Spin dynamics of hopping electrons in quantum wires: Algebraic decay and noise

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We study theoretically the spin decoherence and intrinsic spin noise in semiconductor quantum wires caused by an interplay of electrons hopping between the localized states and the hyperfine interaction of electron and nuclear spins. At a sufficiently low density of localization sites the hopping rates have an exponentially broad distribution. It allows the description of the spin dynamics in terms of closely situated "pairs" of sites and single "reaching" states, from which the series of hops result in electrons localized inside a "pair." The developed analytical model and numerical simulations demonstrate disorder-dependent algebraic tails in the spin decay and power-law singularities features in the low-frequency part of the spin-noise spectrum.

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I. INTRODUCTION

Recent progress in semiconductor nanotechnology and the demand for new hardware elements in prospective quantum technology devices has caused a strong interest in one-dimensional solid-state systems, such as semiconductor nanowires and nanowire-based heterostuctures. There are at least two main reasons for this interest. The first reason is related to the abilities to produce and controllably manipulate electron spin qubits in InSb and InAs nanowires [1,2] and superconductor-semiconductor-nanowire hybrids [3]. The second reason is that, InSb nanowires, due to strong spin-orbit coupling, are important as the hosts of edge Majorana states in such hybrid structures [4–7]. These states, which are of a fundamental interest for quantum theory, are thought to be promising for quantum computation applications as well. Disorder in the nanowires can play a crucial role in the physics of qubits and Majorana states [8], and a variety of disorder regimes, dependent on the growth procedure and doping, is possible [9]. On the other hand, one-dimensionality leads to a strong localization of carriers, and insights into the properties of localized electron states are needed to understand these systems. In addition to spin-orbit coupling, which can be reduced by choosing an appropriate nanowire realization and geometry, III-V semiconductors show a strong hyperfine interaction that is a source of the spin dephasing of localized electrons [10,11]. At a finite temperature, electrons can hop between different sites, and therefore experience randomly fluctuating hyperfine fields. Therefore, the hopping leads to spin relaxation and thus results in a spin noise. Recently, spin-noise spectroscopy experiments [12–14] have made it possible to access information about new regimes of spin dynamics, including a very long-time evolution of electrons and nuclei [15–17]. The width of the spin-noise spectrum is related to the relaxation rate and the spectrum features seen as deviations from the Lorentzian shape can reveal various non-Markovian memory effects [18].

Here, we address the spin relaxation and spin noise in semiconductor quantum wires due to random hyperfine coupling induced by electron hopping between localized states. This disorder-determined relaxation is long and strongly nonexponential. The understanding of this spin relaxation mechanism can be valuable for the analysis of charge and spin transport in semiconductor nanowires and related hybrid structures.

II. MODEL

We consider a nanowire where the electrons are localized at single donors or fluctuations of the wire width. The density of localization sites n and the localization length a satisfy the condition

$$na \ll 1, \tag{1}$$

meaning a weak overlap of the wave functions (Fig. 1). Electrons hop between the sites with the aid of acoustic phonons. At each localization site i the electron spin experiences a random static effective magnetic field with the precession frequency $\mathbf{\Omega}_i$. These frequencies are uncorrelated and isotropically distributed, $\langle \Omega_{i,\alpha} \Omega_{j,\beta} \rangle = \delta_{ij}\delta_{\alpha\beta}\Omega_0^2/3$, where $\alpha,\beta = x,y,z$ enumerate Cartesian components, and the distribution of precession frequencies at a given site is Gaussian with the root mean square of Ω_0 [10,19,20]. Under the condition (1) the electron spin density matrix can be parametrized by the average occupancies N_i and spins $\boldsymbol{S}_i$ at the sites. Here we consider a small electron concentration $N_i \ll 1$, neglect electron-electron interactions, and assume that each site is either empty or singly occupied [21]. The spin dynamics can be described by the kinetic equations [21–23]

$$\frac{d\boldsymbol{S}_i}{dt} + \boldsymbol{S}_i \times \mathbf{\Omega}_i = \sum_j W_{ij}(\boldsymbol{S}_j - \boldsymbol{S}_i), \tag{2}$$

with W_{ij} being the hopping rates between sites i and j. The spin-orbit interaction and hyperfine-unrelated spin-flip processes are disregarded. For the hopping rates we take the minimal model by assuming

$$W_{ij} = \frac{1}{\tau} \exp\left(-2\frac{|x_i - x_j|}{a}\right), \tag{3}$$

where x_i and x_j are the coordinates of the localization sites i and j, respectively, and τ is a prefactor governed by the

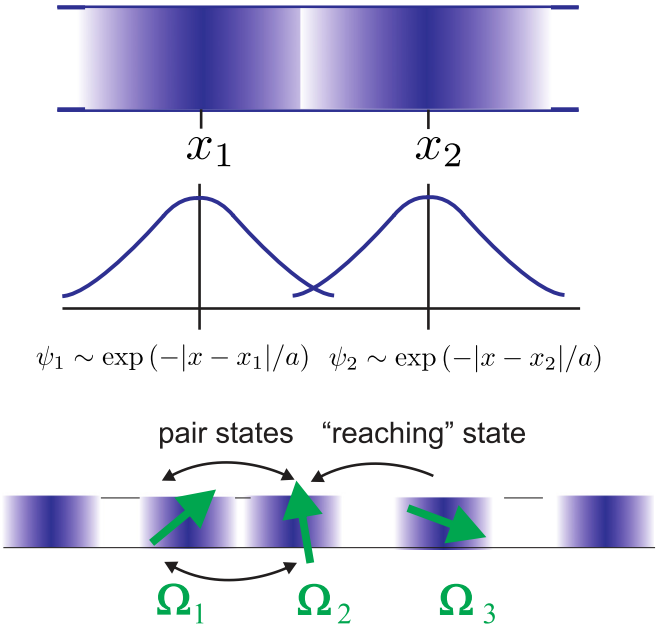

FIG. 1. Upper part: Sketch of a nanowire with localized states, schematically presenting the wave functions beneath the nanowire. Lower part: Illustration of a "pair" and a "reaching" state with hyperfine fields $\mathbf{\Omega}_i$ (green arrows). Note that the distinction between the pairs and the reaching states, which is useful for the analysis of the spin dynamics and the presentation of the results, is not a fundamental feature of one-dimensional systems of localized donor states.

strength of the electron-phonon interaction. The spread of a and τ is disregarded here [21]. The kinetic equation (2) enables us to evaluate the spin dynamics at all relevant time scales.

The condition (1) leads to an exponentially broad spread of the hopping rates. This effect, together with possible multiple returns of hopping electrons to their initial sites, determines the major specific features of the spin dynamics in nanowires. To analyze these phenomena in detail we further consider a realistic situation of rare transitions between the sites, $\Omega_0\tau \gg 1$, assuming, however, that the nuclear spin dynamics controlled by hyperfine coupling with the electron spin, dipole-dipole, or quadrupolar interactions is slow on the time scale of typical hops. Generally, the coupled electron-nuclear spin dynamics may by itself result in nonexponential spin relaxation [24–27]; in our case it results in a cutoff of the algebraic tail in the spin dynamics (see below). In the presented model, the electron spin at a given site i rapidly precesses in the static hyperfine field $\mathbf{\Omega}_i$, and as a result, only its projection onto $\mathbf{\Omega}_i$ is conserved during the typical hop waiting time [10,28]. Then the electron hops to another site j and its spin precesses in the field $\mathbf{\Omega}_j$. Hence, the random hyperfine fields and hopping between the sites serve as a source of spin decoherence and relaxation. The specifics of spin decay in the opposite limit, $\Omega_0\tau \ll 1$, due to the Lévy distribution of waiting times, were studied in Ref. [29]. It is worth stressing that in one-dimensional geometry the electron motion can include multiple returns to the initial sites, which makes spin dynamics particularly involved in such systems [18,30].

It is important that the condition $na \ll 1$, ensuring the exponentially broad distribution of the hopping rates (3), such that in Eq. (2) $|\ln(W_{i,i+1}/W_{i-1,i})| \gg 1$, leads to a situation where for most of the sites the electron hop to its nearest neighbor is exponentially more probable than all other hops. Therefore we are able to divide all the sites into two groups: "pairs," where the hopping within the pair is much faster than the waiting time to hop outside the pair, and the remaining "reaching" ones. For a formal definition of the groups, we consider four sites with the numbers $(k,\ldots,k+3)$ in a row. The sites $(k+1,k+2)$ form a "pair" if for the corresponding positions

$$x_{k+1} - x_k > x_{k+2} - x_{k+1} < x_{k+3} - x_{k+2}, \tag{4}$$

while the sufficient condition for a site, e.g., $k+2$, to be "reaching" is

$$x_{k+1} - x_k < x_{k+2} - x_{k+1} < x_{k+3} - x_{k+2}. \tag{5}$$

A purely geometrical distinction between Eqs. (4) and (5) in systems with $na \ll 1$ acquires a clear physical meaning and allows one to study quantitatively the spin dynamics in terms of the "pair" and "reaching" sites. For the pair sites the nearest-neighbor relation is mutual, i.e., the two pair sites are the nearest neighbors for one another (see Fig. 1; cf. with the cluster model of Ref. [19]). The relaxation of spin on the pair sites is related to multiple hops inside the pair. For reaching sites, the nearest-neighbor relation is not mutual. As a result, the longest waiting time in this situation is that of a hop from the reaching site i to its nearest neighbor j. The subsequent relaxation is due to the hops to other sites that are closer to j than site i and occur much faster than the initial hop $i \to j$. After several hops the electron reaches one of the pair sites and remains in this pair for a sufficiently long time [31].

III. RESULTS

To derive an analytical result for the spin dynamics we take into account hops to the nearest neighbors only [32]. It allows us to evaluate separately the contributions of the two groups of states to the long-time spin dynamics. The relaxation of the spin initially located on a reaching site i at times $t \gg \Omega_0^{-1}$ is determined by the rate of the fastest hop from this site to its neighbor. The expectation value of the spin-z component [33] on the given reaching sites having the distance to the nearest-neighbor close to r_i, can be estimated as $\langle s_{i,z}(t)/s_{i,z}(0)\rangle = s_R(t,r_i) = \exp(-t/\tau_i)K_{\mathrm{KT}}(\Omega_0,t)$, where $\tau_i = \tau\exp(2r_i/a)$. Here, $K_{\mathrm{KT}} = \frac{1}{3} + \frac{2}{3}(1-\Omega_0^2t^2)\exp(-\Omega_0^2t^2/2)$ is the Kubo-Toyabe formula [10,28], which describes the spin precession in the static nuclear field $\mathbf{\Omega}_i$ resulting in the depolarization of transverse to $\mathbf{\Omega}_i$ spin components. Asymptotically (at $t \gg \Omega_0^{-1}$), K_{KT} tends to $1/3$. The electron spin localized on sites k and l forming a pair relaxes according to a similar exponential law $s_P(t,r_{kl},\theta_{kl}) = \exp(-t/\tau_{kl})K_{\mathrm{KT}}(\Omega_0,t)$. Here, r_{kl} is the distance between the sites in the pair and θ_{kl} is the angle between the hyperfine fields at these sites, $\cos\theta_{kl} = (\mathbf{\Omega}_k\cdot\mathbf{\Omega}_l)/(\Omega_k\Omega_l)$, and time constant $\tau_{kl} = \tau\exp(2r_{kl}/a)/(1-|\cos\theta_{kl}|)$ [22,34]. As a result, the disorder-averaged time dependence is given by

$$\left\langle \frac{S_z(t)}{S_z(0)} \right\rangle = \int_0^\infty P_R(r_i)s_R(t,r_i)dr_i + \frac{1}{2}\int_0^\infty dr_{kl}\,P_P(r_{kl})\int_{-1}^{1} d(\cos\theta_{kl})s_P(t,r_{kl},\theta_{kl}). \tag{6}$$

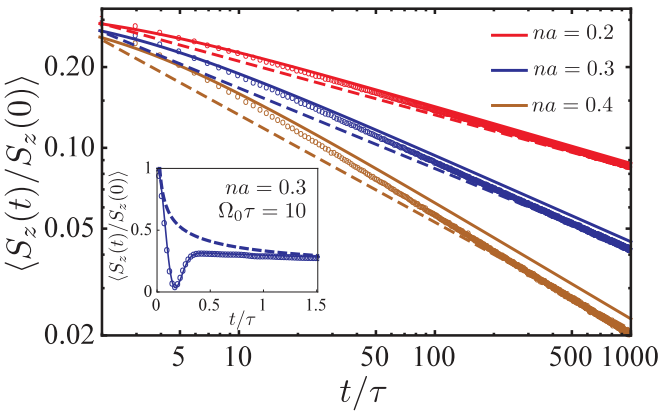

FIG. 2. Comparison of the numerical results (dots) with a model of pair and reaching sites, Eq. (6) (solid lines) and power-law approximation Eq. (7) (dashed lines). The inset shows the initial time interval of the relaxation for $na = 0.3$ and $\Omega_0\tau = 10$. Numerical calculation involved 100 sites and averaging over 5000 realizations of hyperfine fields. Small discrepancies between the large-t behavior in numerical and analytical plots can be attributed to rare hops to not-the-nearest neighbor sites including returns to the reaching sites and jumps out of the pairs.

Here, $P_R(r) = 2ne^{-2nr}(1 - e^{-nr})$ is the probability for a site to be reaching with the distance to its neighbor equal to r and $P_P(r) = 2ne^{-3nr}$ is a probability for a site to be a part of a pair with the distance between sites r, and the Poisson distribution of sites is assumed. Equation (6) demonstrates that the total spin dynamics is given by the weighted average of the electron spins on the reaching and pair sites. The integrals in Eq. (6) can be expressed via special functions [21].

To confirm analytical Eq. (6) we performed numerical simulations based on the kinetic Eqs. (2) and compared the results with the calculation after Eq. (6). In the numerical simulation we allowed hops to any site with probabilities (3). Figure 2 shows very good agreement of the model calculation (solid lines) with numerics (dots) for $na \lesssim 0.4$ without any free parameters.

Now we turn to the detailed analysis of the long-time, $t \gg \tau$, spin dynamics. Figure 2 indicates the power-law relaxation. To support this conjecture, we note that the spin at large $t \gg f\tau$, where the factor $f \gg 1$ [35] is governed by the sites with large distances to its neighbors, i.e., with large $r_i, r_{kl} \gg n^{-1}$ in Eq. (6). The sites with a large distance to its nearest neighbor are typically reaching sites because $P_R(r) \gg P_P(r)$ for r sufficiently larger than n^{-1}, as can be seen from a comparison of Eqs. (4) and (5), and thus the reaching sites serve as a bottleneck for spin relaxation.

The reaching sites' contribution into Eq. (6) can be analytically evaluated at $na \ll 1$ and yields the $t \gg \tau$ asymptotics [21]

$$\left\langle \frac{S_z(t)}{S_z(0)} \right\rangle = \frac{1}{3} C(na) \left(\frac{t}{\tau} \right)^{-na}, \tag{7}$$

where a coefficient $C(na) \sim 1$. Equation (7) clearly demonstrates that the long-time spin dynamics is described by the power law with the exponent controlled by the density of the sites and the localization length. Since the hops from the reaching states serve as a bottleneck for spin relaxation, the long-time spin evolution is controlled by the exponentially broad spread of waiting times for these sites. The numerical simulations show that the asymptotic (7) with $C = 1$ is in good agreement with the numerical results in a wide range of times and parameters na [21]. Only at a small $t \lesssim \tau$ does the asymptotics (7) deviate from the numerical results that agree with the general model, Eq. (6) (see the inset in Fig. 2).

IV. SPIN NOISE

The power-law spin decay results in a zero-frequency anomaly in the spin-noise spectrum. The autocorrelation function $\langle \delta S_z(t) \delta S_z(t') \rangle$ obeys the same set of kinetic equations (2) [23,36]. Defining the spin-noise power spectrum in a standard way,

$$\left(\delta S_z^2\right)_\omega = \int \langle \delta S_z(t) \delta S_z(t') \rangle \exp(i\omega t) dt \tag{8}$$

(see Refs. [20,36–38] for details), we obtain by virtue of Eq. (7) the power-law feature in the spin noise [21]:

$$\left(\delta S_z^2\right)_\omega = \frac{\pi}{12} \frac{\tau n a C(na)}{(\omega\tau)^{1-na}}, \quad \omega\tau \ll 1. \tag{9}$$

The ω^{na-1} feature in the spin-noise spectrum is a direct consequence of the broad distribution of relaxation rates at the reaching sites. In general, the low-frequency spectrum is expected to be $1/\omega^\gamma$. In the above presented model, $\gamma = 1 - na$ and we obtain the "flicker" noise in the low-concentration limit. The exact value of γ depends on the system details [21]. It is noteworthy that the singularity in the spin-noise spectrum at $\omega = 0$ is smeared out due to nuclear spin dynamics: At time scales on the order of the nuclear spin dephasing time T_{2N}, caused, e.g., by the hyperfine coupling with the electron spin, the dipole-dipole coupling between neighboring nuclei, or quadrupolar splittings, the frequencies $\mathbf{\Omega}_i$ in Eq. (2) are no longer static, resulting in a cutoff of the power-law feature in Eq. (9) at $\omega \lesssim 1/T_{2N}$.

Figure 3 shows the spin-noise spectra calculated with Eqs. (6) and (8) in the model of pairs and reaching states for two typical values of $na = 0.2$ and 0.4. In the numerical calculation we have also introduced the exponential cutoff of the spin polarization replacing $K_{\rm KT}(\Omega_0, t)$ in the expression for the spins at the reaching and pair states by the product $K_{\rm KT}(\Omega_0, t) \exp(-t/\tau_s)$, where τ_s is the phenomenological spin relaxation time related, e.g., to the nuclear spin dephasing or the electron activation to the high-energy "extended" states [21]. Three frequency ranges are clearly visible in Fig. 3. At high frequencies $\omega \sim \Omega_0$ ($\Omega_0\tau = 10$ in our calculation) a peak is seen in the spin-noise spectrum. It is related to the electron spin precession in the field of frozen nuclear fluctuation and serves as direct evidence of the hyperfine coupling of the electron and nuclear spins [17]. At this frequency range where $\omega \sim \Omega_0 \gg 1/(f\tau)$ the electron hopping is unimportant and the precession peak is described by the theory developed in Refs. [20,23] (see the dashed lines in Fig. 3). In the range of intermediate frequencies $\tau_s^{-1} \ll \omega \lesssim (f\tau)^{-1}$ the spin-noise spectrum is well described by a power-law asymptotics, Eq. (9) (see the solid lines in Fig. 3). This is a direct consequence of the algebraic tail in the spin relaxation, $S_z(t) \propto t^{-na}$, Eq. (7).

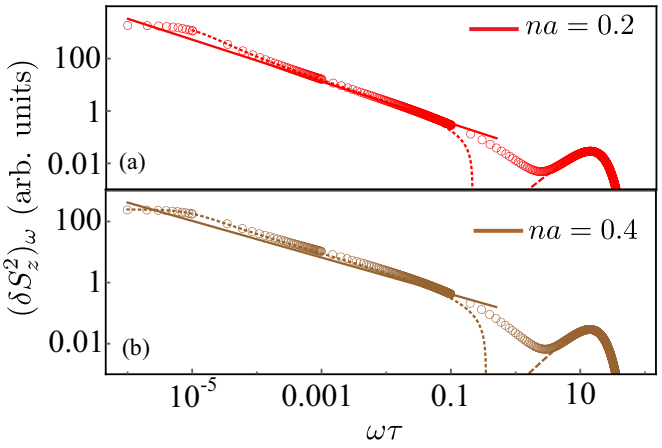

FIG. 3. Spin-noise spectra calculated using Eqs. (6) and (8) (open circles), its power-law asymptotics, Eq. (9) (solid), and spin precession peak (dashed), $\Omega_0\tau = 10$. In the numerical calculation the exponential decay of spin polarization $\propto \exp(-t/\tau_s)$ with $\tau_s/\tau = 10^5$ was included. Dotted lines show asymptotics calculated accounting for the τ_s [21].

Here, the power-law temporal decoherence of spins results in a power-law feature in the spin noise. Finally, at $\omega \lesssim \tau_s$ the algebraic singularity in the spin-noise spectrum is suppressed and $(S_z^2)_\omega$ reaches a constant value $\propto\tau_s$ at $\omega \to 0$. Overall, the ω dependence of the spin-noise power spectrum in the low-frequency domain taking into account the exponential spin relaxation at $t \gtrsim \tau_s$ is described in the Supplemental Material [21]. The power-law features in the spin noise of one-dimensional systems have also been predicted for wires with random spin-orbit coupling and no hyperfine fields [18]. Interestingly, the one-dimensional diffusion in the presence of hyperfine fields does not lead to any power-law singularities in the spin decay and noise [39,40]. Moreover, the distribution (3) at $na \ll 1$ prohibits the diffusive motion of electrons [21].

V. CONCLUSION

We have developed a theory of spin decoherence and spin noise in nanowires by taking into account the key feature of disordered one-dimensional systems such as a strong electron localization resulting in (i) electron hopping transport and (ii) enhanced hyperfine coupling between the electron and host lattice nuclear spins. As a result, the evolution of electron spin density fluctuations is governed by the interplay of hopping electrons and hyperfine interactions. Here, the localization, at least for a low density of sites, results in the exponentially broad distribution of hop waiting times and, consequently, in an algebraic long-time spin decay and in power-law low-frequency singularity in the spin-noise spectrum. It may be expected that the formation of long-time spin decay due to the exponentially wide distribution of waiting times is a general property of hopping electrons: In Ref. [41] it was shown for a model of spin relaxation dominated by spin-orbit coupling.

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[32] The hop to a site that is not a nearest neighbor generally occurs only after a sufficiently long series of hops that already leads to spin relaxation. The nearest-neighbor approximation is not used in the numerical modeling.

[33] Since the considered system is isotropic in the spin space, the same results are valid for the relaxation of any of the spin components.

[34] The spin dynamics for a pair of states is exactly solvable [42,22,43]. Here we use the approximate asymptotics, which works well in the limit of $\Omega_0\tau \gg 1$ (see the Supplemental Material for details).

[35] Formally, $f \sim \exp(2/na)$, which corresponds to the typical waiting time. However, the numerical analysis, as can be seen in Fig. 2, shows that the power-law asymptotics can be established considerably earlier, e.g., at $t \sim 0.1\tau \exp(2/na)$ for $na = 0.2$ (see the Supplemental Material for details).

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