by the contact itself; however, the regime for which the spin current is negative can only be obtained when the spin accumulation is induced by an external source. The quantities on the horizontal and vertical axis are all dimensionless.

accumulation becomes larger and larger, the spin current is no longer independent of $\Delta\mu$ and the existence of the spin accumulation reduces the injected spin current (see Fig. 2, top panel). This phenomenon can be viewed as backflow of spins into the ferromagnetic electrode. Although this is well established for linear models [9–13] the parameters that control it are different here because the backflow is nonlinear (see below).

In principle, the spin current and the spin detection sensitivity of a ferromagnetic Schottky contact can become negative due to the nonlinearity (Fig. 2). However, an external (optical or electrical) source of spins is needed to reach the regime with negative spin current and spin detection sensitivity. If the same ferromagnetic contact is used to create and detect the spin accumulation, the detected spin signal cannot change sign because the point where the spin detection sensitivity changes sign cannot be reached. At very large density of injected current the spin accumulation becomes large, but during the transient build up of the spin accumulation the injected spin current would first approach zero, and beyond this point the spin accumulation does not increase any further. This saturation happens at a value of the spin accumulation for which there is not yet a change in the sign of the spin detection sensitivity (compare the zero crossings in the bottom and top panels of Fig. 2).

B. Spin accumulation and Hanle spin signal

The steady-state spin accumulation is obtained by defining the relation between spin accumulation, injected spin current, and spin resistance r_s of the nonmagnetic material in the usual [5] way ($\Delta\mu = 2J_s r_s$). If we insert expression (8) for the spin current into this we do not obtain an analytic solution, but we can solve for $\Delta\mu$ numerically. The resulting Hanle spin signal, the so-called spin RA product $\Delta V_{\text{spin}}/J$, is shown as a function of the contact RA product in Fig. 3. At large contact resistance, the injected spin current is small and so is the induced spin accumulation. In this regime backflow is negligible and the spin RA product is equal to $P_G^2 r_s$, which is identical to the result of linear transport models. As the junction RA product is reduced below a certain value, the spin RA product decays. This is due to the backflow of spins into the ferromagnet, which becomes important for large $\Delta\mu$ as it limits the injected spin current, as already eluded to. Although this type behavior is also obtained for linear transport (see the solid black curve in Fig. 3), the point where backflow starts to become relevant is different. For linear transport, backflow is significant when the contact RA product $R_0 = V/J$ is smaller than the spin resistance r_s of the semiconductor. However, for the nonlinear transport considered here, the point where backflow sets in is shifted to contact resistances significantly larger than r_s (Fig. 3, symbols). Thus, the nonlinearity enhances the backflow and the contact resistance needed to avoid it is larger than for linear transport.

This result can be understood as follows. The backflow is due to the fact that build up of a spin accumulation reduces the spin polarization of the injected current. In a

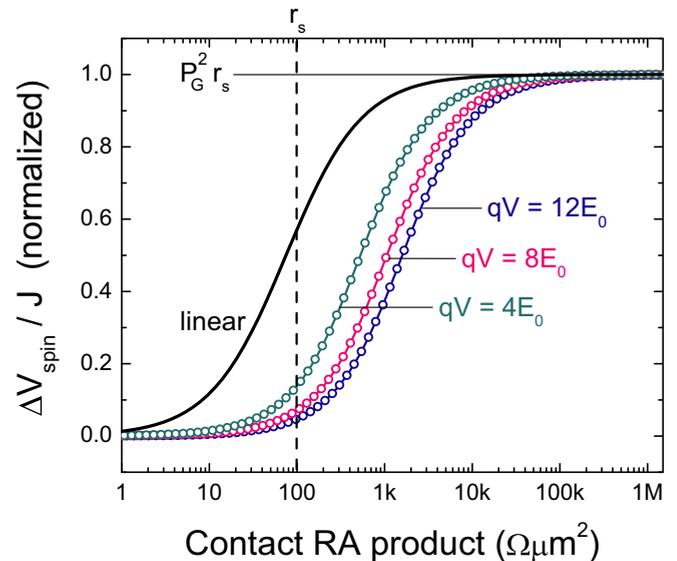


FIG. 3. (Color online) Spin RA product ($\Delta V_{\text{spin}}/J$) versus contact RA product for a rectifying Schottky contact of a ferromagnetic metal and a semiconductor under forward bias ($V < 0$). The contact resistance was varied via the Schottky barrier height Φ_B . The spin RA product is normalized to the value $P_G^2 r_s$ obtained at large contact RA product. The parameters used are $P_G = 50\%$, $r_s = 100 \Omega\mu\text{m}^2$, $T = 300 \text{ K}$, and V was varied from $-4kT/q$ to $-12kT/q$ (symbols). The black solid curve is for linear transport.

linear contact, this is solely due to the change in the number of states that can participate in the tunneling process as the electrochemical potential in the nonmagnetic electrode is shifted up or down (depending on the spin). For instance, if the majority spin is predominantly injected, the upward shift of the electrochemical potential reduces the potential drop across the contact for that spin, and thereby the current of majority spins. The opposite happens for the other spin, so that the spin polarization of the injection current is reduced. For nonlinear transport the backflow is stronger because the shifts in the electrochemical potential induce stronger changes in the current due to the nonlinearity, and thus a stronger reduction of the injected spin current. The value of $\Delta\mu$ for which backflow sets in is of the order of a mV for the parameters used here ($E_0 = kT = 25.8$ meV). These features make the nonlinearity relevant for the design of devices such as spin transistors with a FM source and drain contact, since these typically require large spin accumulation and small contact resistance to obtain a large magnetic response and high speed operation.

We can gain some additional insight by using the approximate expression (9) for the spin current in the weakly nonlinear regime, for which an analytic solution for the spin accumulation can be obtained:

$$\Delta\mu = 2 P_G J r_s \left(\frac{R_0}{R_0 + \left(\frac{-qV}{E_0}\right)r_s} \right). \quad (10)$$

The term between brackets in Eq. (10) describes the reduction of the spin accumulation due to the backflow. Whereas for linear transport this term is given by $R_0/(R_0 + r_s)$, we find that an additional factor $-qV/E_0$ appears. Since this factor is larger than unity for thermionic emission in the forward bias regime under consideration, the effective spin resistance that controls the backflow is a factor of $-qV/E_0$ larger than r_s .

C. Spin detection with a nonmagnetic contact

A noteworthy aspect is that for a contact with a nonmagnetic metal ($P_G = 0$), the spin current injected into the semiconductor is zero, but the spin-detection sensitivity is not (see Fig. 4). This is readily understood. If transport across the contact is nonlinear, then the change in current induced by raising the electrochemical potential by $\Delta\mu/2$ for one spin direction is not compensated by the change in current due to the lowering of the electrochemical potential by $\Delta\mu/2$ for the other spin. The presence of a spin accumulation thus changes the total charge current across the contact. Hence, a nonmagnetic contact with strongly nonlinear transport can be used to electrically detect a spin accumulation (created by some external means, such as optically, or electrically from a nearby ferromagnetic injector). Note, however, that for a nonmagnetic contact the sign of the spin voltage ΔV_{spin} does not depend on the sign of $\Delta\mu$, but is solely determined by the sign of the nonlinearity (i.e., by the sign of the second derivative $\partial^2 J/\partial V^2$). Also note that what we consider here is exclusively due to the nonlinearity of the transport *across* the detector contact interface. It should be distinguished from effects due to the nonlinearity of the transport *within the nonmagnetic channel*, which in the presence of a spin accumulation has been shown to lead to charge voltages that can be detected by a contact with a nonmagnetic electrode

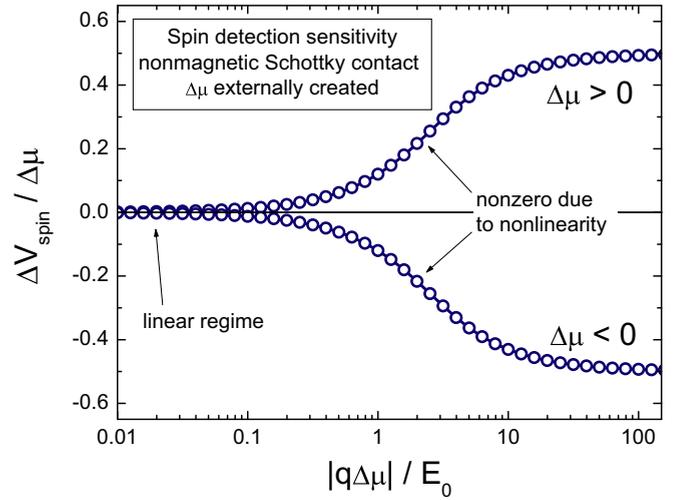


FIG. 4. (Color online) Spin detection sensitivity ($\Delta V_{\text{spin}}/\Delta\mu$) calculated for a rectifying Schottky contact of a *nonmagnetic* metal and a semiconductor under forward bias ($V < 0$). The result is shown as a function of the spin splitting relative to E_0 , for $P_G = 0$. The spin accumulation is created by an external source and can be positive or negative, which yields opposite signs of the spin detection sensitivity, but note that the sign of the spin voltage ΔV_{spin} is always positive. The quantities on the horizontal and vertical axis are dimensionless.

[30,31]. This does not require nor rely on nonlinear transport across the interface between the channel and the nonmagnetic electrode. Similarly, the detection method we propose here does not require or rely on nonlinearity of the transport within the nonmagnetic channel.

IV. DISCUSSION

Let us compare our results to previous works [22,26,27] that consider the effect of the nonlinearity on the spin signals. Those previous descriptions do not include the ratio of $\Delta\mu$ and E_0 and thus do not capture the associated physics. When $\Delta\mu$ is small, the transport parameters are essentially constant in the energy window defined by the spin accumulation, and this feature must be reflected in the description of the effect of the nonlinearity on the spin signals. Another notable feature of previous works [22,26] is the appearance of a multiplicative factor $(\partial V/\partial J)/(V/J)$ in the expression for the spin voltage [22,26], suggesting that spin signal enhancement occurs if the differential resistance is larger than the regular resistance V/J . Our results show that the effect of nonlinearity on the magnitude of the spin signal in general cannot be described by including this multiplicative factor (see also the Appendix). In our explicit evaluation the ratio of differential resistance and resistance does not appear, even though the transport by thermionic emission is highly nonlinear and rectifying [32]. Perhaps most strikingly, for reverse bias the $\partial V/\partial J$ is much larger than V/J , but the spin signal is not enhanced, and in fact, the spin detection sensitivity goes to zero at reverse bias, as already noted in Sec. III A. Another example that shows that the magnitude of the spin signal does not track $(\partial V/\partial J)/(V/J)$ is an Esaki diode. In the

regime of negative differential resistance the Fermi level of the n-type semiconductor is aligned with the band gap of the other (p-type) semiconductor. Creating a spin splitting in the n-type semiconductor does not change the current because states around the Fermi energy of the n-type electrode do not contribute to the current. Hence, the spin detection sensitivity is zero. The differential resistance, however, is not zero. Hence, care should be taken not to use the ratio of $(\partial V/\partial J)$ and (V/J) in order to judge whether or not the spin-detection sensitivity deviates from the linear result.

Let us finally discuss whether the transport nonlinearity can enhance the detectable spin signal and thereby explain the results of experiments on spin transport in FM/I/SC tunnel devices. For various semiconductors (GaAs [16], Si [4,5,24,33–36], Ge [25,37–43] as well as oxide semiconductors [44–46]) these devices exhibit Hanle spin signals that are orders of magnitude larger than what is expected from the theory previously developed for spin injection into nonmagnetic metals [9–13]. To explain the discrepancy, the role of localized states in the tunnel oxide or at its interface with the semiconductor has been considered [16–18,35,47,48]. In particular, spin transport by two-step tunneling via localized interface states was modeled and predicted to yield greatly enhanced spin signals due to spin accumulation in those interface states [16]. Because the predictions of this model were shown to be inconsistent with experiments [5,33,36], extended versions [18,19,48] of the two-step tunneling model [16] have recently been developed. Nevertheless, some of the predictions of those extended models [18,48] are also in disagreement with experiments on electrical spin injection [49] and thermal spin injection by Seebeck spin tunneling in similar FM/I/SC structures [50–53]. The origin of the large spin signals and whether localized states play a role is thus still unclear. With this in mind, a recent experiment [23] has focused on a direct Schottky contact of a metallic ferromagnet (Mn_5Ge_3) and a semiconductor (Ge), in which the absence of a tunnel oxide eliminates all sources of spin signal enhancement that rely explicitly on localized states associated with the oxide [16–18,35,47,48]. Nevertheless, the observed spin signals [23], that have all the characteristic features of spin accumulation and spin precession due to the Hanle effect, were found to be up to 4 orders of magnitude larger than predicted by linear transport models [9–13]. Since the studied Mn_5Ge_3 /Schottky contacts exhibited highly rectifying current-voltage characteristics, the question arises whether the nonlinear transport can affect the spin signal magnitude. Indeed, in some previous reports it was argued that spin signals might be enhanced if transport is nonlinear [22,26].

Our explicit evaluation shows that a spin signal enhancement due to nonlinearity is unlikely. First of all, our results show that in the regime where nonlinearity is important ($|q\Delta\mu| > E_0$), the effect is to *reduce* the spin detection sensitivity, not to enhance it. In fact, it is straightforward to show that nonlinearity in general reduces the spin detection sensitivity because current-voltage characteristics are typically superlinear [i.e., the conductance $(\partial J/\partial V)$ increases with bias voltage]. The spin detection sensitivity is enhanced only in special cases where transport is sublinear. Second, even if nonlinearity is present, the induced spin accumulation is generally small enough to ensure that $|q\Delta\mu| \ll 2E_0$, in

which case the spin current, spin-detection sensitivity, and spin voltage signal are well described by the expressions previously derived for linear transport. For instance, for strongly rectifying transport by thermionic emission we have $E_0 = kT$, but since $|q\Delta\mu|$ is typically a fraction of a meV in experiments conducted so far, the condition $|q\Delta\mu| \ll 2E_0$ is satisfied at the temperatures used in the experiments. For transport with weaker rectification, the value of E_0 is larger, and the nonlinearity is even less likely to play a role. Thus, our explicit evaluation establishes that the common practice, which is to compare the spin signal magnitude to that predicted by models that assume perfectly linear transport, is justified even for semiconductor junctions that exhibit significant rectification. Nevertheless, the effect of nonlinearity might be observable for devices in which a large spin accumulation is induced in the semiconductor channel using a spin injection contact with large spin polarization and very small RA product, while a separate and highly rectifying contact is used for spin detection.

V. SUMMARY

The theory presented here serves as a basis for the interpretation of spin transport in rectifying ferromagnet/semiconductor Schottky contacts. It provides a quantitative means to assess whether nonlinear transport modifies the spin current, spin-detection efficiency, and detectable spin voltage. The theory highlights the role of the magnitude of the induced spin splitting relative to the energy scale that parametrizes the degree of nonlinearity. Even for semiconductor junctions that exhibit significant rectification and nonlinearity, the spin accumulation is generally small enough for it to be justified to compare the spin signal magnitude to that predicted by models that assume perfectly linear transport. If the spin accumulation is large enough, the nonlinearity is important, but it does not enhance the spin voltage. Rather, it reduces the spin-detection sensitivity. It also enhances the backflow of spins into the ferromagnetic injector and its detrimental effect on the injected spin current. In order to suppress the backflow, one needs a larger contact resistance than what is deduced from linear transport models. It was also shown that the nonlinearity enables a means to detect a spin accumulation in a semiconductor, using a nonlinear contact with a nonmagnetic metal electrode.

APPENDIX: EFFECT OF NONLINEAR CONDUCTANCE ON SPIN-DETECTION SENSITIVITY

In this appendix we discuss how the nonlinear conductance of a ferromagnetic contact affects its spin-detection sensitivity, and in particular we examine whether or not the spin-detection sensitivity is modified by a factor $(\partial V/\partial J)/(V/J)$, as argued in previous works [22,26]. It is shown here that this multiplicative factor appears as a result of the (incorrect) assumption that the nonlinearity does not result in a change of the conductance when a spin accumulation is induced, but only when the bias voltage changes.

In order to illustrate this, we consider transport that, to first order, is linear in the voltage V and incorporate the nonlinearity by using a conductance $G(V, \Delta\mu)$ that is a function of the

bias voltage *and* the spin accumulation. In the absence of a spin accumulation the voltage across the contact is V_0 and the currents for each spin are simply given by

$$J^\uparrow = G_0 \left(\frac{1 + P_G}{2} \right) V_0, \quad (\text{A1})$$

$$J^\downarrow = G_0 \left(\frac{1 - P_G}{2} \right) V_0, \quad (\text{A2})$$

where the G_0 denotes the conductance for $V = V_0$ and $\Delta\mu = 0$. The total current J is then $G_0 V_0$. In the presence of a nonzero spin accumulation, the voltage changes by an amount ΔV in order to keep the total current unchanged, and the currents become

$$J^\uparrow = G(V, \Delta\mu) \left(\frac{1 + P_G}{2} \right) \left(V_0 + \Delta V + \frac{\Delta\mu}{2} \right), \quad (\text{A3})$$

$$J^\downarrow = G(V, \Delta\mu) \left(\frac{1 - P_G}{2} \right) \left(V_0 + \Delta V - \frac{\Delta\mu}{2} \right). \quad (\text{A4})$$

Importantly, the conductance $G(V, \Delta\mu)$ deviates from G_0 not only because the voltage has changed by ΔV , but also because the electrochemical potential in the nonmagnetic electrode is shifted by $\Delta\mu/2$ with respect to the average electrochemical potential (either up or down, depending on the spin orientation). In general ΔV and $\Delta\mu$ are small compared to V_0 , so that we can write

$$J^\uparrow = \left(G_0 + \frac{\partial G}{\partial V} \Delta V + \frac{\partial G}{\partial \mu} \frac{\Delta\mu}{2} \right) \left(\frac{1 + P_G}{2} \right) \times \left(V_0 + \Delta V + \frac{\Delta\mu}{2} \right), \quad (\text{A5})$$

$$J^\downarrow = \left(G_0 + \frac{\partial G}{\partial V} \Delta V - \frac{\partial G}{\partial \mu} \frac{\Delta\mu}{2} \right) \left(\frac{1 - P_G}{2} \right) \times \left(V_0 + \Delta V - \frac{\Delta\mu}{2} \right). \quad (\text{A6})$$

From the requirement that the total current with and without spin accumulation is the same and equal to $G_0 V_0$, and neglecting higher order terms proportional to $(\Delta V)^2$, $(\Delta\mu)^2$, or $\Delta V \Delta\mu$, we obtain the voltage change ΔV as

$$\Delta V = \left(\frac{P}{2} \right) \Delta\mu \left[\frac{G_0 + \left(\frac{\partial G}{\partial \mu} \right) V_0}{G_0 + \left(\frac{\partial G}{\partial V} \right) V_0} \right]. \quad (\text{A7})$$

The extra factor between the straight brackets represents the modification of the spin-detection sensitivity due to the nonlinearity of the transport across the contact. In order to obtain the change in the spin-detection sensitivity, one thus needs to evaluate the derivatives $\partial G/\partial V$ and $\partial G/\partial \mu$, which depend on the particulars of the transport across the contact. It is instructive to consider the spin-detection sensitivity for two limiting cases:

If $\partial G/\partial \mu = 0$, then

$$\frac{\Delta V}{\Delta\mu} = \left(\frac{P}{2} \right) \left[\frac{G_0}{G_0 + \left(\frac{\partial G}{\partial V} \right) V_0} \right] = \left(\frac{P}{2} \right) \left[\frac{\partial V/\partial J}{V/J} \right]. \quad (\text{A8})$$

If $\partial G/\partial \mu = \partial G/\partial V$, then

$$\frac{\Delta V}{\Delta\mu} = \left(\frac{P}{2} \right). \quad (\text{A9})$$

We thus find that the multiplicative factor of $(\partial V/\partial J)/(V/J)$ discussed in previous works [22,26] appears as a consequence of setting $\partial G/\partial \mu$ to zero. In general this is not justified and $\partial G/\partial V$ as well as $\partial G/\partial \mu$ are nonzero. For instance, a change in voltage across an oxide tunnel barrier will change the energy of the tunneling electrons with respect to the maximum of the potential barrier and thereby changes the tunnel conductance. However, when a spin accumulation is created, the associated shifts of the electrochemical potential (up or down depending on the spin) also change the energy of the tunneling electrons with respect to the barrier maximum and thus the conductance. Similar statements can be made for tunneling through a Schottky barrier, where the effective width and height of the barrier change upon application of a voltage but also upon creation of a spin accumulation. While this does not mean that $\partial G/\partial V$ and $\partial G/\partial \mu$ are identical, the nonzero $\partial G/\partial \mu$ counterbalances the effect of the nonzero $\partial G/\partial V$. This removes most of the multiplicative factor $(\partial V/\partial J)/(V/J)$ and yields a spin-detection sensitivity that, despite the nonlinearity, is close to the result $\Delta V/\Delta\mu = P/2$ obtained for linear transport.

Note that the above analysis applies to systems in which transport to first order is linear, such as tunneling transport. For thermionic emission over an energy barrier, as discussed in the main text, the transport equations are different, and this needs to be considered when evaluating the spin-detection sensitivity [29].

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