Entanglement of Electron Spin and Orbital States in Spintronic Quantum Transport

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An electron within a mesoscopic (quantum-coherent) spintronic structure is described by a single wave function which, in the presence of both charge scattering and spin-orbit coupling, encodes an information about entanglement of its spin and orbital degrees of freedom. The quantum state—an improper mixture—of experimentally detectable spin subsystem is elucidated by evaluating quantum information theory measures of entanglement in the scattering states which determine quantum transport properties of spin-polarized electrons injected into a two-dimensional disordered Rashba spin-split conductor that is attached to the ferromagnetic source and drain electrodes. Thus, the Landauer transmission matrix, traditionally evaluated to obtain the spin-resolved conductances, also yields the reduced spin density operator allowing us to extract quantum-mechanical measures of the detected electron spin-polarization and spin-coherence, thereby pointing out how to avoid detrimental decoherence effects on spin-encoded information transport through semiconductor spintronic devices.

PACS numbers: 03.65.Ud, 03.67.-a, 72.25.-b

Recently, a considerable effort has been devoted to gain control over a “neglected” property of an electron—its spin—and demonstrate how it can be exploited as a carrier of information [1]. This field of research, dubbed spintronics, is envisioned to bring new paradigms for both classical and quantum information processing. Manipulation of spins as possible carriers of classical information, when combined with traditional electronics manipulating the charge, offers exciting possibilities for novel devices that would process, store, and communicate information on the same chip [2]. Furthermore, phase-coherent dynamics of spin-1/2 as a generic two-level system has been one of the most natural candidates for a qubit in quantum computers [3]. The attempts to utilize long-lived (because of the weak coupling to environmental forces) spin quantum states in semiconductors, either as spin-polarized currents or solid state qubits, is currently at the basic research phase where various conceptual problems are to be surmounted before functional devices can be transferred to an engineering phase. Besides pursuits of efficient room temperature injection [4] from a ferromagnetic source (metallic or semiconducting) into a non-magnetic semiconductor, or tunability of spin-dependent interactions [5], some well-known concepts of the spin physics are to be reexamined in this new guise. For instance, one would like to know the fate of the spin-polarization of injected electrons (which can change its properties or diminish altogether due to exposure to various controlled [6] or uncontrolled spin-dependent interactions, respectively) in the course of transport through complicated solid-state environment, thereby building a firm quantum-mechanical ground for the understanding of what is actually measured in the final stage of experiments in spintronics [4].

The essential features of spin dynamics are captured by two key time scales: spin relaxation $T_1$ and spin decoherence $T_2$ time [7]. The time $T_1$ is classical in nature (i.e., it does not involve any superpositions of quantum states) since it determines lifetime of an excited spin state (aligned along the external magnetic field) [8]—as studied since 1950s by, e.g., exciting a nonequilibrium population of spin-polarized electrons in the skin depth of a metal, where microwave radiation is absorbed in an electron spin-resonance experiment and the diffusion of spins into the bulk is then traced [9]. On the other hand, the spin decoherence time $T_2$ has received increased attention in quantum engineering of single spins where during $T_2$ relative phase in the superpositions of $|\uparrow\rangle$ and $|\downarrow\rangle$ spin quantum states is well-defined [8]. Thus, long $T_2$ ensures enough time for quantum coherence in quantum computing with spintronic qubits [10] or in exploiting spin interference effects in the envisaged semiconductor spintronic devices ($T_2$ can reach 100 ns thereby allowing for the transport of coherent spin states over length scales $L_2 < 100 \mu m$ [8]). The principal modes of decoherence and relaxation are exchange coupling with nuclear or other electronic spins, as well as the spin-orbit (SO) coupling to impurity atoms and defects [6,11].

While paramount problems in spin injection [4] are currently under scrutiny, efficient detection of spin in solid state systems, whose weak coupling to the environment serves as an impediment here, remains an equal challenge [6]. Surprisingly enough, there are many different notions of spin-polarization of electrons detected via transport measurements in metallic [11] or semiconductor [12] spintronic structures. On the other hand, strict quantum-mechanical description of both spin-polarization and spin-coherence is unique: the quantum state of a spin subsystem has to be described by a spin density operator. The spin density operator $\hat{\rho}_s$ makes it possible to predict the result of a measurement of any quantum-mechanical observable related to spin only, thereby accounting for both transport [11] and optical [1,6,12] (which are particularly relevant for detec-
FIG. 1: The von Neumann entropy (solid) and polarization (dashed) of the spin quantum state of a detected electron in the right lead of a Ferromagnet-Semiconductor-Ferromagnet structure where spin-↑ electron is injected from the left lead into the central region (modeled on a tight-binding lattice 100 × 10) with Rashba SO interaction and disorder (disorder-averaging is performed over 10000 samples) characterized by the strengths tso = α/2n and W, respectively. The orbital state of the injected electron is chosen to correspond to the first (the lowest subband) conducting channel in the Landauer scattering picture of transport, except for tso = 0.01 entropy curves that depict all of the twenty spin-polarized channels, exhibiting similar features for each (↑ or ↓) spin species.

FIG. 1: The von Neumann entropy (solid) and polarization (dashed) for each (curves that depict all of the twenty spin-polarized channels, exhibiting similar features for each (↑ or ↓) spin species.

The electron spin as physical observable is described by a density operator \[ \hat{\rho}_s = \frac{1 + \mathbf{P} \cdot \mathbf{\sigma}}{2} \]. (1)

The vector \( \mathbf{P} \) quantifying the “purity” of the quantum state of also provides a strict quantum-mechanical notion of spin-polarization |\( \mathbf{P} \)| for spintronic experiments. For example: (i) \( |\mathbf{P}| = 1 \) stands for a pure quantum state; (ii) \( |\mathbf{P}| = 0 \) stands for a non-pure state (mixture or statistical superposition) that is completely unpolarized; (iii) for intermediate values \( 0 < |\mathbf{P}| < 1 \), spin-\( \frac{1}{2} \) particle is partially spin-polarized mixture. Any pure quantum state can be viewed as a coherent superposition \( |\Sigma \rangle = \cos(\theta/2)|\uparrow\rangle + e^{i\phi} \sin(\theta/2)|\downarrow\rangle \), which, being an eigenvector of \( \mathbf{\sigma} \cdot \mathbf{P} \), is fully polarized in the direction \( \mathbf{P} = (\theta, \phi) \) specified in terms of the angles \( \theta \) and \( \phi \) on a Bloch sphere [14]. In this formal language, the dynamics of spin decoherence and spin relaxation follows a simple ‘chain of events’: a pure state \( |\Sigma\rangle\langle\Sigma| = \left( \begin{array}{cc} \cos^2 \frac{\theta}{2} & \frac{1}{2} e^{-i\phi} \sin \frac{\theta}{2} \\ \frac{1}{2} e^{i\phi} \sin \frac{\theta}{2} & \sin^2 \frac{\theta}{2} \end{array} \right) \).
decoheres into \( \begin{pmatrix} \cos^2 \frac{\theta}{2} & 0 \\ 0 & \sin^2 \frac{\theta}{2} \end{pmatrix} \), on the time scale \( T_2 \) due to entanglement to the environment (such vanishing of the diagonal elements of a density operator is the general phenomenology of any decoherence process [16]); the remaining diagonal elements equilibrate on the scale \( T_1 \) yielding finally \( \begin{pmatrix} \rho_{zz}^{T} & 0 \\ 0 & \rho_{xx}^{T} \end{pmatrix} \) (typically \( T_2 < T_1 \)) [17].

The spin-polarized electron injected into quantum-coherent spintronic structure remains in a pure state \( |\Psi\rangle \), which is a principal feature of mesoscopic system studied over the past two decades by fabricating nanoscale samples and measuring transport at low enough temperatures ensuring that the sample size \( L < L_o \) is smaller than the dephasing length \( L_o \) (determined by inelastic processes) [17]. However, traditional mesoscopic experiments probe the quantum coherence of orbital wave functions, where on the scale \( L_o \) one observes quantum interference effects due to the preservation of relative phase in the superpositions of spatial states of an electron. On the other hand, vector \( |\Psi\rangle \) is a pure state in the tensor product of the orbital Hilbert space and the spin Hilbert space, \( |\Psi\rangle \in \mathcal{H} = \mathcal{H}_o \otimes \mathcal{H}_s \). In general, this state does not have to be separable, meaning that it cannot be decomposed into a tensor product of two vectors \( |\Phi\rangle \otimes |\sigma\rangle \) (unless the orbital and spin coherence, i.e., \( L_o \) and \( L_2 \), are completely independent [18]). Instead, \( |\Psi\rangle \) is a superposition of uncorrelated states \( |\phi_a\rangle \otimes |\sigma\rangle \) comprising a basis in \( \mathcal{H} \): \( |\Psi\rangle = \sum_{a,\sigma} c_{a,\sigma} |\phi_a\rangle \otimes |\sigma\rangle \), where \( |\phi_a\rangle \in \mathcal{H}_o \) is a basis in the orbital factor space \( \mathcal{H}_o \). Thus, when the interplay of SO interaction and scattering at impurities, boundaries or interfaces takes place, orbital and spin quantum subsystems become entangled. Since their individuality is lost, they cannot be assigned a pure state vector any more. Nevertheless, the result of a measurement of any spin observable, described by an operator \( \hat{A}_s \) acting in \( \mathcal{H}_s \), is accounted by \( \langle \hat{A}_o \rangle = \text{Tr}_s [\hat{A}_o \hat{\rho}_s] \). Here the reduced density operator \( \hat{\rho}_s = \text{Tr}_o \hat{\rho} = \sum_{a} (|\phi_a\rangle \langle \phi_a|) \) is obtained by partial tracing, over the orbital degrees of freedom, of the pure state density operator \( \hat{\rho} = |\Psi\rangle \langle \Psi| \). Equivalently, \( \hat{\rho}_o = \text{Tr}_s \hat{\rho} \) plays the same role in the measurement of spatial observables. However, the knowledge of \( \hat{\rho}_s \) and \( \hat{\rho}_o \) does not exhaust all non-classical correlation between electron orbital and spin degrees of freedom embodied in \( |\Psi\rangle \), i.e., \( \hat{\rho} \neq \hat{\rho}_s \otimes \hat{\rho}_o \) except when the full state is separable \( |\Psi\rangle = |\Phi\rangle \otimes |\sigma\rangle \).

These concepts are usually discussed in the context of composite systems of two particles (like the notorious Einstein-Podolsky-Rosen states violating the Bell inequalities [18]). In fact, recent diffusion of the ideas of quantum information theory has led to reexamination [19] of many-body correlations in quantum systems by quantifying the entanglement in their wave functions (which are available in condensed matter physics only in a limited number of exactly or variationally solvable models). Nonetheless, the formalism is the same for any composite quantum system, regardless of whether the subsystems are particles or additional internal degrees of freedom—the joint Hilbert space \( \mathcal{H} \) of a multipartite system is always constructed as a tensor product of the Hilbert spaces of quantum subsystems. The entanglement between subsystems is manifestation of linear superpositions of states in \( \mathcal{H} \). It can be quantified using the von Neumann entropy of a density operator, e.g., in the case of bipartite systems \( S(\hat{\rho}_s) = -\text{Tr} [\hat{\rho}_s \log_2 \hat{\rho}_s] = S(\hat{\rho}_s) \). Essentially, any measure of the entanglement in the pure bipartite state is just a function of the eigenvalues of \( \hat{\rho}_s \) or \( \hat{\rho}_o \) (quantifying entanglement of pure-multipartite or mixed-bipartite states is far more intricate problem [14]). Evidently, the entropy of a pure state is zero [e.g., for fully-polarized spin \( S(|\Sigma\rangle\langle\Sigma|) = 0 \)], and becomes positive for mixtures.

It is insightful to recall a fundamental conceptual difference between the mixed states of entangled subsystems, the so-called improper mixtures [20], and proper mixtures stemming from subjective lack of knowledge when insufficient filtering of an ensemble takes place during a quantum state preparation [18]. Textbook examples of proper mixtures are: conventional unpolarized currents, where \( \rho_{\uparrow\uparrow} = \rho_{\downarrow\downarrow} = 1/2 \) gives rise to \( \hat{\rho}_s = \hat{I}_s/2 \); or thermal equilibrium states in macroscopic solids [14]. Although one uses the same mathematical tool \( \hat{\rho}_o \) in Eq. (1) for both proper and improper mixtures, no real statistical ensemble of different spin states exists within the conductor that would correspond to improper mixtures (the full state is still pure). Injection of partially polarized current, i.e., proper mixture, can lead to an entangled mixed bipartite state in the opposite lead.

These formal tools offer a strict quantum-mechanical route toward understanding the spin-polarization of electrons in a paradigmatic two-terminal spintronic device [2], where two-dimensional electron gas (2DEG) in a semiconductor heterostructure is attached to two ferromagnetic leads. The non-magnetic part of the device can be modeled by a single-particle Hamiltonian [13]

\[
\hat{H} = \left( \sum_m \varepsilon_m |m\rangle \langle m| + t \sum_{m,n} |m\rangle \langle n| \right) \otimes \hat{I}_s + \frac{\alpha \hbar}{2 a^2 t} (\hat{v}_x \otimes \hat{\sigma}_y - \hat{v}_y \otimes \hat{\sigma}_x).
\]  

Here the orbital part \( (\hat{I}_s) \) is a unit operator in \( \mathcal{H}_s \) is a standard tight-binding Hamiltonian defined on a square lattice \( N_x \times N_y \) where electron can hop, with hopping integral \( t \) (a unit of energy), between nearest-neighbor s-orbitals \( |r\rangle = \psi(r - m) \) located on the lattice sites \( m = (m_x, m_y) \). In clean samples \( \varepsilon_m \) is constant, while in disordered ones random potential is simulated by taking \( \varepsilon_m \) to be uniformly distributed over the interval \([-W/2, W/2] \). The SO term \( \hat{v} = (\hat{v}_x, \hat{v}_y, \hat{v}_z) \) is the velocity operator, acting effectively as an “entangler”, is the
Rashba interaction which arises from the asymmetry along the z-axis of the confining quantum well electric potential that creates a two-dimensional (2D) electron gas (xy-plane) on a narrow-gap semiconductor (such as InAs) surface. This type of SO coupling, which is different from the more familiar impurity induced and position dependent ones in metals, is particularly important for spintronics since its strength \( \alpha \) can be tuned in principle by an external gate electrode. It is, therefore, envisaged as a tool to control the precession (i.e., unitary quantum evolution of coherent superpositions of spin states) of injected spin-polarized electrons during their ballistic flight, thereby modulating the current in the opposite lead of the spin-FET.

The spin-polarized electrons are injected from the left ferromagnetic lead into 2DEG, and then either \( \uparrow \) or \( \downarrow \) -electrons (or both) are collected in the right lead (which are semi-infinite in theory). To study entanglement in such open mesoscopic system, where electrons can escape from the sample through the leads, we use the fact that pure states of injected and collected electrons are linear superpositions of asymptotic scattering “channels” in the Landauer picture of quantum transport. However, in spintronics each channel \( |n\sigma\rangle \) (at the Fermi energy \( E_F \) in the leads) is fully spin-polarized and denotes a separable state vector \( \langle r | n \sigma \rangle^\pm = \Phi_n(y) \exp(\pm ik_n x) \otimes |\sigma\rangle \), which is characterized by a real wave number \( k_n \), transverse wave function \( \Phi_n(y) \) defined by quantization of transverse momentum in the leads of a finite cross section (with hard wall boundary conditions implemented here), and a spin factor state \( |\sigma\rangle \). When injected electron is prepared in the channel \( |n\sigma\rangle \equiv |n, \sigma\rangle \), a pure state will emerge in the other lead \( |\tau\rangle \equiv |n', \sigma'\rangle \) if the coherent superposition introduces a transmission matrix \( t \), which is defined in the basis of incoming spin-polarized channels of the injecting lead and outgoing channels in the detecting lead. It encodes a unitary transformation that the central region performs on the incoming electronic wave function from the left lead. To compute the \( t \)-matrix efficiently, we switch from wave functions to a single-particle real \( \otimes \) spin space Green function (which is an inverse of the non-Hermitian operator \( \hat{H} + \Sigma \), with self-energy \( \Sigma \) modeling the open quantum system attached to the external leads), as elaborated in more detail in Ref. 13.

To each of the outgoing pure states we assign the density operator as the projector onto that state

\[
\hat{\rho}_{\text{out}}^{n\sigma} = \sum_{n', \sigma'} t_{n', n, \sigma, \sigma'} |n'\rangle \langle n'| \otimes |\sigma'\rangle \langle \sigma'| ,
\]

(3)

where all matrices here depend on \( E_F \). Taking partial trace, which is technically just the sum of all \( 2 \times 2 \) block matrices along the diagonal of \( \hat{\rho}_{\text{out}}^{n\sigma} \), we obtain the exact reduced density operator for the spin subsystem

\[
\hat{\rho}_{\text{s}}^{n\sigma} = \sum_{n', \sigma'} t_{n', n, \sigma, \sigma'} |n'\rangle \langle n'| \otimes |\sigma'\rangle \langle \sigma'| .
\]

(4)

From \( \hat{\rho}_{\text{s}}^{n\sigma} \) we can extract: the components of the polarization vector \( \mathbf{P} = (p_x, p_y, p_z) \) defined by Eq. 1, \( \mathbf{P} = \text{Tr} \left[ \hat{\rho}_{\text{s}} \sigma \right] \); and the von Neumann entropy of improper mixture generated by spin-orbit entanglement, \( S(\hat{\rho}_{\text{s}}) = -\frac{1}{2} \left( 1 + |\mathbf{P}| \right) \log_2 \left( \frac{1}{2} (1 + |\mathbf{P}|) \right) - \frac{1}{2} \left( 1 - |\mathbf{P}| \right) \log_2 \left( \frac{1}{2} (1 - |\mathbf{P}|) \right) \). Since the von Neumann entropy (a standard measure of the degree of entanglement in bipartite pure quantum states) is a function of the eigenvalues of a hermitian operator, it is essentially a measurable quantity. Moreover, the case of spin-\( \frac{1}{2} \) is rather unique: the spin density operator \( \hat{\rho}_{\text{s}} \), the spin polarization \( \mathbf{P} \), and the degree of entanglement \( S(\hat{\rho}_{\text{s}}) \equiv S(\mathbf{P}) \) are all obtained once the average components of the spin operator \( \langle \hat{\sigma}_x / 2 \rangle, \langle \hat{\sigma}_y / 2 \rangle, \langle \hat{\sigma}_z / 2 \rangle \) have been measured.

We are now fully armed to revisit the results of Fig. 1 for injection of electrons that are spin-polarized along the direction of transport (as in the spin-FET proposal), denoted as the \( x \)-axis here, through a mesoscopic conductor modeled on a 100 \( \times \) 10 lattice. Within the conductor electrons experience different strengths of the disorder \( W \) and the Rashba SO coupling \( t_{\text{so}} = \alpha / 2a \) (\( a \) is the lattice spacing). We rely here on the quantum intuition, rather than the “unreliable” classical one that invokes picture of spin precession whose axis changes every time the electron momentum is knocked out due to the scattering off impurities—the so-called Dyakonov-Perel (DP) mechanism. Such process diminishes electron spin-polarization \( |\mathbf{P}| < 1 \) by entanglement, as signaled by \( S > 0 \) in Fig. 1 which is sensitive even to small disorder \( W = 1 \) and negligible \( t_{\text{so}} = 10^{-3} \) [around the band center a mean free path is roughly \( \ell \approx 30((\ell / W)^2) \). Moreover, our quantum framework goes beyond classical insight, which predicts that spin-diffusion length is independent of the mean free path (the so-called motional narrowing effect): further increasing of the disorder impedes the DP decoherence mechanism thereby restoring the partial quantum coherence of the mixed state of the spin subsystem. This is demonstrated by the decrease of entropy \( S_{W=5} < S_{W=1} \) when rather strong disorder \( W = 5 \) is introduced into the conductor with fixed and uniform \( t_{\text{so}} \). However, we see that partial spin-polarization for a very wide range of parameters exhibits an oscillatory structure (that is not seen in naive measures of spin-polarization) as a function of \( E_F \) at which the zero-temperature quantum transport occurs. In fact, the most interesting case occurs for \( t_{\text{so}} = 0.01 \), corresponding to currently achievable strengths of the Rashba SO coupling, where polarization reaches \( |\mathbf{P}| \approx 0.95 \) at discrete values of \( E_F \). To evade spin-charge entanglement, the spin-FET would have to operate in a strictly ballistic transport regime. Nonetheless, Fig. 1 suggest that careful crafting of the device parameters makes possible...
to “purify” almost completely the quantum state of the spin subsystems, therefore restoring spin coherence, even when charge scattering takes place in the presence of the engineered SO interaction.

In summary, it is shown that quantum information style analysis of spin-orbit entanglement in the scattering states of quantum transport theory provides a thorough understanding of the state of transported spins through spintronic devices, ultimately accounting for any spin detection experimental scheme. Although the amplitudes of the Landauer transmission matrix elements directly yield conductance, we demonstrate that analysis of both their phases and amplitudes reveals “nonequilibrium” spin-orbit entanglement. The spin polarization, spin coherence, and the degree of entanglement are all extracted from the reduced spin density operator, whose dynamics is formulated for nonequilibrium steady transport state without invoking any master equations of ‘open quantum system’ approaches [16] (note that the reduced density operator no longer obeys the von Neumann equation, whereas the total wave function evolves according to the Schrödinger equation). The principal insight gained for the future of spin-FET devices is that, due to any scattering mechanism (even without disorder, scattering can occur at the interfaces and boundaries, particularly at the lead-semiconductor interface due to difference in electronic states with and without the Rasha SO coupling [7, 11]), they will operate with mixed spin states, rather than with the originally proposed [2] pure ones. The full quantum coherence of spin states can be preserved only in single-channel wires.

I thank E. I. Rashba and J. Fabian for enlightening discussions.