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We report progress in calculati g-factors in quantum dots, excha dipolar magnetic fields for nuclea spin transistors. Our new propos photon detection (Bell detection) polarized packets at room tempe closer to 2 than previously expect	ons of spin coherence and spin trange interactions in Si/Ge quantun ar spin, spontaneous spin polariza al for electron-spin based teleport . We find that electric transport in rature. We also predict that orbita ted. These calculations may be o	ansport properties in r n dots, tuning of spin o tion generation and ne ation is mediated by s nonmagnetic semicon I angular momentum o f use in semiconducto	hanoscale geometries, including calculations of coherence times for electron spin, tuning of ew designs for spin-based teleportation and single photons and does not require correlated nductors is unstable to the formation of spin- quenching in quantum dots will drive g factors or spintronic devices or quantum computation.
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Statement of Problem:

Recent experimental advances in generating, transporting, and detecting coherent spin-polarized populations of electron and nuclear spin in semiconductors have demonstrated that these effects can be harnessed in nanoscale electronics as the basis of novel devices. The breadth of these experiments is staggering. Optical generation and probing of coherent electron spin populations demonstrated spin coherence times exceeding 100 ns and spin diffusion lengths exceeding 100 μ m. Electrical spin injection from the magnetic semiconductors GaMnAs and BeMnZnSe has also been demonstrated in device structures, specifically in the spin-polarized LED.

Scope of Program

Major advances in theoretical understanding of the generation, transport, and detection of coherent spin populations in nanostructures are now desperately required. Theoretical work must contribute to the field in several ways: it must provide a framework for understanding the recent experiments, it must suggest unusual new phenomena which can be inferred from these experiments, and it must incorporate these phenomena in realistic models of device operation and performance. The work must also be able to identify specific systems and geometries that most strongly exhibit the desired effects. In order to be of best use to this field the work must also be very responsive to issues as they arise in the experimental community.

This grant supports a broad theoretical effort which is closely coordinated with current and proposed experimental efforts in this field. The efforts can be classified into four directions:

1) Accurate calculations of spin coherence times for electronic systems in nanoscale structures:

2) Theory of inhomogeneous spin transport and spin injection in nonmagnetic and magnetic semiconductors

3) Theory of nuclear spin coupling to electronic spin, and the implications for all-optical manipulation of nuclear spin

4) Theory of Si/Ge quantum dots in inhomogeneous electric fields

Summary of Most Important Results:

Accurate calculations of spin coherence times for electronic systems in nanoscale structures:

The dominant mechanism for spin decoherence in bulk and quantum well systems, particularly near room temperature, is precessional decoherence. We have exhaustively explored the origins of this mechanism, which can be traced to inversion asymmetry in the material or nanostructure itself. We predicted several orders of magnitude tuning of the spin lifetime in (110) semiconductor quantum wells. These results were applied to design new spin transistors. We also predicted the properties of collective spin excitations and spin lifetimes in quantum dots.

The tuning of spin lifetimes in (110) InAs/AISb and GaAs/AIGaAs quantum wells has also been demonstrated. The tuning range of spin lifetimes with electric field in InAs/AISb quantum wells, grown at HRL, is smaller than the range in GaAs/AIGaAs systems, but the scale of the spin lifetimes is very different. GaAs/AIGaAs quantum wells are tunable from ~1ns to ~10ns at 170K, whereas InAs/AISb quantum wells are tunable from ~6ps to ~30ps at 300K. These very short spin lifetimes are important for achieving small-scale coherent spin devices (e.g. a nonmagnetic spin transistor), and if the ~30ps lifetime in the absence of a field can be lengthened, the on-off ratios possible in these spin transistors would be competitive with CMOS. Theoretical calculations suggest a much greater range of tuning is possible than was seen experimentally. The InAs/AISb work has appeared in *Applied Physics Letters*. The GaAs/AIGaAs work has appeared in *Physical Review Letters*. Theoretical calculations suggest a much greater range of tuning is possible than was seen experimentally.

A new type of spin transistor was proposed based on such tunable spin lifetimes, and was calculated to be competitive with 2018 low standby power CMOS from the ITRS roadmap. The nonmagnetic spin transistor is based on the InAs/GaSb/AISb material system. The spin orbit interaction in this system is exceptionally strong, and as a result the spin filtering effects of carriers moving through the structure are large enough to be visible at room temperature. By varying a gate voltage in the designed structure the spin lifetime can be reduced by several orders of magnitude. This device has significant gain, but does not require depletion of the conductive channel of the device to achieve the "off" state. We hope this structure would be a lower-power transistor than typical CMOS transistors. This work was performed in collaboration with T. F. Boggess' group at U. Iowa and has appeared in *Applied Physics Letters.*



Measured and calculated spin relaxation rates for an InAs/AISb (110) quantum well. The tuning range is about a factor of 5. The experiment is shown on the left, theory on the right. The theoretical spin lifetime at high electric field is similar to experiment, but at small electric field is much longer than seen experimentally. The sample was grown at HRL and prepared by K. Holabird, A. Hunter, D. H. Chow and J. J. Zinck. Optical measurements of spin lifetimes were done at U. Iowa and theory also done at U. Iowa. This work has appeared in Applied Physics Letters.



Measured and calculated spin relaxation rates for a GaAs/AlGaAs (110) quantum well. The tuning range exceeds an order of magnitude. Red circles are the experiment, black circles the theory for the perfect structure. The red square is the calculation for the quantum well with a single 2 monolayer thick disordered interface. This work has appeared in Physical Review Letters.

We also, in a related work, were able to show that spin lifetimes in the InAs/GaSb/AlSb system were much longer for (110) superlattices than for (001) superlattices. The difference was larger than a factor of 30. We explained this as due to the crystal symmetry of the superlattice in an identical way to the situation for GaAs/AlGaAs. This work, in collaboration with T. F. Boggess' group at U. Iowa, has appeared in *Physical Review B*.

Our exploration of the properties of dynamical spin-polarized excitations in quantum wells also extended to collective modes in quantum wells. Here we considered the dynamics of collective modes in quantum wells with both bulk inversion asymmetry and structural inversion asymmetry. These collective modes were split in energy by the spin-orbit interaction in the quantum wells, suggesting an alternate way to probe the spin orbit interaction in these nanostructures. This is the subject of the paper above co-authored with Ullrich that has appeared in *Physical Review B*.

We also obtained an extensive series of results on g-factors in quantum wells. Here we found orbital quantization effects, whereby the presence of the Landau levels created structures in the dependence of the g-factor on magnetic field and density. Examples are shown in the figures below. As the g-factors will change rapidly with density or field near the places where new Landau levels

become occupied, these calculations will provide guidance for where g-factor tunability will be greatest.



On the left is the density of states for a large magnetic field (so the structure is easier to see). On the right is the g factor for Landau level n as a function of magnetic field.

We have also been able to calculate theoretically some spin lifetimes in self-assembled quantum dots, and compare with experimental measurements on such dots at U. Iowa (dots from D. Deppe's group at UT Austin). The electron spin lifetimes were of the order of 100 ps and the hole spin lifetimes were about a factor of 4 shorter. As these spin lifetimes were shorter than those seen in some other optical measurements, and very much shorter than those seen in electrical measurements at very low temperatures in lithographic dots, we developed a theoretical understanding of spin lifetimes at elevated temperatures in such dots. The picture is that phonons in the lattice can scatter from the electrons in the quantum dots, and lead to decoherence. A simple calculation of spin-orbit effects in phonon scattering led to spin relaxation times comparable to the experimentally-observed spin relaxation times at hose temperature is negligible, however, leading to the much longer spin relaxation times at those temperatures seen in other experiments in lithographic quantum dots.

Finally, we prepared and submitted a paper describing an extensive set of spin coherence time calculations for a wide variety of bulk and quantum well III-V and II-VI systems, comparing with all of the literature we were aware of. This paper describes fully the theoretical framework within which we calculate these spin coherence times, and presents many new results on systems. This should provide an excellent resource for researchers interested in predictions of spin lifetimes and spin coherence times in just about any III-V or II-VI system.

Theory of inhomogeneous spin transport and spin injection in nonmagnetic and magnetic semiconductors

We have predicted a new mechanism for the spontaneous generation of spin-polarized packets at room temperature in nonmagnetic semiconductors. This effect, which we refer to as the spin Gunn effect, is a spintronic analog of the Gunn effect. We have discovered that the mobility of an electron

gas is dependent on the spin polarization of the electron gas, and in addition the mobility of that polarized electron gas is highly spin-dependent. As a result, whenever inhomogeneous electric fields are present in a system the drift current is different for spin-up and spin-down carriers, leading to an accumulation of spin polarization. We propose that at room temperature in nonmagnetic GaAs or InP (materials in which the ordinary Gunn effect produces spontaneous time-dependent inhomogeneous electric fields), spin-polarized pulses of current should form with room-temperature spin polarization ~90%. This work appeared in *Physical Review Letters*.



(Left) Schematic of an unpolarized electron sea, showing the scattering time for electrons is the same for up and down spins no matter what the scattering mechanism is. (Right) Schematic of a polarized electron sea, showing that the scattering time for electrons differs for up and down spins, and can be larger or smaller for the majority spins, depending on the scattering mechanism.

We also have proposed a spintronic analog to the heterojunction bipolar transistor (HBT), referred to as the heterostructure unipolar spin transistor (HUST). The HBT was proposed to eliminate leakage current from the base to the emitter under operating conditions of the bipolar transistor. The HUST similarly eliminates the leakage current from the base to the collector under the operating conditions of the unipolar spin transistor. This work has appeared in *Journal of Applied Physics.*



(Left) Original proposal of the homojunction unipolar spin transistor, showing the dropping of the barrier for carriers to leak from base to collector. (Right) new proposal of the heterostructure unipolar spin transistor, showing that the barrier for majority carriers to leak from base to collector is high.

A previously unresolved problem in spin LED's was the degree of circular polarization for in-plane emission in GaMnAs spin-LED's. Naïve calculations indicated that the polarization should be very small. We performed more accurate calculations and traced the size of the effect to the maintenance of orbital coherence upon injecting spin-polarized holes from the barrier in the spin-LED into the emitting quantum well. Our calculations are consistent with the measurements of the UCSB Awschalom group and also of those of Ohno at Tohoku University. This work has been submitted to *Applied Physics Letters.*

An exceptionally large magnetoresistive effect (3000%) was discovered in GaMnAs nanoconstrictions by the Molenkamp group in 2003. We provided the first theory of this effect, arguing that the enhancement of the magnetoresistive effect originated from the dependence of the tunnel barrier on the relative magnetization of the two regions on either side of the barrier. For parallel magnetization

the barrier is much thicker and taller for one spin direction, whereas for antiparallel magnetization the barrier is the same for each spin direction. This dramatically enhances the magnetoresistance. The first paper on this effect, a combined theory/experiment work, has appeared in *Physical Review Letters*.



Upper left: scanning electron micrograph of the GaMnAs double nanoconstriction. Upper right: resistance of the double nanoconstriction structure, showing 3000% magnetoresistance. Lower left: barriers for parallel magnetoresistance. Lower right: barriers for antiparallel magnetoresistance.

We have also derived a drift-diffusion equation for spin polarization in semiconductors by consistently taking into account electric-field effects and nondegenerate electron statistics. This has two extremely significant consequences. First, we identify a high-field diffusive regime that has no analogue in metals. In this regime there are two distinct spin diffusion lengths, upstream and downstream relative to the electric field. Specifically, spin polarization can be transported by the electric field downstream over distances orders of magnitude greater than the intrinsic spin diffusion length. Also, spin polarization upstream is substantially suppressed.

Perhaps the most surprising (and technologically important) consequence of this is that in this highfield regime the spin injection from a ferromagnetic metal into a semiconductor is enhanced by several orders of magnitude. We suggest that the unusual current dependence observed in spin injection experiments involving both ferromagnetic semiconductors and ferromagnetic metals may be traceable to this high-field regime. Furthermore this derivation permits a way around the "conductance mismatch" argument of Schmidt, *et al.*, without employing a tunnel barrier. Thus it might be of use in spin injection into InAs, which naturally forms good Ohmic contacts.

Finally, in collaboration with the Awschalom group at UCSB we have proposed a magnetic bipolar transistor. We predict that the presence of a magnetic base in such a structure has a dramatic spin filtering effect on current flowing from the emitter to the collector. This work has appeared in *Applied Physics Letters*.

Theory of nuclear spin coupling to electronic spin, and the implications for all-optical manipulation of nuclear spin

We have calculated the magnetic fields arising from polarized nuclei in semiconductor quantum wells. These magnetic fields have three components. There is a dipolar magnetic field from the nuclei acting on the electrons, a hyperfine field from the nuclei acting on the electrons, and a hyperfine field from the nuclei acting on the electrons acting on the nuclei. We have calculated each of these in turn, and predicted the detailed time dependence of these fields under the conditions of optical pumping (dynamic nuclear polarization). We believe these fields could be used to manipulate electron spins by changing the overlap of the electron spin wavefunction with the nuclei.



Induced dipolar field from the nuclei as a function of time and position across a parabolic quantum well. This highly localized magnetic field could be used to manipulate spins by electrically pushing them back and forth across the region of nuclear polarization.

We have also explored tuning the nuclear spin relaxation time in nanostructures and applied our results to parabolic quantum wells. In order to estimate the effect of the direct interaction between electron and nuclear spins we have evaluated both the nuclear and electronic spin decoherence times due to the hyperfine coupling for low dimensional semiconductor systems. We then derived general formulae applicable to nanostructures for the nuclear and electronic T₁ and T₂ from the hyperfine interaction. The central physical quantity is the electronic local density of states (ELDOS) at the nuclei. We predict that the dominant process for nuclear T₁ in GaAs QW's (and T₂ in others) can be tuned with an electric field by modifying the ELDOS at particular locations. For a parabolic QW (PQW) electric-field tuning of nuclear spin relaxation by many orders of magnitude is possible; this tuning is possible at temperatures at least as high as 30K and is robust to nuclear spin diffusion. We have also calculated the effects of nuclear spin diffusion properly by considering the ELDOS and inhomogeneous nuclear magnetization. These calculations indicate non-exponential long-time nuclear dynamics. This work has appeared in *Physical Review Letters*.

For GaAs QW's we propose two different experimental configurations to demonstrate the electric field tunability of the nuclear T_1 . The same approaches can be used to tune nuclear T_2 and electronic spin decoherence in other material systems. In the first configuration, the T_1 of Ga and As nuclei in the nanostructure depends on the occupancy of conduction subbands, decreasing stepwise as the number of occupied conduction subbands (and hence the density of states) increases. Manipulation of the QW density, and implicitly the number of occupied subbands, can be accomplished with a gate voltage, permitting the manipulation of T_1 . In the second configuration, we consider a single delta-doped layer of a different material (such as In) inserted at a specific position inside the QW. The tunability of T_1 of these nuclei comes from the change in the electronic wave functions due to the applied electric field.



The position dependence of $(T_{1n}T)^{-1}$ for different values of the external electric field [(a) thick PQW and (c) thin PQW]. The field dependence of $(T_{1n}T)^{-1}$ for δ -doped layers situated at different position across the QW [(b) thick PQW and (d) thin PQW].

Theory of Si/Ge quantum dots in inhomogeneous electric fields

We proposed a new method of teleportation, using only single photons (no photon Bell states), from a spin state in one quantum dot to the spin state in another quantum dot. The process involves sequential entanglement of a single photon with a single spin. First a "destination spin" is entangled with a photon in a microcavity through Faraday rotation. Then the photon (now entangled with the destination spin) is sent to the "origin" and kept until teleportation is desired. When teleporting a spin is to occur, the photon is entangled with the spin at the origin. We now have a three-particle entangled state (two spins and one photon). Measurement of the polarization direction of the photon and of the origin spin yields two bits of classical information. When these are sent to the destination, and single-spin rotations are done (or not) based on those bits, the state of the destination spin becomes identical to the original state of the origin spin, thus completing teleportation. This work has appeared in *Physical Review Letters.* The analysis in this paper applies to general dots, not just to Si/Ge quantum dots.



(Left) schematic of a multi-qubit teleportation scheme. (Right) schematic of the teleportation apparatus for a single qubit, including the microcavities in which the spin and photon interact.

We have also performed our first calculations of the g factors of quantum dots. We find an entirely new effect that dramatically changes the values of these g factors from those calculated previously. Similar to the effect known for paramagnetic impurities in solids (van Vleck theory), the presence of the quantum dot confining potential quenches the orbital angular momentum in the quantum dot. Thus the g factor found for quantum dots is much closer to g=2 than previously expected. We have compared with experimental measurements, which appear in decent agreement with our calculations. Our calculations have been done in a full quantum dot calculation that includes the multiband electronic structure, strain, piezoelectric effects, deformation potentials, and shape. We predict that measurements of the g factors of electrons and holes, both in the growth direction and in-plane, will provide a detailed image of the shape of the quantum dot. This work has appeared in *Physical Review Letters*.



(Left) the g factor for a colloidal InAs quantum dot as a function of the transition energy (size) of the dot. In the limit of large dots the g factor approaches the bulk value. For smaller dots the g factor differs greatly from other calculations coming from quantum confinement. (Right) growth-direction g factor for self-assembled InAs/GaAs quantum dots as a function of transition energy, showing good agreement with experimental measurements for big quantum dots.

We also explored two-qubit gates in Si/Ge quantum dots. One of the significant challenges in realizing quantum information processing based on Si/Ge quantum dots is to perform two-qubit gates. The key to an accurate quantum XOR, for example, is precise control of the overlap of the wavefunctions of two adjacent dots under the application of an electric field. We have found that the spatially indirect character of the electronic states of a Si/Ge quantum dot permit this kind of precise control. Shown in the figure below is the wavefunction for a single excess electron in a quantum dot for an applied field of 24 mV/nm and an applied field of 26 mV/nm. The difference is startling, as the electron moves from being confined at the apex of the dot to being confined at the base of the dot. This suggests a pseudo-digital way of manipulating the electron spins of two adjacent dots. If we assume that these two dots are separated by 35 nm, then if both electrons are confined at the apex of their respective dot the exchange interaction is ~20 microeV. If both electrons are confined at the base of the base of the exchange interaction is the much larger ~500 microeV. If, however, one electron is at the base and the other at the apex, then the exchange interaction is negligible.



electronic wavefunction for an electric field of (a) 24 mV/nm and (b) 26 mV/nm. (c) schematic of exchange interaction between two dots separated by 35 nm as the electric field is modified. We assume the switching field from the apex to the base differs for the two dots.

A quantum dot spin LED provides a test of carrier spin injection into a qubit, as well as a means of analyzing carrier spin injection in general and local spin polarization. The polarization of the observed light is, however, significantly influenced by the dot geometry so the spin may be more polarized than

the emitted light would naively suggest. We have calculated carrier polarization-dependent optical matrix elements using 8-band strain-dependent k.p theory for InAs/GaAs self-assembled quantum dots (SAQDs) for electron and hole spin injection into a range of quantum dot sizes and shapes, and for arbitrary emission directions. The observed circular polarization does not depend on whether the injected spin-polarized carriers are electrons or holes, but is strongly influenced by the SAQD geometry and emission direction. Calculations for typical SAQD geometries with emission along [110] show light that is only ~5% circularly polarized for spin states that are 100% polarized along [110]. Therefore observed polarizations of ~1% imply a spin polarization within the dot of ~20%. We also find that measuring along the growth direction gives near unity conversion of spin to photon polarization, and is the least sensitive to uncertainties in SAQD geometry. This work has appeared in *Physical Review Letters*.



Left: Polarization as a function of spin polarization and light emission direction for a SAQD, Middle: Polarization along [110], and Right: Polarization along [110], both as a function of elongation.

We have also performed calculations for Si/Ge quantum dots. Shown below are the wavefunctions for 2nm by 8nm Ge dots in Si. The electron wavefunction is in red, the hole wavefunction in blue. We calculate that for these dots the optical transitions are indirect, and the band gap is about 0.5 eV. For optical generation of spin polarized carriers we predict the spin polarization generated by 100% circularly polarized light will be 83% for such dots. We are currently engaged in exploring the fidelity for generation and detection of spin polarized carriers via circularly polarized light.



Electron (red) and hole (blue) wavefunctions in a germanium dot.

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Papers presented at meetings, but not published in conference proceedings

Invited:

M. E. Flatté, "Performance of a Spin-Based Field-Effect Transistor", Fourth International Conference on the Physics and Applications of Spin-Related Phenomena in Semiconductors (PASPS-IV), Sendai, Japan, August 17, 2006.

M. E. Flatté, "Quantum teleportation and other applications of spin-photon entanglement in semiconductors", Spin and Charge Effects at the Nanoscale (SCEN06), Pisa, Italy, June 5, 2006.

M. E. Flatté, "Spin-based quantum computation in semiconductors", Spin and Charge Effects at the Nanoscale (SCEN06), Pisa, Italy, June 3, 2006.

M. E. Flatté, "Spin-dependent phenomena in semiconductors", Spin and Charge Effects at the Nanoscale (SCEN06), Pisa, Italy, June 1, 2006.

M. E. Flatté, "Optospintronics: open theoretical issues", KITP Spintronics Conference, Santa Barbara, California, March 20-24, 2006.

M. E. Flatté, "Teleportation of electronic many-qubit states via single photons", American Physical Society March Meeting, Baltimore, Maryland, March 13, 2006.

M. E. Flatté and K. C. Hall, "Performance of spin-based current-gating devices", The 3rd International Symposium on System Construction of Global Network Oriented Information Electronics (IGNOIE 05), Sendai, Japan, January 31, 2006

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Report of Inventions:

"Nonmagnetic semiconductor spin transistor", patent application filed February 28, 2005. Inventors: Kimberley C. Hall, Wayne H. Lau, Kenan Gundogdu, Michael E. Flatté, and Thomas F. Boggess.

"Bipolar Spin Transistors and Applications of the Same", patent application filed May 26, 2004. Inventors: Michael Edward Flatté, Zhi Gang Yu, Ezekiel Johnston-Halperin, David Awschalom.