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Universal spin-polarization fluctuations in one-dimensional wires with magnetic impurities

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We study conductance and spin-polarization fluctuations in one-dimensional wires with spin-5/2 magnetic impurities (Mn). Our tight-binding Green function approach goes beyond the mean field thus including *s-d* exchange-induced spin-flip scattering. In a certain parameter range, we find that spin-flip suppresses conductance fluctuations while enhancing spin-polarization fluctuations. More importantly, spin-polarization fluctuations attain a *universal value* 1/3 for large enough spin-flip strengths. This intrinsic spin-polarization fluctuation may pose a severe limiting factor to the realization of steady spin-polarized currents in Mn-based one-dimensional wires.

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I. INTRODUCTION

Spin-related effects in solid state heterostructures give rise to a rich variety of fascinating physical phenomena. These spin-dependent properties also underlie a potential technological revolution in conventional electronics.[1] This paradigm is termed "Spintronics." A particularly interesting theme within this emerging field is spin-polarized transport in semiconductor heterostructures. This topic has attracted much attention after the fundamental discovery of exceedingly long spin diffusion lengths in doped semiconductors[2] followed by the seminal spin injection experiments in Mn-based heterojunctions.[3]

Theoretically, a number of works have addressed issues connected with spin-polarized transport. These include, for instance: spin filtering,[4] spin waves,[5] and quantum shot noise,[6]—all in ballistic semimagnetic tunnel junctions—and mesoscopic conductance fluctuations in Rashba wires.[7] Spin-dependent phenomena in connection with localization effects should bring about exciting interesting physics.

Here we investigate conductance *and* spin-polarization fluctuations for transport through one-dimensional wires with spin-5/2 magnetic impurities, e.g., Mn-based II-VI alloys such as ZnSe/ZnMnSe/ZnSe. The experimental feasibility of these wires has already been demonstrated.[8,9] In these systems, the conduction electrons interact with the localized *d* electrons of the Manganese via the *s-d* exchange coupling.[10] UCF in Mn-based submicron wires was first experimentally studied in Ref. 8. We describe transport within the Landauer formalism[11] and calculate the relevant transmission coefficients via noninteracting tight-binding Green functions.[12]

We treat the *s-d* interaction beyond the usual mean-field theory thus accounting for spin flip scattering. In a certain parameter range we find that spin-flip scattering suppresses conductance fluctuations[13] (below the UCF value for strictly one-dimensional wires) while enhancing the corresponding spin-polarization fluctuations. More importantly, we show that the spin-polarization fluctuations attain a *universal value* $\langle(\delta\zeta)^2\rangle = 1/3$ for strong spin-flip scattering. This large spin-polarization fluctuation may pose a fundamental obstacle to attaining steady spin-polarized currents in Mn-based wires.

II. HAMILTONIAN MODEL

We consider a one-dimensional tight-binding chain (see Fig. 1), of N spin $s=5/2$ magnetic impurities coupled to ideal leads (sites $n<1$ and $n>N$). We separate the electronic and impurity-spin degrees of freedom and treat the latter classically (static scatterers). The two-component electron wave function, $\psi=(\psi_\uparrow,\psi_\downarrow)$ is then governed by the Schrödinger equation with a Hamiltonian

$$\mathbf{H}=\begin{pmatrix}\mathbf{H}_0 & \mathbf{0}\\ \mathbf{0} & \mathbf{H}_0\end{pmatrix}+\begin{pmatrix}\mathbf{H}_{\uparrow\uparrow} & \mathbf{H}_{\uparrow\downarrow}\\ \mathbf{H}_{\downarrow\uparrow} & \mathbf{H}_{\downarrow\downarrow}\end{pmatrix}. \tag{1}$$

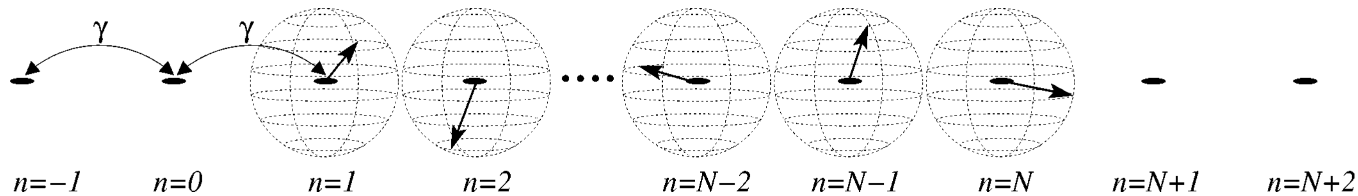

FIG. 1. One-dimensional tight-binding chain with N magnetic $s=5/2$ impurities (mutually uncorrelated, each spin equally distributed among the six spin states) coupled to ideal impurity-free leads (sites $n<1$ and $n>N$).

Here $\mathbf{H}_0$ is spin independent, with elements[12]

$$\{\mathbf{H}_0\}_{nm} = 2\gamma\delta_{nm} - \gamma\delta_{nm+1} - \gamma\delta_{nm-1} + V_n\delta_{nm}, \qquad (2)$$

where V_n is the potential at site n and $\gamma = \hbar^2/2ma^2$, with a being the "lattice constant." In the leads $\mathbf{H}_0$ itself gives rise to the usual dispersion relation $\varepsilon(k) = 2\gamma(1-\cos ka)$.

In the following, $\sigma = \uparrow \equiv 1/2$ and $\sigma = \downarrow \equiv -1/2$. We restrict ourselves to zero magnetic field so that the block matrices $\mathbf{H}_{\sigma\sigma}$ have elements given by

$$\{\mathbf{H}_{\sigma\sigma}\}_{nm} = \delta_{nm} J_z \sigma S_{n,z} \qquad (3)$$

which is a Heisenberg-like interaction of the spin of the electron (σ) with the z-component spin of the impurity $S = (S_x, S_y, S_z)$. The off-diagonal block matrix $\mathbf{H}_{\uparrow\downarrow} = \mathbf{H}_{\downarrow\uparrow}^\dagger$ contains the interaction of the electron spin with the x and y components of the impurity spins which leads to spin-flip:

$$\{\mathbf{H}_{\uparrow\downarrow}\}_{nm} = \delta_{nm}[J_x S_{n,x} - iJ_y S_{n,y}]/2. \qquad (4)$$

We consider a sufficiently weak coupling between the impurity spins so that they can be considered mutually uncorrelated, i.e., no magnetic ordering. The z-component of each spin is equally distributed among the six spin states and the x and y components are uniformly distributed with the constraint that $S^2 = S_x^2 + S_y^2 + S_z^2 = s(s+1)$; see Fig. 1.

III. TRANSPORT PROPERTIES

We study transport in the low-temperature linear response limit within the Landauer formalism[11]:

$$g = \frac{e^2}{h}\sum_{\sigma\sigma'} \mathbf{T}_{\sigma\sigma'}(\varepsilon_F). \qquad (5)$$

Here $\mathbf{T}$ is a 2×2 matrix with the elements $\mathbf{T}_{\sigma\sigma'}$ being the transmission probability of an electron from a state with spin σ' in one lead to a state with spin σ in the other lead. From Eq. (5) we now define the degree of spin polarization

$$\zeta \equiv \frac{I_\uparrow - I_\downarrow}{I_\uparrow + I_\downarrow} = \frac{\mathbf{T}_{\uparrow\uparrow} + \mathbf{T}_{\uparrow\downarrow} - \mathbf{T}_{\downarrow\uparrow} - \mathbf{T}_{\downarrow\downarrow}}{\mathbf{T}_{\uparrow\uparrow} + \mathbf{T}_{\uparrow\downarrow} + \mathbf{T}_{\downarrow\uparrow} + \mathbf{T}_{\downarrow\downarrow}}, \qquad (6)$$

which we will focus on in this paper.

Green function method. The transmission matrix $\mathbf{T}$ is related to the retarded Green function

$$\mathbf{G}(\varepsilon) = [\varepsilon \cdot \mathbf{1} - \tilde{\mathbf{H}} - \mathbf{\Sigma}(\varepsilon)]^{-1} \qquad (7)$$

via the Fisher-Lee relation[14]

$$\mathbf{T}_{\sigma\sigma'}(\varepsilon) = [\hbar v(\varepsilon)]^2 |\{\mathbf{G}_{\sigma\sigma'}(\varepsilon)\}_{N1}|^2, \qquad (8)$$

where $v = \hbar^{-1}\partial\varepsilon/\partial k$ is the group velocity in the leads. In Eq. (7) the $2N\times 2N$ matrix $\tilde{\mathbf{H}}$ is the Hamiltonian truncated to the N lattice sites with magnetic impurities. The effect of coupling to the leads is contained in the $2N\times 2N$ retarded self-energy matrix with elements[12]

$$\{\mathbf{\Sigma}_{\sigma\sigma'}(\varepsilon)\}_{nm} = -\gamma e^{ik(\varepsilon)a}\delta_{\sigma\sigma'}\delta_{nm}(\delta_{1n} + \delta_{Nn}). \qquad (9)$$

N=1 case. A chain with a single impurity is a simple illustrative example where analytical progress is possible. After performing the straightforward matrix inversion in Eq. (7) we find

$$\zeta(\varepsilon) = \frac{-V_1 J_z S_z}{V_1^2 + \varepsilon(4\gamma - \varepsilon) + (JS)^2}, \qquad (10)$$

where $J = (J_x, J_y, J_z)^T$. In zero magnetic field $\langle S_z\rangle = 0$ and $\langle S_z^2\rangle = 35/12$. This implies that $\langle\zeta\rangle = 0$ both with and without spin-flip, whereas the fluctuations are finite. The analytical averaging is of course complicated by the presence of S_z in the denominator, but for isotropic coupling $J_x = J_y = J_z = J_0$, we have $(JS)^2 = J_0^2 s(s+1)$ so that S_z only shows up in the numerator, i.e.,

$$\langle(\delta\zeta)^2\rangle = \frac{35}{12}\frac{V_1^2 J_0^2}{[V_1^2 + \varepsilon(4\gamma - \varepsilon) + J_0^2 s(s+1)]^2}. \qquad (11)$$

In the absence of spin-flip ($J_x = J_y = 0$) the fluctuations are enhanced due to the replacement of $s(s+1) \rightarrow S_z^2 < s(s+1)$ in the denominator (the final expression for the fluctuations is much more complicated) and this means that spin-flip will lower the fluctuations of ζ. Of course this trend is strictly valid for $N=1$, but in a limited parameter range this trend is still true for larger N values.

Finite N case. For a finite number of impurities the problem is not analytically tractable and we study the problem numerically by generating a large ensemble (typically 10^5 members) of spin configurations. For each spin configuration we calculate Eqs. (7) and (8) numerically. In our simulations we use the following parameters: $\varepsilon_F = \gamma$, $J_z = \gamma/2$, $V_n = 0$ (i.e., we neglect *spatial disorder*), and varying spin-flip coupling strengths $0 \leq J_x = J_y \leq \gamma$.

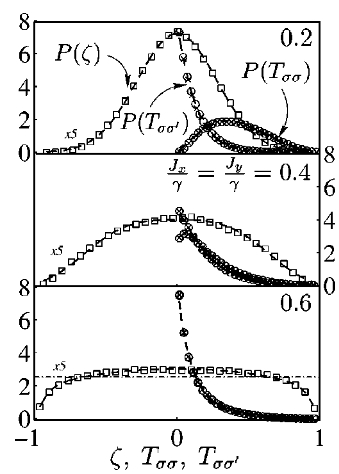

FIG. 2. Distributions $P(\zeta)$, $P(T_{\sigma\sigma})$, and $P(T_{\sigma\sigma'})$ for different spin-flip scattering strengths $J_x = J_y$ in the case of $N=10$. The dash-dotted line in the lowest panel indicates the uniform limit $P(\zeta) = 1/2$ [note the magnification of $P(\zeta)$ by of factor of 5] attained for strong enough spin-flip scattering.

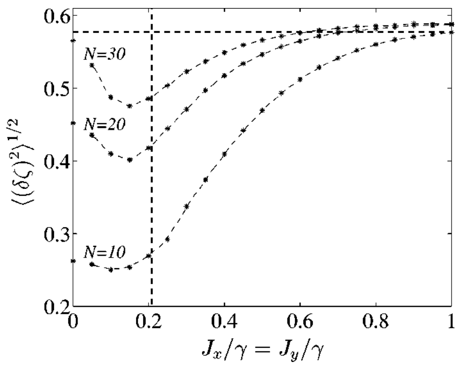

FIG. 3. Average fluctuations $\langle(\delta\zeta)^2\rangle^{1/2}$ as a function of spin-flip strength for $N=10$, 20, and 30. The dashed horizontal line indicates the universal value $1/\sqrt{3}$ obtained from the uniform limit $P(\zeta)=1/2$. The vertical dashed line indicates where the spin-flip rate is comparable to $|J_z\sigma|/\hbar$.

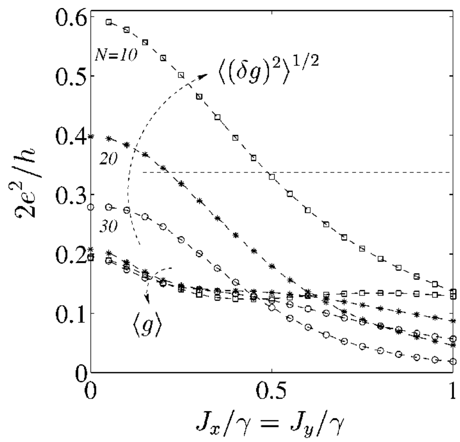

FIG. 4. Average conductance $\langle g\rangle$ and its fluctuations $\langle(\delta g)^2\rangle^{1/2}$ as a function of the spin-flip scattering strength for $N=10$, 20, and 30. The conductance fluctuations are much more sensitive to spin-flip than the average conductance: the former is strongly suppressed for increasing spin-flip rates.

IV. RESULTS AND DISCUSSIONS

Figure 2 shows the distributions $P(\zeta)$, $P(T_{\sigma\sigma})$, and $P(T_{\sigma\sigma'})$ for $N=10$ and increasing strengths of the spin-flip coupling $J_x=J_y$. The distribution $P(\zeta)$ is symmetric around $\zeta=0$, which implies that on average there is no spin filtering, $\langle\zeta\rangle=0$. The distribution $P(\zeta)$ first gets narrower for spin-flip in the $[0,0.15\gamma]$ range (not shown) and then broadens as spin-flip further increases. For sufficiently strong spin-flip scattering the distribution approaches that of the uniform limit in which $P(\zeta)=1/2$. In this limit $P(T_{\sigma\sigma})$ and $P(T_{\sigma\sigma'})$ coincide, and so do all average transmission probabilities $\langle T_{\sigma\sigma'}\rangle$. As we discuss below, the initial narrowing and subsequent broadening of $P(\zeta)$ with spin flip gives rise to a minimum in the fluctuation of ζ (Fig. 3).

Universal spin-polarization fluctuations. In the limit of a short spin-flip length $\ell_\sigma \ll L$ we in general find a uniform distribution $P(\zeta)=1/2$ (Fig. 2). This uniform distribution yields the universal value $\langle(\delta\zeta)^2\rangle=1/3$ for the spin-polarization fluctuations. Figure 3 clearly shows that this universal value is attained for increasing spin flip strengths and is indeed independent of *N*. Interestingly, Fig. 3 also shows a minimum at around $J_x=J_y=0.15\gamma$. This minimum can be attributed to two competing energy scales: the longitudinal ($\sim J_z$) and the transverse ($\sim J_x,J_y$) parts of the *s-d* exchange interaction [Eqs. (3) and (4), respectively]. A simple ''back-of-the-envelope'' calculation shows that these two competing scales are equal for $J_x=J_y=J_z/\sqrt{2s(s+1)/3}\gamma=0.208\gamma$. The vertical dashed line in Fig. 3 indicates this value. Observe that $\langle(\delta\zeta)^2\rangle$ becomes larger for increasing *N*. This happens because $P(\zeta)$ broadens for larger *N*'s (the traversing electrons see a wider region with random spins). This is similar to the broadening due to increasing spin flip strength.

We should mention that the distribution $P(\zeta)$, and consequently $\langle(\delta\zeta)^2\rangle$, change dramatically for $\varepsilon_F<J_z$. In this regime, $P(\zeta)$ becomes U shaped (not shown) because of the dominant filtering due to the ''end states'' with $S_{j,z}=\pm 5/2$. This *qualitatively* different $P(\zeta)$ yields a monotonically decreasing $\langle(\delta\zeta)^2\rangle$ as a function of spin-flip strength. Here the universal $\langle(\delta\zeta)^2\rangle=1/3$ value is approached from above for large spin-flip strengths ($J_x=J_y\sim\gamma$).

Suppression of conductance fluctuations. Whereas the fluctuations in the spin polarization ζ remain finite in the strong spin-flip scattering regime (Fig. 3), we find that the fluctuations of the conductance *g* are strongly suppressed in this limit. This is illustrated in Fig. 4 which shows the average conductance and its fluctuations as a function of spin-flip scattering for $N=10$, 20, and 30. Note that $\langle(\delta g)^2\rangle^{1/2}$ is much more sensitive to spin-flip than $\langle g\rangle$. In addition, for all *N* we essentially have $\langle(\delta g)^2\rangle^{1/2}>\langle g\rangle$ for $J_x=J_y\to 0$ and $\langle(\delta g)^2\rangle^{1/2}\lesssim\langle g\rangle$ for $J_x=J_y\to\gamma$. Figure 4 clearly shows the conductance fluctuations get suppressed for increasing *N*. The horizontal dashed line shows the UCF value $(0.73/2=0.365$, see, e.g., Ref. 15) for a one-dimensional wire in the metallic regime. The spin-related *conductance* fluctuations do not approach a finite value for increasing spin-flip scattering. It actually seems to go to zero. This is in contrast to the *spin-polarization* fluctuations (Fig. 3), which attain a universal value $\langle(\delta\xi)^2\rangle^{1/2}=1/\sqrt{3}$ for strong spin-flip scattering. Incidentally, we observe that $\langle(\delta g)^2\rangle^{1/2}$ and $\langle(\delta\zeta)^2\rangle^{1/2}$ also present contrasting behavior for increasing *N* (and $\varepsilon_F>J_z$): the former is suppressed while the latter is enhanced (cf. Figs. 3 and 4).

Spin disorder as spatial disorder. To some extent, the *s-d* site interaction considered here plays the role of spatial disorder in the system with a mean free path ℓ_J. Let us consider first the case with no spin-flip (i.e., $J_x=J_y=0$). In this case, the term $J_z\sigma S_{n,z}$ acts as a ''random'' spin-dependent potential along the chain (here the site potential has some internal structure). As shown in Fig. 4 the conductance fluctuations for zero spin-flip scattering are larger than, slightly above, and slightly below, the UCF value for $N=10$, 20, and 30, respectively. For increasing *N* we go from the metallic regime ($L=Na\ll\ell_{J_z}$) with vanishing fluctuations and a Gaussian $P(g)$ strongly peaked near $g\sim 2e^2/h$ to the strongly localized regime ($L\gg\ell_{J_z}$) where it is well known that $P(g)$ is strongly peaked near $g\sim 0$ with a log-normal distribution so that fluctuations can be comparable to the mean value.[16] This is in accordance with numerical studies with different continuous distributions of the ''on-site'' potential (e.g., Gaussian or uniform distributions).[17] In Fig. 4 the ''small'' mean values $\langle g\rangle$, for $N=10, 20$, and 30, indicate the onset of localization with fluctuations comparable to the mean value. As N becomes larger conductance fluctuations are as expected suppressed.[16,18]

Role of spin-flip scattering. Spin-flip clearly suppresses conductance fluctuations (Fig. 4). This can be understood from Eq. (4) being a *complex* number with a random phase which makes spin-flip act as a source of ''decoherence'' (the total wave function is, of course, fully coherent). Furthermore, spin-flip mixes all the $S_{n,z}$ components on each site thus smoothing the potential seen by the traversing electron and hence reducing conductance fluctuations. This is true for both $\varepsilon_F > J_z$ [except for the window $(0,0.15\gamma)$ in which $P(\zeta)$ narrows] and $\varepsilon_F < J_z$.

''Truly'' universal fluctuations. Why is $\langle(\delta\zeta)^2\rangle^{1/2}$ universal even for short spin-flip lengths $\ell_\sigma \ll L$ (strong spin-flip scattering) while $\langle(\delta g)^2\rangle^{1/2}$ is clearly suppressed below the usual UCF value in this limit? It is well known that conductance fluctuations are suppressed in the incoherent limit.[15] More specifically, in one-dimensional wires with $\ell_\varphi \ll L$, ℓ_φ is some ''dephasing length,'' the suppression factor is $\sqrt{L/\ell_\varphi}$ (see Ref. 12). Interestingly, we can likewise understand the suppression of $\langle(\delta g)^2\rangle^{1/2}$ seen in our simulations by viewing spin-flip scattering as producing ''dephasing'' with $\ell_\varphi \sim \ell_{J_{x,y}}$.[19] For the spin-polarization fluctuations, however, the picture is slightly different: here we divide our system into $N_L = L/l_\varphi$ segments. To each of these we can associate an average spin polarization $\langle\zeta_i\rangle = 0\,(i{:}1..N_L)$ and a corresponding spin-polarization fluctuation $\langle(\delta\zeta_i)^2\rangle$. Neither $\langle\zeta_i\rangle$ nor $\langle(\delta\zeta_i)^2\rangle$ are additive quantities like $\langle g\rangle$ and $\langle(\delta g)^2\rangle$ (''extensive versus intensive'' properties). Sensible *global* averages for the whole system are then $\overline{\zeta} \equiv (1/N_L)\Sigma_i\langle\zeta_i\rangle = 0$ and $\overline{(\delta\zeta)^2} \equiv (1/N_L)\Sigma_i\langle(\delta\zeta_i)^2\rangle$. We should expect $\overline{(\delta\zeta)^2} = \langle(\delta\zeta_i)^2\rangle \equiv \langle(\delta\zeta)^2\rangle$ if the system is *ergodic*. Hence universal spin-polarization fluctuations are not suppressed for large spin-flip scattering in contrast to conductance fluctuations.

IV. CONCLUDING REMARKS

Spin-flip scattering in Mn-based wires reduces conductance fluctuations while enhancing spin-polarization fluctuations in a limited parameter range. Remarkably, spin-polarization fluctuations reach a universal value 1/3 for large spin-flip scattering in which the conductance fluctuations vanish. This universal value should manifest itself in time- and polarization-resolved photoluminescence measurements. More important, these sizable spin fluctuations may limit the possibilities for steady spin injection in these systems.

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