Theory of NMR in semiconductor quantum point contact devices

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We describe how a local nonequilibrium nuclear polarization can be generated and detected by electrical means in a semiconductor quantum point contact device. We show that measurements of the nuclear-spin-relaxation rate will provide clear signatures of the interaction mechanism underlying the "0.7" conductance anomaly. Our analysis illustrates how nuclear-magnetic-resonance methods, which are used extensively to study strongly correlated electron phases in bulk materials, can be made to play a similarly important role in nanoscale devices.

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I. INTRODUCTION

The confinement of electrons to nanoscale regions in semiconductor devices leads to the formation of low-dimensional quantum systems, which are highly susceptible to quantum fluctuations. Electron-electron interactions can then have dramatic effects. Indeed, experimental studies of nanoscale semiconductor devices have uncovered evidence of many very interesting strong-correlation phenomena—including the Kondo[1] effect, spin-charge separation,[2] and the "0.7 effect."[3]

The 0.7 effect refers to a series of anomalous features that are observed in the conductance of quantum point contact (QPC) devices.[3,4] The anomalous conductance features observed are believed to arise from electron-electron interactions in the quasi-one-dimensional (1D) geometry of the QPC, but the question of how interactions lead to these conductance anomalies is hotly debated. Many theoretical models have been proposed to account for the observations: including spontaneous spin polarization,[5–8] the Kondo effect,[4,9,10] and the spin-incoherent Luttinger liquid.[11] These theories make similar predictions for the conductance, the property that is usually measured, precluding a conclusive experimental distinction between them.

In this paper, we show that the nature of the electronic state responsible for the 0.7 effect can be uncovered through a variant of nuclear-magnetic resonance (NMR). NMR is a very powerful tool that is widely used to study strongly correlated electronic phases in bulk materials. The very small active volume in a QPC would make it extremely difficult to perform a conventional NMR measurement, owing to the small number of nuclei coupled to the electrons. Here we describe how NMR can be performed on a QPC by generating and detecting a *local* nonequilibrium nuclear-spin polarization. We then turn to discuss the nuclear-spin-relaxation rate in the vicinity of the 0.7 effect. We show that different interaction mechanisms that can lead to similar features in conductance have very different effects on the nuclear-spin-relaxation rate. We identify clear experimental signatures which distinguish between different proposed scenarios for the 0.7 effect. Our work shows how electrical manipulation of local nuclear-spin polarization opens the possibility of performing NMR in nanoscale electronic systems.

II. GENERATING AND DETECTING NUCLEAR SPIN POLARIZATION

The local NMR scheme that we propose relies on the possibility to generate a nonequilibrium nuclear-spin polarization in the vicinity of a QPC. This can be achieved in various ways using purely electrical means. Current-induced breakdown of the $\nu=2/3$ fractional quantum Hall state[12] has been used to create large local nuclear polarizations in QPCs.[13] Alternatively, a nonequilibrium nuclear polarization can be achieved by the selective backscattering of the spin-polarized edge states of the $\nu=2$ quantum Hall state;[14–16] this creates a region in which the edge states are out of spin equilibrium and their relaxation leads to a local dynamic nuclear-spin polarization. Simple gate geometries can be envisaged for which this nonequilibrium spin polarization is placed at the center of a second point contact. In both these methods the dynamic nuclear polarization is generated at nonzero magnetic field, so its use in probing electron systems at low field would require a field sweep that is shorter than the nuclear-spin equilibration time.[17] A recent proposal has shown that, through spin-orbit coupling, it is possible to generate a local dynamic nuclear-spin polarization in a biased quantum wire at zero magnetic field.[18]

The presence of nuclear polarization in the vicinity of the QPC can be detected by its effect on the two-terminal conductance. The effect arises from the Overhauser shift of the electronic Zeeman energy from hyperfine contact interactions. For GaAs devices, even a small change in the nuclear polarization can shift the Zeeman energy by a substantial fraction of k_BT, leading to a sizeable change in conductance of the QPC. To illustrate the sensitivity of this resistive detection scheme, we model the device by a quasi-1D wire with Hamiltonian

$$H=\sum_{s,k,\sigma}\left[\epsilon_s+\frac{\hbar^2k^2}{2m}+\frac{\sigma}{2}g\mu_BB\right]\hat{c}^{\dagger}_{nk\sigma}\hat{c}_{nk\sigma}+A_s\sum_i\vec{I}_i\cdot\vec{S}(\mathbf{R}_i), \tag{1}$$

where $\epsilon_s\equiv\hbar\omega_y(s+1/2)$ are the edges of the in-plane subbands (we assume that the out-of-plane subband spacing $\hbar\omega_z$ is very large) and $\sigma=\pm$ are the spin polarizations. $\vec{I}_i$ is the spin of nucleus i at location $\mathbf{R}_i$, which is coupled to the

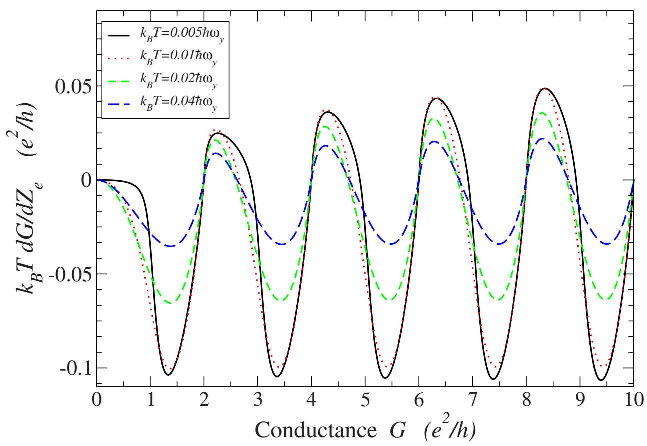

FIG. 1. (Color online) The sensitivity of the QPC device to small changes in the nuclear polarization at fixed gate voltage is conveniently represented by $\frac{dG}{dZ_e}|_n$. This is plotted as a function of the conductance (which varies with gate voltage) for a noninteracting electron gas with subband spacing $\hbar\omega_y$ and $Z_e=0.03\hbar\omega_y$.

electronic spin density $\vec{S}(\mathbf{r})$ via the hyperfine contact interaction. The net electron Zeeman energy, with Overhauser shift, is therefore

$$Z_e \equiv g\mu_B B + A_s n_{\text{nuc}}\langle I^z\rangle, \tag{2}$$

where n_{nuc} is the nuclear density. We neglect the nuclear Zeeman energy, assuming it to be small compared to electronic energy scales. For quantitative estimates we choose parameters for typical GaAs QPCs.[19]

The linear conductance of the quasi-1D wire is

$$G(\mu,Z) = \frac{e^2}{h}\sum_{s,\sigma} f(\epsilon_s + \sigma Z_e/2), \tag{3}$$

where $f(z)\equiv[e^{(z-\mu)/k_BT}+1]^{-1}$, T is the temperature, and μ is the chemical potential. Owing to the importance of electrostatic forces, a fixed gate voltage, V, on the QPC fixes the 1D electron density in the channel, $n=c(V-V_0)/e$ (where c is the capacitance per unit length and V_0 the pinch-off voltage). Thus, the sensitivity of G to small changes in nuclear polarization [hence Z_e (2)] at fixed gate voltage can best be expressed by the derivative of G with respect to Z_e *at fixed particle density*, n.

Figure 1 shows $\frac{\partial G}{\partial Z_e}|_n$ over a range of temperatures as a function of G (which eliminates device-specific properties). The conductance is most sensitive to changes in Z_e when G is away from a quantized value. The conductance changes by $\sim 0.01e^2/h$ when Z_e changes by $\sim k_BT/10$: for GaAs at $T=50$ mK, this corresponds to a change in the fractional nuclear polarization of $\Delta I^z/(2I)\simeq 0.3\%$.

By monitoring the rate of change of the two-terminal conductance, the nuclear-spin-relaxation rate, T_1^{-1}, for nuclei in the QPC may be measured. Nuclear-spin relaxation is dominated by coupling to the electrons and is determined by their low-frequency spin dynamics via[21]

$$T_1^{-1}(\mathbf{R}) = \frac{A_s^2}{2\hbar^2}\int_{-\infty}^{\infty} dt\langle S^+(\mathbf{R},t)S^-(\mathbf{R},0)\rangle, \tag{4}$$

where the angled brackets denote thermal and quantum averages. Since there are many nuclei per electron (of the order of 10^6) the gradual nuclear depolarization leads to a smooth evolution of G over the time scale T_1; this time is much longer than electronic time scales (see below) so many electrons pass through the QPC and contribute to the measurement of G.

We shall calculate the nuclear-spin-relaxation rate for an electron gas on the first conductance riser, $0\le G\le 2e^2/h$,[22] where experiments show the appearance of the anomalous conductance features of the 0.7 effect.[3] We first calculate the nuclear–spin-relaxation rate for a noninteracting electron gas before turning to consider the effects of electron-electron interactions within several simple theoretical models of the 0.7 effect.

III. NONINTERACTING 1D ELECTRON GAS

We consider a noninteracting electron gas described by Eq. (1). Restricting attention to the lowest subband ($s=0$) and focusing on nuclei at the center of the quantum wire, we find from Eq. (4)

$$T_1^{-1} = \Gamma_0 \int_{|Z_e|/2}^{\infty} \frac{f(\epsilon)[1-f(\epsilon)]}{\sqrt{\epsilon^2+(Z_e/2)^2}}d\epsilon, \tag{5}$$

where

$$\Gamma_0 \equiv \frac{2\pi A_s^2 m}{\hbar^3 w_y^2 w_z^2} \tag{6}$$

is a characteristic rate and $w_y w_z$ is the root-mean-square transverse area of the lowest subband. For a typical GaAs QPC,[19] $\Gamma_0\simeq 0.5$ Hz. The value of Γ_0 is very sensitive to the value of $w_y w_z$. Our main results, below, concern the dependence of T_1^{-1} on gate voltage and temperature and are independent of this overall scale.

In Fig. 2(a) we show the conductance G and relaxation rate T_1^{-1} as a function of electron density (controlled by gate voltage) for a small Zeeman energy ($Z_e \ll k_BT$). There is a maximum in T_1^{-1} close to the midpoint of the conductance riser. Increasing the electronic Zeeman energy to $Z_e\sim k_BT$ [Fig. 2(b)] leads to the emergence of a plateau at $G=e^2/h$; this is accompanied by a suppression of the peak in T_1^{-1}.

It is instructive to compare these results with the conventional Korringa expression for the nuclear-spin-relaxation rate of a metal, $T_1^{-1}\propto \rho_\uparrow\rho_\downarrow T$, where $\rho_{\uparrow,\downarrow}$ are the densities of states for the two spin species at the Fermi level. The Korringa expression applies when $k_BT\ll\mu$, which for the quantum wire implies that $G\simeq 2e^2/h$. In this regime, we do find that $T_1^{-1}\propto(1/n^2)T$, consistent with the Korringa expression; increasing the Zeeman energy leads to a small *increase* in T_1^{-1}, consistent with an expected increase in $\rho_\uparrow\rho_\downarrow$ at fixed n. However, the Korringa expression does not account for the most dramatic signatures in T_1^{-1}. These occur on the conductance riser, $0\lesssim G\lesssim 2e^2/h$, where $k_BT\sim\mu$. In this regime, we

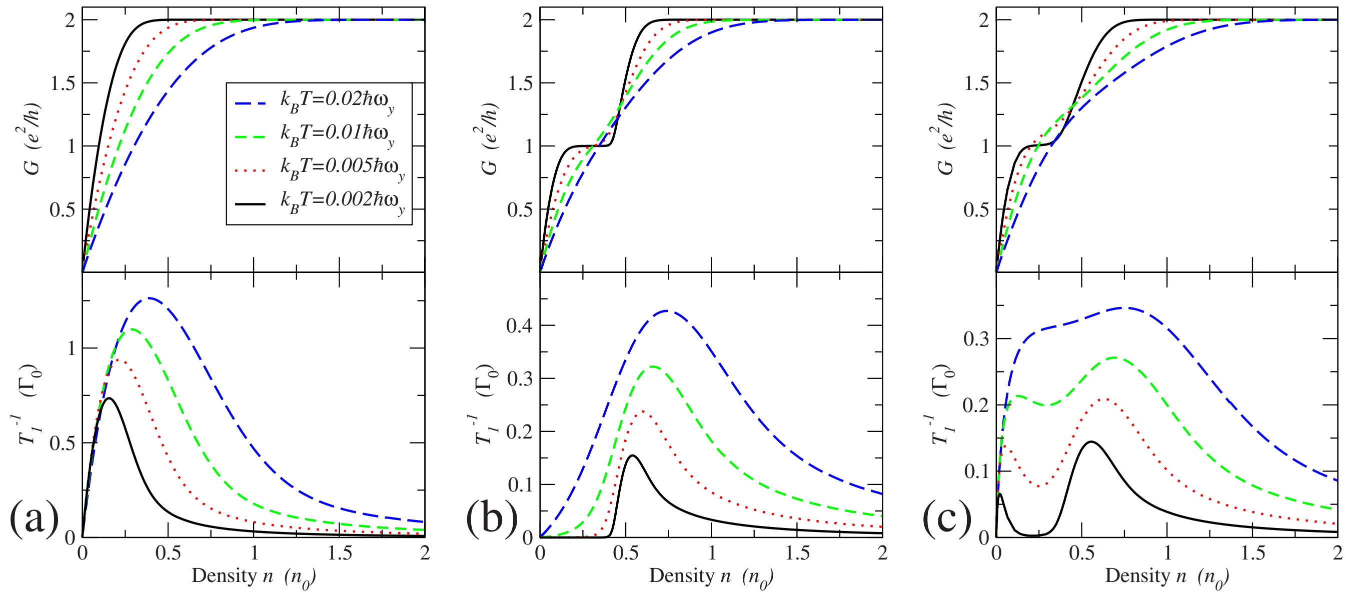

FIG. 2. (Color online) Conductance (top panels) and nuclear-spin-relaxation rate (bottom panels) for a quasi-1D electron gas on the first conductance riser. (a) Noninteracting electron gas with small Zeeman energy, $Z_e=0.001\hbar\omega_y$. (b) Noninteracting electron gas with larger Zeeman energy, $Z_e=0.05\hbar\omega_y$. (c) Electron gas with exchange-enhanced spin splitting [Eq. (7)] with $Z_e=0.001\hbar\omega_y$ and $\gamma=0.1\hbar\omega_y/n_0$. The electron density n is in units of $n_0\equiv\sqrt{m\omega_y/\pi\hbar}$. A typical quantum wire has subband spacing $\hbar\omega_y=20$ K (Ref. 20), for which the illustrated temperatures are T=40, 100, 200, and 400 mK.

find that T_1^{-1} increases more slowly than linear in T. An increase in the Zeeman energy leads to a dramatic *decrease* in the height of the peak in T_1^{-1}; at the same time, the position of the maximum shifts to lie in the regime $e^2/h\lesssim G\lesssim 2e^2/h$ where both spin species are occupied [compare Figs. 2(a) and 2(b)].

IV. EXCHANGE-ENHANCED SPIN SPLITTING

The importance of exchange-enhanced spin splitting was recognized by Thomas *et al.*[3] and has been explored theoretically by various authors.[5] Reilly and co-workers[6,7] provided a simple phenomenological theory that can successfully reproduce many features of the 0.7 effect. The electron gas is assumed to experience a density-dependent exchange splitting, leading to an effective Zeeman energy,

$$Z_{\rm eff}=Z_e+\gamma n, \tag{7}$$

where γ is a phenomenological parameter. (We note that a linear dependence of exchange energy on n is expected for Coulomb interactions, with $\gamma\propto e^2/\epsilon$. However, this model[6,7] overlooks the possible collapse of the spin splitting at larger densities, as found in some microscopic models.[8]) Treating the system as a noninteracting gas with this exchange-enhanced Zeeman splitting leads to the results shown in Fig. 2(c), where γ has been chosen to give conductance features similar to those of the 0.7 effect.[6] Comparing the results for T_1^{-1} with those for noninteracting electrons at the same bare Zeeman energy, Fig. 2(a), one sees that the main effect of exchange is a strong suppression of the peak in T_1^{-1}. This is consistent with the result discussed above that increasing the Zeeman energy leads to a suppression of T_1^{-1}. However, the exchange enhancement of the Zeeman energy leads to a qualitatively new feature: there are now two peaks in T_1^{-1} as a function of density. At very small densities exchange interactions are negligible and T_1^{-1} rises as for the noninteracting gas with small Zeeman energy, Fig. 2(a); at higher densities the increase in exchange splitting at first causes a reduction in T_1, leading to a second peak similar to that for a large Zeeman energy, Fig. 2(b). The observation of a double-peak structure in T_1^{-1} as a function of density (gate voltage) is a clear signature of a density-dependent exchange-enhanced spin splitting.

V. "KONDO" MODEL

Within the "Kondo" model for the 0.7 effect,[4,9] one of the electrons is assumed to become trapped in a quasi-bound state and to behave as a spin-1/2 "impurity" exchange coupled to the rest of the electron gas.[9,10] This exchange coupling, J_K, leads to a low energy scale, the Kondo temperature, $k_BT_K\sim\epsilon_F e^{-1/J_K\rho(\epsilon_F)}$ [$\rho(\epsilon_F)$ is the density of states at the Fermi level]. For $Z_e\ll k_BT_K$, which is the regime that we shall consider here, the conductance for the QPC shows an interesting temperature dependence, with a crossover from $G<2e^2/h$ for $T\gtrsim T_K$ to $G\simeq 2e^2/h$ for $T\ll T_K$.[4,9]

This crossover should be accompanied by dramatic changes in the nuclear-spin-relaxation rate. The nuclear-spin relaxation in the QPC is dominated by the fluctuations of the impurity spin.[23] The fastest rate is for those nuclei located close to the impurity, which are coupled to the impurity spin with an energy scale $A_d\sim A_s/(w_xw_yw_z)$, where $w_xw_yw_z$ is the mean volume of the impurity. Relating Eq. (4) to the impurity dynamical susceptibility, we can make use of known results in limiting cases. For $T\gg T_K$, the coupling of the impurity spin to the electron gas is relatively weak. Using the results of Ref. 24 we find

$$T_1^{-1} = 2\frac{A_d^2 S(S+1)}{3\pi\hbar(k_B T)[J_K\rho(\epsilon_F)]^2}, \tag{8}$$

where $S=1/2$ for the spin-1/2 impurity.[25] For $T \ll T_K$, the Kondo singlet is well formed and the system behaves as a local Fermi liquid. From Ref. 26, one then recovers a Korringa law for the nuclear-spin-relaxation rate with

$$T_1^{-1} = \frac{2\pi(k_B T)A_d^2}{\hbar(g_s\mu_B)^4}\chi_{\mathrm{imp}}^2, \tag{9}$$

where χ_{imp} is the static Kondo impurity susceptibility, which is a universal function of T/T_K and tends to a constant as $T \to 0$.[27] The nuclear-spin-relaxation rate is a nonmonotonic function of T, passing through a maximum at $T \sim T_K$ with a maximum rate of order

$$\Gamma_{\mathrm{Kondo}} \simeq \frac{A_d^2}{\hbar k_B T_K} = \frac{A_s^2}{\hbar k_B T_K (w_x w_y w_z)^2}. \tag{10}$$

This nonmonotonic temperature dependence of T_1^{-1} is characteristic of the Kondo physics. It is qualitatively distinct from the case of noninteracting electrons or electrons with exchange-enhanced Zeeman energy, for which T_1^{-1} increases monotonically with T.

VI. SPIN-INCOHERENT LUTTINGER LIQUID

Finally, we consider the possibility that the electron system in the QPC behaves as a strongly interacting 1D wire. Strong repulsive interactions lead to pronounced local charge-density wave order and a suppression of the exchange interaction energy scale J_{LL}, with $J_{\mathrm{LL}} \ll \epsilon_F$.[11]

At low temperatures $T \ll J_{\mathrm{LL}} \ll \epsilon_F$ the system should behave as a Luttinger liquid. Nevertheless, since it is coupled to Fermi liquid leads the conductance is $G=2e^2/h$ and is insensitive to the electron-electron interactions.[28] Applying the general approach of bosonization to the spin susceptibility of the repulsive 1D electron gas leads to the prediction[29] that as $T \to 0$, $T_1^{-1} \sim T^{K_\rho}$, with $K_\rho < 1$ for repulsive interactions. Thus, the nuclear-spin-relaxation rate is sensitive to the formation of a Luttinger liquid.

As temperature is increased, the 1D electron gas enters the regime of the "spin-incoherent" Luttinger liquid,[11,30] $J_{\mathrm{LL}} \ll k_B T \ll \epsilon_F$. The conductance is then expected[11] to be $G \simeq e^2/h$. The spin-incoherent Luttinger liquid is characterized by an enhanced nuclear-spin-relaxation rate. This arises from the existence of low-energy spin-flip excitations, of bandwidth J_{LL}, which decouple from the electronic motion. Treating the spin-flip excitations as a spin chain with lattice constant $1/n$ and exchange energy J_{LL}, one finds for $k_B T \gg J_{\mathrm{LL}}$

$$T_1^{-1} \sim \Gamma_{\mathrm{SILL}} \equiv \frac{I A_s^2 n^2}{\hbar w_y^2 w_z^2 J_{\mathrm{LL}}}. \tag{11}$$

Since $J_{\mathrm{LL}} \ll \epsilon_F$, the relaxation rate (11) is parametrically enhanced as compared to that for the noninteracting electron gas (5). In the spin-incoherent Luttinger liquid regime T_1^{-1} is expected to be large and weakly temperature dependent.

In summary, we have shown how NMR methods can be used to explore novel electronic phenomena in nanoscale semiconductor devices and that measurements of $1/T_1$ can discriminate between different theoretical models of the 0.7 effect. We hope that this work will stimulate both experimental studies of nuclear-spin relaxation in QPCs, and theoretical investigations of nuclear-spin relaxation within in more detailed models of the 0.7 effect.

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