Dynamic nuclear polarisation in biased quantum wires with spin-orbit interaction

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received 10 October 2007; accepted in final form 21 January 2008
published online 20 February 2008

PACS 85.75.-d – Magnetoelectronics; spintronics: devices exploiting spin polarised transport or integrated magnetic fields
PACS 71.70.Ej – Spin-orbit coupling, Zeeman and Stark splitting, Jahn-Teller effect
PACS 72.25.Pn – Current-driven spin pumping

Abstract – We propose a new method for dynamic nuclear polarisation in a quasi-one-dimensional quantum wire utilising the spin-orbit interaction, the hyperfine interaction, and a finite source-drain potential difference. In contrast with current methods, our scheme does not rely on external magnetic or optical sources which makes independent control of closely placed devices much more feasible. Using this method, a significant polarisation of a few per cent is possible in currently available InAs wires which may be detected by conductance measurements. This may prove useful for nuclear-magnetic-resonance studies in nanoscale systems as well as in spin-based devices where external magnetic and optical sources will not be suitable.

The ability to locally manipulate spin has been the subject of intense research recently. In particular, local control of nuclear polarisation in the vicinity of quantum dots and in wires has diverse uses such as in nuclear-magnetic-resonance (NMR) studies\textsuperscript{[1]} or for control of nuclear spins in devices where external magnetic fields and/or optical sources will not be suitable or convenient as for instance in non-magnetic spin-filtering\textsuperscript{[2]} and qubits\textsuperscript{[3]}. In some very beautiful recent experiments related to spin-based qubits, dynamically-generated nuclear polarisation has been used to control the decoherence of electron spins in quantum dots\textsuperscript{[4,5]}. Nuclear polarisation can also be used to manipulate the electron spin-splitting in quantum wires\textsuperscript{[6]} without using a magnetic field. Local control of nuclear polarisation in quantum wells using a gate contact has now been demonstrated\textsuperscript{[7]}; however, the polarisation itself involved the use of an optical source. In this letter, we propose a new method for dynamically generating and controlling nuclear polarisation, locally and without using magnetic and optical sources, in a nonequilibrium quasi-one-dimensional quantum wire with spin-orbit interaction.

By local we mean the nuclear polarisation is within the wire and not in the bulk surroundings. We argue that the role of spin-orbit interaction in creating a spin-polarised electron distribution cannot in this scheme be replaced with an external magnetic field. We estimate the magnitude and build-up time for the polarisation as around 2.5% and 200 s, respectively, in typical InAs quantum wires which compares favourably with other methods. We discuss possible ways in which the nuclear polarisation may be detected and measured, as for instance through a measurement of the two-terminal conductance\textsuperscript{[6,8]}.

The Overhauser effect\textsuperscript{[9]} is used for dynamically polarising nuclei through their hyperfine coupling with electrons using a magnetic field and an external radio source tuned to the electron Zeeman splitting. The electron spin resonance (ESR) inducing radio source tends to equalise (saturate) the numbers of spin-up and -down electrons even though they have different Zeeman energies — this implies that the chemical potentials of the two spin species must be different and the spin distribution is not in equilibrium. The electron spins at the higher chemical potential ultimately relax with a spin flip to equalise the chemical potentials; and some of these spins can be exchanged with the nuclei. In this manner, a nonzero nuclear polarisation is built up. The key requirement for the Overhauser scheme is the creation of a nonequilibrium electron spin distribution. This usually involves pumping and saturation of the electron spins. In the presence of a magnetic
field, saturation may be attained by, besides ESR, hot electrons [10], or optically through unpolarised light [11]. Hot electrons have been used to generate nuclear polarisation in InSb [12] subjected to a Zeeman field, and more recently, in GaAs [13]. In the so-called optical Overhauser effect, electron spin pumping is achieved using circularly polarised light [11]. However these methods all involve the use of physically large external sources of magnetic field and light making local control of nuclear polarisation difficult, which is the main motivation of our work.

Spin-orbit interaction offers one way where the electron spin degeneracy can be lifted without using an external field. The lifting of electron spin degeneracy by a spin-orbit interaction differs in many ways from that in a magnetic field. In particular, no electron spin polarisation \( \sigma \) can be created solely through spin-orbit interaction in a single sub-band quantum wire carrying a current [14]. However, it can be shown that in a quasi-one-dimensional model where the spin-orbit coupling mixes different sub-bands, it is possible to obtain a finite \( \sigma \) by passing an electric current through the wire [15]. This will be the model we shall consider. Spin-orbit interaction in semiconductor devices is usually of the Rashba or Dresselhaus kind. For simplicity, our analysis focuses on a Rashba interaction, but our results will hold even in the presence of a Dresselhaus interaction.

For strong spin-orbit coupling, the left- and right-moving charges in the lowest two sub-bands of transverse momentum quantisation can become, at sufficiently large wave-vectors, completely spin-polarised with opposite spin orientations for the two directions [15]. In the same multi-band model, we show that a small (partial) \( \sigma \) occurs even when the spin-orbit coupling is weak, typical in quantum wires. As the left- and right-moving electrons have overall opposite polarisations, an applied potential difference creates an equilibrium electron spin distribution. Therefore, we show how nuclear polarisation develops in the quantum wire due to the hyperfine coupling of the nuclei with the nonequilibrium electrons.

It is important to note that merely polarising the conduction electron spins does not in general lead to dynamic nuclear polarisation. We discuss later that dynamic nuclear polarisation is not possible by simply using an external magnetic field to polarise the conduction electrons instead of spin orbit interaction.

Let us first discuss how spin-orbit coupling in a quasi-one-dimensional wire can lead to electron spin polarisation. Consider a two-dimensional gas (2DEG) of electrons in the \((x, z)\)-plane. The geometry of the quantum wire is such that the electrons are confined in the \(y\)- and \(z\)-directions and the transport “channel” is along the \(x\)-axis. We assume a hard-wall confinement at \(z = 0\) and \(z = W\), and at \(y = 0\) and \(y = \delta\). The Hamiltonian of the 2D electrons is

\[
H = \frac{1}{2m}(p_x^2 + p_z^2) + V(z) + H_{SO},
\]

where

\[
H_{SO} = \frac{\hbar k_{SO}}{m} (\sigma_z p_x - \sigma_x p_z)
\]

is the Rashba spin-orbit interaction arising from the 2DEG’s asymmetric confinement in the \(y\)-direction. Its interaction strength, \(k_{SO}\), may be controlled by an external gate voltage [16]. \(\sigma_x\) and \(\sigma_z\) are Pauli matrices in the space of electron spin.

In the absence of the Rashba interaction, the scattering states are labelled by the sub-band index \(n\) of transverse-momentum quantisation:

\[
\psi_{n \kappa \sigma} = e^{i k_x x} \sin(k^{(n)}_z) z |\sigma\rangle,
\]

where \(k^{(n)}_z = n\pi/W, n = 1, 2, \ldots\), and the energy eigenvalues are \(E^{(0)}_n(k_z) = \frac{\hbar^2 k_z^2}{2m} + \frac{hn\pi^2}{2mW^2}. |\sigma\rangle = |\uparrow\rangle, |\downarrow\rangle\) are the eigenstates of \(\sigma_z\). The \(\sigma_z p_x\) term in eq. (2) respects this sub-band quantisation but the \(\sigma_x p_z\) term mixes sub-bands whose indices differ by an odd number as well as the spin eigenstates of \(\sigma_z\). It is convenient to regard this mixing term as a perturbation, and the rest as the bare Hamiltonian. Then, the spatial part of the bare eigenstates has the same form (eq. (3)) as that in the absence of spin-orbit interaction. The matrix elements of the second term in the spin-orbit interaction are

\[
H'_{SO} = \frac{\hbar^2 k_{SO}}{mW} \frac{2n'}{n'^2 - n^2} |1 - (-1)^{n'|n}| \delta_{\sigma,-\sigma'},
\]

where \(n'\) is such that the electrons are confined in the \(y\)- and \(z\)-directions and the transport “channel” is along the \(x\)-axis. The energy eigenvalues of \(H_{trunc}\) are

\[
E_{n\sigma(1)} = \frac{\hbar^2 k_z^2}{2m} \pm \frac{\hbar^2 k_{SO}k_z}{m},
\]

\(n = 1, 2\), and \(\Delta_{SO} = \frac{\hbar^2 k_{SO}k_z}{mW}\). The eigenvalues of \(H_{trunc}\) are

\[
\epsilon_{1a(2b)} = \frac{E_{21} + E_{21}}{2} \pm \frac{1}{2} \sqrt{(E_{21} - E_{11})^2 + 4\Delta_{SO}^2},
\]

\[
\epsilon_{1b(2a)} = \frac{E_{11} + E_{21}}{2} \pm \frac{1}{2} \sqrt{(E_{21} - E_{11})^2 + 4\Delta_{SO}^2}.
\]

The eigenvectors are also easily found. In the spin basis \(|\uparrow\rangle, |\downarrow\rangle\), we have

\[
\psi_{1a} = e^{i k_x x} \sqrt{\frac{2}{W'}} N_1 a \left( \frac{\sin(\pi z/W)}{i g_{1a}(k_z) \sin(2\pi z/W)} \right),
\]

\[
\psi_{1b} = e^{i k_x x} \sqrt{\frac{2}{W'}} N_1 b \left( \frac{ig_{1b}(k_z) \sin(2\pi z/W)}{\sin(\pi z/W)} \right),
\]
The mixing functions \( g_{1a,b}(k_x) \) have been re-expressed as functions of energy \( E \) as \( \sigma_e \) is to be calculated at a fixed \( E \) rather than a fixed \( k_x \). Clearly, in the absence of inter-sub-band mixing, \( \langle \sigma_z(E) \rangle \) is zero. When the spin-orbit interaction is weak (\( k_{SO}W < 1 \)), and the energy is far from the region of sub-band mixing, the mixing functions \( g_{1a(b)} \) will be small compared to unity and \( \langle \sigma_z(E) \rangle \approx 2(\langle g_{1b}(E,k_{SO}) \rangle^2 - \langle g_{1a}(E,k_{SO}) \rangle^2) \). In this regime, the energy-wave vector relations for the 1a and 1b sub-bands to \( O(k_{SO}^2) \) are, respectively, \( k_x \approx -k_{SO} \pm \sqrt{2mE/h^2 - \pi^2/W^2} \) and \( k_x \approx k_{SO} \pm \sqrt{2mE/h^2 - \pi^2/W^2} \), which we can use to express \( g_{1a} \approx -\Delta_{SO}/(E_{2\uparrow} - E_{1\uparrow}) \) and \( g_{1b} \approx -\Delta_{SO}/(E_{2\downarrow} - E_{1\downarrow}) \) as functions of \( E \):

\[
\langle \sigma_z(E) \rangle = g_{1b}(E,-k_{SO}) - 2mW^2\Delta_{SO} \left[ 1 + \frac{4k_{SO}W^2}{3\pi^2} (-k_{SO} \pm k_{F}^{(1D)}) \right].
\]

Here \( k_{F}^{(1D)} = \sqrt{2mE/h^2 - \pi^2/W^2} \) is the 1D Fermi wave vector in the n = 1 sub-band in the absence of Rashba coupling. It follows that for weak spin-orbit coupling, the electron spin polarisations for right (R) movers and left (L) movers at energy \( E \) are, respectively,

\[
\langle \sigma_z(E) \rangle_{RL} \approx \pm 6 \left( \frac{16}{\pi^2} \right)^3 (k_{SO}W)^3 (k_{F}^{(1D)}W)
\]

Note that unlike an external magnetic field, the right and left movers have an opposite net polarisation for both strong and weak Rashba coupling. Thus, by imposing a net electrical current which imbalances the left- and right-moving electrons, we are able to satisfy one of the requirements for the Overhauser effect; namely, we have a non-equilibrium distribution of electron spin. Spin-orbit-interaction–mediated electron spin polarisation can be controlled non-magnetically also by applying a local strain [19]; however, this will not fulfil our requirement of compact external sources.

In fig. 2 we show a numerical calculation for the electron spin polarisation \( \langle |\sigma_z| \rangle \) for the lowest two sub-bands (1a and 1b) as a function of the dimensionless spin-orbit interaction \( k_{SO}W \) at different values of the energy \( E \), using eq. (12). The range of values of energy shown spans, approximately, the range of Fermi energy over which only the two lowest sub-bands (1a and 1b) are occupied. Note that the polarisation undergoes a significant change when \( k_{SO}W \) reaches some large value; this is especially true at low energies. One can understand this change by looking at the spin structure of the 1a and 1b sub-bands in fig. 1b. When the energy is small enough, the two sub-bands have opposite spin polarisations, and total polarisation is the difference of the polarisations of the two. As \( k_{SO}W \) is increased, the sub-bands move down in energy until, eventually, the energy will exceed the value at which both sub-bands have the same polarisation, which causes a significant increase in \( \langle |\sigma_z| \rangle \).
The rate of change of transition probability for a hyperfine-mediated scattering, say with $\Delta m_I = -1$, is

$$w_{kk'} = \frac{8\pi}{\hbar} GA^2 \nu_f,$$  \hspace{1cm} (16)$$

where $\nu_f = m_j/(2\pi\hbar^2 k_{hyp}^2)$ is the (1D) density of final states and $G = \sum_{n,m=-l} |I_{n-m,1}|^2 = \frac{3}{2} I (I + 1)$, is the appropriate average value of $|I|^2$ assuming that the nuclear moments are unpolarised. We now obtain an expression for the rate of electron flips $w(R \downarrow; L \uparrow)$ from the right-moving $|\downarrow\rangle$ state to the left-moving $|\uparrow\rangle$ state following the general prescription of ref. [20]. The distribution functions of the right-moving and left-moving electrons are $f_{R(L)}^{n,s}(k_x) = \exp[\epsilon_{n,s}(k_x) - \mu_{R(L)}]/k_B T$. The energies $\epsilon_{n,s}(k_x)$ have been obtained in eq. (7) and eq. (8). We have not considered magnetic fields here but that can also be incorporated in principle. The rate of electron flips per nucleus from $R \downarrow$ to $L \uparrow$ is

$$w(R \downarrow; L \uparrow) = \int_{k_{min}}^{k_{max}} dw_{kk'} f_{R}^{n,s}(k_x) [1 - f_{L}^{n',s'}(k'_x)].$$  \hspace{1cm} (17)$$

Here $k_{min}$ and $k_{max}$ correspond to the minimum and maximum values of $k_x$ at which the 1 $\uparrow$ and 2 $\downarrow$ bands cross (see fig. 1). We assume that the temperature is low compared to the inter sub-band separation as well as the potential difference and choose the left and right chemical potentials to lie in the energy band where spin polarisation is possible. The energy conservation condition for the above transition is $\epsilon_{n,s}(k_x) = \epsilon_{n',s'}(k'_x)$. Starting with unpolarised nuclei, the initial rate of change of the polarisation $\langle I_z \rangle$ per nucleus at the centre of the wire is $-w(R \downarrow; L \uparrow) - w(L \uparrow; R \downarrow)$, i.e.

$$\frac{d\langle I_z \rangle}{dt} = -\frac{8\pi}{\hbar} GA^2 (\mu_L - \mu_R) \sum_{n,s,n',s'} \nu_{ns,n's'}.$$  \hspace{1cm} (18)$$

Here scattering from $L \uparrow$ to $R \downarrow$ is suppressed because $\mu_R < \mu_L$. For $I = 1/2$ or at long times in general, $\langle I_z \rangle + I$ will decay exponentially. A spin-down nuclear polarisation is thus built up.

When spin-orbit coupling is weak, and the Fermi energy is far from the (avoided) intersection of the sub-bands, we have shown earlier that the right movers in the $n = 1$ sub-bands can have either spin orientation with a small excess of spin-down electrons. Likewise the left movers have a small excess of spin-up electrons. Thus spin-flip backscattering of spin-down right movers is not completely cancelled by the spin-flip backscattering of the spin-up right movers. Forward scattering does not contribute as in this case the two competing spin-flips occur at the same rate. The initial rate of change of $\langle I_z \rangle$, therefore,
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is suppressed by a factor $|\langle \sigma_z(\epsilon_F) \rangle|$. The initial rate $T_n^{-1}$ of build-up of the polarisation ($I_z$) of a nucleus is

$$T_n^{-1} = \frac{8\pi}{\hbar} GA^2 |\langle \sigma_z(\epsilon_F) \rangle| \Delta \mu \sum_{n,ns,n's'} \nu_{ns} \nu_{n's'}$$

$$\approx \frac{3GA^2}{4} \frac{m^2 k_{SO}^3}{9 \pi^2} \left( \frac{W}{\delta} \right)^2 \Delta \mu,$$  \hspace{1cm} (19)

where $\Delta \mu = |\mu_L - \mu_R|$ and $\nu_{n,s} \approx m/(2\pi \hbar^2 k_F^{(1D)})$. We used eq. (14) for $|\langle \sigma_z(\epsilon_F) \rangle| \ll 1$, which is the expected experimental situation. We considered only the lowest sub-bands. At finite temperatures exceeding $|\Delta \mu|/k_B$, the polarisation build-up rate decreases by an amount proportional to the temperature owing to Korringa relaxation. Equation (19) is the main result of the paper.

Figure 3 shows a numerical calculation for $T_n$ for an InAs/GaSb heterostructure with effective electron mass $m = 0.027m_e$, $I_{As} = 3/2$ and $I_{In} = 9/2$, and confinement ratio $(W/\delta)^2 = 10$ (typical ratio of sub-band energy spacings in GaAs devices). The atomic density is $3.6 \times 10^{28}$ m$^{-3}$, hyperfine couplings are of the order of $100 \mu$eV per atom (see, e.g., ref. [21]), and the Rashba coupling from ref. [16] is $k_{SO} = 1.4 \times 10^{-7}$ m$^{-1}$. The average value of $G$ is 9.5. For a small potential difference $\Delta \mu = 1$ meV $\lesssim \epsilon_F$, and using $\epsilon_F = h^2 (k_F^{(1D)})^2 / 2m \approx \Delta \mu$, we estimate from eq. (19) $T_n \approx 200$ s. Estimating $W \approx 1/k_F^{(1D)}$, we have $\langle I_z \rangle / I \approx 2.5 \times 10^{-2}$ for In atoms. The build-up rate is very sensitive to the spin-orbit coupling strength and the confinement asymmetry. The small number of polarised spins may pose a considerable problem for detection by conventional NMR. Though the situation can be further improved by having multiple quantum wires parallel to each other, this is not ideal.

We would like to suggest two methods of detection. Firstly, because $\langle I_z \rangle \neq 0$, the final term of the hyperfine Hamiltonian (15) produces an effective magnetic field. By applying an in-plane magnetic field as a reference, it is possible to infer the strength of the effective hyperfine field and hence the polarisation from two-terminal conductance measurements [6,8]. Secondly, since polarised radioactive nuclei have an anisotropic decay pattern [22], it should be possible to detect polarisation by measuring the beta decay statistics [23]. In this case, $^{114}$In possesses a half-life of 50 days, and may prove suitable.
Dipolar interactions of the nuclei will reduce the steady-state nuclear polarisation through spin diffusion out of the boundary of the quantum wire, and spin-flip processes that do not conserve total spin. Small magnetic fields can be used to strongly suppress such processes [24].

In conclusion, we have shown how gate-controlled local dynamic nuclear polarisation is possible in a quasi–one-dimensional wire with spin-orbit interaction subjected to a finite source-drain potential. A significant polarisation of a few percent can be easily attained in present InAs devices in about 200 s, and may be detected by conductance measurements [6,8]. The polarisation is very sensitive to the strength of (gate-controlled) spin-orbit coupling as well as the asymmetry of confinement in the quantum wire. This method may prove useful in NMR studies in semiconductor devices and in the local control of electron spin decoherence in spin-based devices.

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VT thanks the support of TIFR and a DST Ramanujan Fellowship (sanction no. 100/IFD/154/2007-08). ACHC thanks Trinity college, Cambridge for support. NRC acknowledges support by EPSRC grant GR/S61263/01.

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