



Spintronics: electron spin coherence, entanglement, and transport

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The prospect of building spintronic devices in which electron spins store and transport information has attracted strong attention in recent years. Here we present some of our representative theoretical results on three fundamental aspects of spintronics: spin coherence, spin entanglement, and spin transport. In particular, we discuss our detailed quantitative theory for spin relaxation and coherence in electronic materials, resolving in the process a long-standing puzzle of why spin relaxation is extremely fast in Al (compared with other simple metals). In the study of spin entanglement, we consider two electrons in a coupled GaAs double-quantum-dot structure and explore the Hilbert space of the double dot. The specific goal is to critically assess the quantitative aspects of the proposed spin-based quantum dot quantum computer architecture. Finally, we discuss our theory of spin-polarized transport across a semiconductor/metal interface. In particular, we study Andreev reflection, which enables us to quantify the degree of carrier spin polarization and the strength of interfacial scattering.

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1. Introduction

There has been a great deal of recent interest in the concept of spintronics [1] where active control and manipulation of electron spin in semiconductors and metals provide the basis of a novel quantum technology. Possible applications of spintronics include high-speed magnetic filters, sensors, quantum transistors, and spin qubits for quantum computers [2, 3]. More fundamental research will, however, be needed before practical spintronic devices can be demonstrated, as much remains to be understood about spin coherence, spin dynamics, and spin transport. In this paper we discuss some of our recent theoretical work on understanding spin dynamics in electronic materials.

The existing spintronic architectures [1, 4] and the proposed solid-state quantum computing schemes [3] rely on the relatively long spin coherence times of conduction electrons. Indeed, in the simplest spintronic scheme—the spin injection [5]—electrons with a definite spin polarization are supplied into a nonmagnetic metal or semiconductor from a ferromagnetic electrode. The farther (longer) the electrons in the nonmagnetic sample carry the spin coherence, the more useful the device is. Similarly, if an electron spin represents a qubit in a solid-state quantum computer, the longer the spin survives, the more reliably it can store information. The question of how spins of mobile electrons (and holes) lose their spin coherence is thus of the utmost importance for spintronic technology and for solid-state quantum computing. Unfortunately, the physical

picture of spin decoherence (or relaxation) we now have is far from complete. Most information comes from experiments, but experimental data are still scarce and often incomplete. The existing theories seem to provide a broad conceptual framework for understanding spin decoherence in metals and semiconductors, but the acute absence of realistic calculations for concrete materials makes it difficult to validate these theories. The hope is that with more complete experimental and theoretical understanding we will be able to choose or build materials with the longest decoherence times possible. In this paper we discuss, as an example, our detailed quantitative theory [6–8] of spin relaxation and coherence in a simple metal, Al.

One challenge of spintronics is to study the possibility of using (electron or nuclear) spins as quantum bits (qubits) in a quantum computer (QC). QC has drawn growing attention in recent years because it can deliver significant speed-up over classical computers [2] for some problems due to inherent superposition and entanglement of a quantum system. Various QC architectures have been proposed, including several solid state models that may possess the important feature of scalability. We study a QC model [3] in which a double quantum dot in the GaAs conduction band serves as the basic elementary gate for a QC with the electron spins in the dots as qubits. The two-electron exchange coupling provides the necessary two-qubit entanglement required for quantum computation. Using a molecular orbital approach [9], we determine the excitation spectrum of two horizontally coupled quantum dots with two confined electrons, and study its dependence on an external magnetic field [10]. We particularly focus on the electron exchange coupling and double occupation probability, which are two crucial parameters for a QC architecture.

Since potential spintronic devices are typically heterojunctions [5], it is important to understand how transport across the interface between different materials depends on the degree of carrier spin polarization and the interfacial transparency. Significant progress has been made in manipulating spin dynamics in semiconductors [11], including various methods to create spin-polarized carriers [12], such as employing a novel class of ferromagnetic semiconductors [13] and spin injection from a ferromagnet [14]. These advances, together with tunable electronic properties (such as carrier density and Fermi velocity) and well-established fabrication techniques, provide a compelling reason to study hybrid semiconductor structures in the context of spintronics [1]. In particular, we consider spin-polarized transport in the semiconductor/superconductor hybrid structures, which for low applied bias is governed by Andreev reflection [15]. Our aim is also to motivate study of the interplay between spin polarization and Andreev reflection in other areas, such as mesoscopic physics and quantum computing.

2. Spin coherence in electronic materials

Spins of conduction electrons decay because of the spin-orbit interaction and momentum scattering. At low temperatures ($T \lesssim 20$ K) spin relaxation is caused by impurity scattering and is temperature independent. At higher temperatures electrons lose spin coherence by colliding with phonons (phonons can induce a spin flip because in the presence of a spin-orbit coupling electronic Bloch states are not spin eigenstates). Spin relaxation rate $1/T_1$ increases as temperature increases, with the growth becoming linear above the Debye temperature. This mechanism, discovered by Elliott [16] and Yafet [17], is the most important spin relaxation mechanism in metals and semiconductors with inversion symmetry. It gives typical values of T_1 on the nanosecond scale, in agreement with experiment. To our knowledge the longest T_1 in a metal has been reported to be a microsecond, in a very pure Na sample at low temperatures [18]. The situation is much more complicated in semiconductors [8]. Many interesting semiconductors such as GaAs lack inversion symmetry, so other mechanisms, in addition to the Elliott–Yafet one, become important [8]. These mechanisms operate differently in different temperature regions, doping, and magnetic, strain, and confinement fields, so that sorting out the relevant mechanism(s) for a given material is a tremendous task which is yet to be carried out. Magnitudes of T_1 in semiconductors are also typically nanoseconds, but recent experimental studies [11] in II–VI and III–V systems show that T_1 can be artificially enhanced [8]. It seems, however, that intrinsic elec-

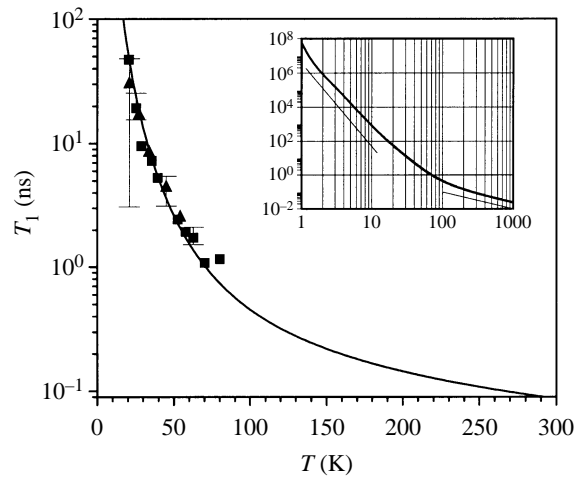


Fig. 1. Calculated phonon-induced spin relaxation time T_1 in Al as a function of temperature T . Symbols with error bars are experimental data from [5, 19] and the inset is a larger-scale log–log plot. There is good agreement between the theory and the experiment, but the absence of experimental data at temperatures above 100 K makes the calculation a prediction which is particularly useful for spintronic applications at room temperature.

tronic properties may not allow T_1 in technologically interesting materials to be longer than a microsecond at room temperature.

Spin relaxation is very sensitive to the electronic band structure. Our *ab initio* calculation [6, 7] of T_1 in Al, whose result is shown in Fig. 1, shows that bandstructure anomalies such as the Fermi surface crossing of a Brillouin zone boundary or an accidental degeneracy line, can enhance spin relaxation (reduce T_1) by orders of magnitude. Since such anomalies are ubiquitous in polyvalent metals (the Fermi surfaces of monovalent metals are well contained within the first Brillouin zone boundary and thus are free of anomalies), we gave them a special name: spin hot spots. Whenever an electron jumps in or out (as a result of a collision) of a spin hot spot, the electron's chance of flipping spin is greatly enhanced. As a result, $1/T_1$ in Al and other polyvalent metals is much greater than what one would naively expect. This is indeed what is measured [20]: While monovalent alkali and noble metals have their spin relaxation rates in accordance with simple estimates based on the Elliott–Yafet theory, polyvalent metals (only Al, Be, Mg, and Pd have been measured so far) have $1/T_1$ larger than expected by typically one to three orders of magnitude. Take as an example Al and Na. They have similar atomic numbers, so one would expect that their corresponding spin–orbit couplings would also be similar (as is the case in the atomic state [17]), giving similar spin relaxation rates. However, the corresponding T_1 at the Debye temperatures (150 K for Na and 390 K for Al) are about 20 ns in Na and 0.1 ns in Al! This huge difference is caused by the presence (absence) of spin hot spots in polyvalent Al (monovalent Na).

The current fashion for electron spin aside, spin relaxation in electronic materials is a beautiful and important subject of its own. The field itself began in the 1950s with the advent of CESR (conduction electron spin resonance), but after some initial breakthroughs the subject went dormant until the current surge inspired by spintronics. The experimental focus has so far been on the simplest elemental metals like the alkali and the noble metals, and on just a handful of interesting semiconductors. This is understandable from the point of view of technological applications, but not quite right from the point of view of fundamental physical understanding. What is clearly needed is catalogue of temperature-dependent spin relaxation times for different metals and semiconductors, a systematic study of the effects of impurities, alloying, and surfaces and interfaces. Theory should have the same goal: performing realistic calculations of T_1 for different metals within the existing framework laid out by Elliott and Yafet, and similarly for semiconductors taking into account other spin relaxation mechanisms as well.

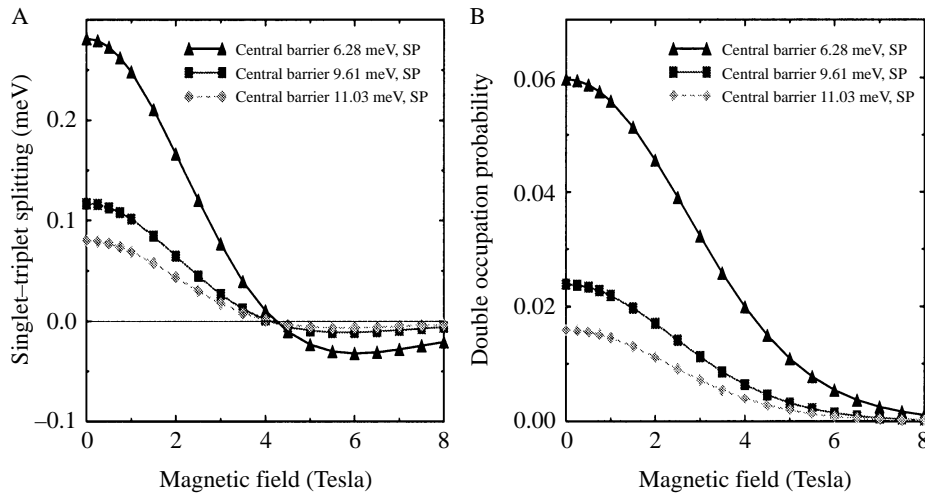


Fig. 2. Calculated magnetic field dependence of A, the spin singlet–triplet splitting and B, double occupation probability in the singlet state for a two-electron double quantum dot. The dot size is 30 nm in radius, and the inter-dot distance 40 nm. There is a singlet–triplet crossing at about 4 Tesla, which is a result of competing Coulomb repulsion, exchange, and single particle kinetic and potential energies. DOP is relatively high at low magnetic fields, but is quickly suppressed as magnetic field increases.

3. Electron entanglement through exchange interaction in a double quantum dot

The exchange coupling (the splitting of the lowest singlet and triplet states) and the double occupation probability (the probability that the two electrons occupy the same orbital state in one dot) in a double dot are two important parameters for the spin-based quantum dot quantum computer (QDQC). The exchange coupling between two electrons establishes the necessary entanglement between spins, and determines how fast quantum gates can be. Quantum computation has very low tolerance for errors (it requires an error rate below 10^{-4}), so that precise control and small errors are imperative for a QC. In a QDQC, individual quantum dots are tags which distinguish different qubits. If during a gating action two electrons jump onto a single quantum dot, their original tag information will be lost, which will result in an error. Thus, in designing a QDQC, double occupation probability (DOP) has to be minimized for the states that belong to the QDQC Hilbert space. Figure 2 shows our numerical results on the magnetic field dependence of (A) the exchange coupling with three different central barrier heights, and (B) the ground state DOP. The latter clearly decreases as B field increases. Physically, as B increases, the single-electron atomic wavefunctions are squeezed so that the inter-dot wavefunction overlap decreases, while the ‘on-site’ Coulomb repulsion energy for a single dot increases. The ground state DOP can also be seen in Fig. 2 to decrease significantly with increasing central barrier strength separating the two dots, as one would expect.

As shown in Fig. 2, at zero magnetic field it is difficult to have both a vanishing DOP for a small error rate and a sizeable exchange coupling for fast gating, because the exchange coupling and the DOP have similar dependence on the inter-dot barrier and inter-dot distance. On the other hand, finite magnetic fields may provide finite exchange coupling for QC operations with small errors. However, a finite magnetic field will produce a Zeeman splitting in the triplet state, causing additional phase shifts. Therefore, a swap gate [3] in a QC would have to include additional single-qubit operations to correct the effects of these phase shifts [10]. This added complexity inevitably prolongs the gating time of a two-qubit operation, which in turn increases the chance of an error due to spin relaxation. Another implication of a finite magnetic field is small exchange coupling—about an order of magnitude smaller than that at zero field. This means that the two-qubit operations will last as long as 10 ns, requiring the spin coherence time to be longer than 10 μ s in a semi-

conductor quantum dot. Whether GaAs or other electronic materials can provide such favorable environment for electron spins is yet to be determined, and many other questions need to be answered before practical spin-based QDQC can be realized. These questions include, but are not limited to, the effects of stray fields, the implication of a chosen geometry, and the effects of external noise introduced through active control.

4. Spin transport

The presence of spin-polarized carriers gives rise to both modified charge transport and intrinsic spin transport, absent in the unpolarized case. Each of these aspects provides information about the degree of spin polarization which can be utilized in spintronics. Here, we focus on the transport of spin-polarized carriers across the semiconductor/metal interface where the metal is in the superconducting state. The study of semiconductor/superconductor (Sm/S) hybrid structures has several important ramifications. Already in the context of spin-unpolarized transport [21], it has been demonstrated [22] that this configuration can be used to examine the interfacial transparency which for a Sm/normal metal is typically limited by a native Schottky barrier. In the presence of spin-polarized carriers, Sm/S structure can also serve to quantify the degree of spin polarization of a semiconductor and probe both potential and spin-flip interfacial scattering [12]. To understand such sensitivity to spin polarization and different types of interfacial scattering it is important to consider the process of Andreev reflection [15] which governs the low bias transport. In this two-particle process, an incident electron of spin $\sigma = \uparrow, \downarrow$ on a Sm/S interface is reflected as a hole belonging to the opposite spin subband, back to the Sm region while a Cooper pair is transferred to the superconductor. The probability for Andreev reflection at low bias voltage is thus related to the square of the normal state transmission coefficient and can have stronger dependence on the junction transparency than the ordinary single-particle tunneling. For spin-polarized carriers, with different populations in two spin subbands, only a fraction of the incident electrons from a majority subband will have a minority subband partner in order to be Andreev reflected. In the superconducting state, for an applied voltage smaller than the superconducting gap, single particle tunneling is not allowed in the S region and the modification of the Andreev reflection amplitude by spin polarization or junction transparency will be manifested in transport measurements.

Prior to work from Ref. [12] the spin-dependent Andreev reflection was addressed in the context of ferromagnet/S junctions [23] and calculations were performed assuming the equality of the effective masses [24] in the two regions across the interface. Such an assumption is inadequate for the Sm/S hybrid structures. We adopt here the scattering approach from Ref. [12] and solve the Bogoliubov–de Gennes [12, 24] equations in a ballistic regime. At the flat interface between the Sm and S region we model the interfacial scattering by Z_σ and F , orbital and spin-flip scattering strengths, respectively. $Z_\uparrow \neq Z_\downarrow$ can describe magnetically active interface and the effects of spin-filtering. We represent spin polarization by X , the ratio of spin subband splitting and the Fermi energy. In Fig. 3 we give normalized low-temperature results [12] for the three-dimensional charge conductance, $G_3 \equiv G_{3\uparrow} + G_{3\downarrow}$, as a function of the ratio of bias voltage, eV , and the superconducting gap, Δ . Displayed charge conductance, which is calculated for vanishing interfacial scattering strength, depends strongly on the spin polarization X . The inset shows the effect of orbital and spin-flip scattering at a fixed spin polarization of $X = 0.4$ [12], $G_{S3} \equiv G_{S3\uparrow} - G_{S3\downarrow}$. To study the intrinsic spin transport, it is convenient to define spin conductance. For $eV < \Delta$ and any spin polarization $G_{S3} = 0$, since $G_{S3\uparrow, \downarrow}$ are each proportional to the corresponding spin component of the quasiparticle current and that there is no quasiparticle tunneling below the superconducting gap. For the unpolarized case, $X = 0$, $G_{S3\uparrow} \equiv G_{S3\downarrow}$ and the spin conductance vanishes identically. For $eV > \Delta$, G_{S3} is a sensitive function of X and could be used to determine the degree of the spin polarization. Experimental studies of spin-polarized Sm/S junctions should provide an important test for feasibility of spintronic devices based on hybrid semiconductor structures, as well as stimulate future theoretical studies considering, for example, nonequilibrium processes, realistic band structure, and diffusive regime.

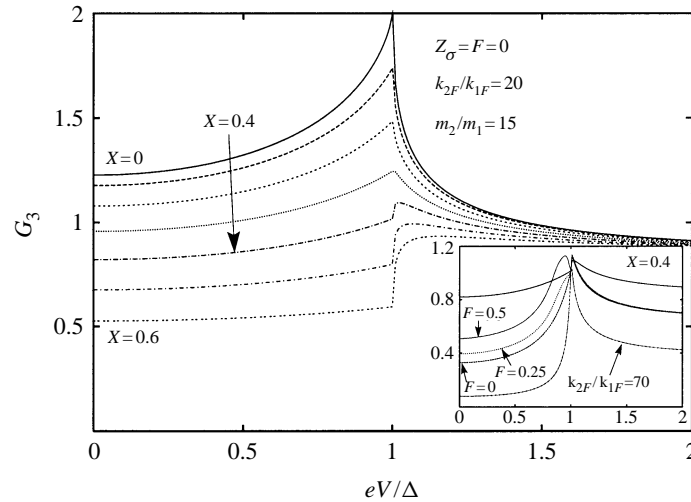


Fig. 3. Normalized charge conductance $G_3(eV/\Delta)$. Curves from top to bottom represent $X = 0, 0.1, 0.2, 0.3, 0.4, 0.5, 0.6$ at $Z_\sigma = F = 0$. The inset shows $X = 0.4$ results. The upper four curves (from top to bottom at zero bias) have Z_σ and F values of $(0,0)$, $(0.5,0.5)$, $(0.5,0.25)$, and $(0.5,0)$. For the bottom curve, which corresponds to $k_{2F}/k_{1F} = 70$, the Z_σ and F values are $(0,0)$. Here the effective masses and the Fermi wave vectors are denoted by m_i and k_{if} , where $i = 1, 2$ correspond to the Sm and S regions, respectively.

5. Conclusion

We studied several issues related to spintronics. First, we demonstrated the importance of band structure effects in spin relaxation and established that special subtle features (spin hot spots) of electronic structure have profound effects on the magnitude of the spin relaxation rate in electronic materials. Since spin hot spots can be artificially induced, our work also shows a way of tailoring spin dynamics of conduction electrons. Next, our study of a quantum dot hydrogen molecule showed that the goal of having both a reasonable exchange coupling and a vanishingly small error rate can only be achieved at finite magnetic fields (4–8 Tesla), and one has to consider many factors (such as fast gating time, precise control, low error rate, etc) to produce a realistic spin-based quantum computer. Finally, we demonstrated that the low-temperature spin-polarized transport in Sm/S structures may serve as a sensitive and quantitative probe for determining the degree of spin polarization and the strength of interfacial scattering. In contrast to the unpolarized case, the junction transparency can be enhanced with the increase of the Fermi velocity mismatch in the two regions.

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References

- [1] G. Prinz, *Phys. Today* **48**, 58 (1995); *Science* **282**, 1660 (1998).
- [2] A. Steane, *Rep. Prog. Phys.* **61**, 117 (1998).
- [3] D. Loss and D. DiVincenzo, *Phys. Rev.* **A57**, 120 (1998); G. Burkard, D. Loss, and D. DiVincenzo, *Phys. Rev.* **B59**, 2070 (1999).
- [4] J. Gregg *et al.*, *J. Magn. Magn. Mater.* **175**, 1 (1997).
- [5] M. Johnson and R. H. Silsbee, *Phys. Rev. Lett.* **55**, 1790 (1985).
- [6] J. Fabian and S. Das Sarma, *Phys. Rev. Lett.* **81**, 5624 (1998); *J. Appl. Phys.* **85**, 5057 (1999).
- [7] J. Fabian and S. Das Sarma, *Phys. Rev. Lett.* **83**, 1211 (1999).

- [8] J. Fabian and S. Das Sarma, *J. Vac. Sci. Technol.* **B17**, 1708 (1999).
- [9] R. McWeeny, *Methods of Molecular Quantum Mechanics* (Academic Press, San Diego, 1992).
- [10] X. Hu and S. Das Sarma, LANL Preprint quant-ph/9911080. To appear in *Phys. Rev. A*.
- [11] D. D. Awschalom and J. M. Kikkawa, *Phys. Today* **52**, 33 (1999).
- [12] I. Žutić and S. Das Sarma, *Phys. Rev.* **B60**, 16322 (1999).
- [13] H. Ohno, *Science* **281**, 951 (1998).
- [14] P. R. Hammar, B. R. Bennett, M. J. Yang, and M. Johnson, *Phys. Rev. Lett.* **83**, 203 (1999).
- [15] A. F. Andreev, *Zh. Eksp. Teor. Fiz.* **46**, 1823 (1964).
- [16] R. J. Elliott, *Phys. Rev.* **96**, 266 (1954).
- [17] Y. Yafet, *Solid State Physics*, edited by F. Seitz and D. Turnbull (Academic, New York, 1963) Vol. 14.
- [18] W. Kolbe, *Phys. Rev.* **B3**, 320 (1971).
- [19] D. Lubzens and S. Schultz, *Phys. Rev. Lett.* **36**, 1104 (1976).
- [20] P. Monod and F. Beuneu, *Phys. Rev.* **B19**, 911 (1979).
- [21] C. J. Lambert and R. Raimondi, *J. Phys.: Condens. Matter* **10**, 901 (1998); C. W. J. Beenakker, *Rev. Mod. Phys.* **69**, 731 (1997), give reviews of unpolarized transport in Sm/S junctions and address Andreev reflection in mesoscopic physics.
- [22] S. De Franceschi, F. Giazotto, F. Beltram, L. Sorba, M. Lazzarino, and A. Franciosi, *Appl. Phys. Lett.* **73**, 3890 (1998).
- [23] V. A. Vas'ko *et al.*, *Appl. Phys. Lett.* **73**, 844 (1998); R. J. Soulen Jr. *et al.*, *Science* **282**, 85 (1998); S. K. Upadhyay *et al.*, *Phys. Rev. Lett.* **81**, 3247 (1998).
- [24] M. J. M. de Jong and C. W. J. Beenakker, *Phys. Rev. Lett.* **74**, 1657 (1995); J.-X. Zhu *et al.*, *Phys. Rev. B* **59**, 9558 (1999); I. Žutić and O. T Valls, *Phys. Rev.* **B60**, 6320 (1999); *ibid.*, **61**, 1555 (2000); S. Kashiwaya *et al.*, *Phys. Rev.* **B60**, 3572 (1999).