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Quantum non-demolition measurements of single donor spins in semiconductors

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We propose a technique for measuring the state of a single donor electron spin using a field-effect transistor induced two-dimensional electron gas and electrically detected magnetic resonance techniques. The scheme is facilitated by hyperfine coupling to the donor nucleus. We analyze the potential sensitivity and outline experimental requirements. Our measurement provides a single-shot, projective, and quantum non-demolition measurement of an electron-encoded qubit state.

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Semiconductor implementations of quantum computation have become a vibrant subject of study in the past decade because of the promise quantum computers (QCs) hold for radically altering our understanding of efficient computation, and the appeal of bootstrapping the wealth of engineering experience that the semiconductor industry has accumulated. A promising avenue for implementing quantum computing in silicon was proposed by Kane\(^1\), suggesting the use of phosphorous nuclei to encode quantum information. However, while the long coherence times of the nuclei are advantageous for information storage tasks, their weak magnetic moment also results in long gate operation times. In contrast, donor electrons in Si couple strongly to microwave radiation and permit the fast execution of gates; and while electron spin decoherence times are shorter than their nuclear counterparts, the tradeoff of faster operation times for decreased robustness to noise could be appropriate to implementing a fault-tolerant QC. This has led several authors to suggest the use of electron spin qubits as a variant on the original Kane architecture here.

An integral part of any quantum computation architecture is the capacity for high-fidelity qubit readout. While small ensembles of donar spins have been detected\(^2\) and single spin measurements have been demonstrated (e.g. \(3\)), detection of spin states of single donor electrons and nuclei in silicon has remained elusive. In this paper we analyze spin dependent scattering between conduction electrons and neutral donors\(^2\) as a spin-to-charge-transport conversion technique, and show that quantum non-demolition (QND) measurements of single electron spin-encoded qubit states are realistically achievable when mediated via nuclear spin states. Such a measurement will also be of value to the developing field of spintronics\(^2\). Our readout takes advantage of two features: i) the ability to perform electron spin resonance spectroscopy using a high-mobility two-dimensional electron gas (2DEG), and ii) the hyperfine shift induced on dopant electron Zeeman energies by the dopant nuclear spin state. We examine these two aspects separately in the following and then outline our proposed protocol for qubit readout.

The low-energy, low-temperature Hamiltonian describing the electron and nuclear spins of a phosphorous dopant in a static magnetic field, \(\mathbf{B} = \mathbf{B}_z\) is

\[
H = \frac{1}{2} [g_e \mu_B \mathbf{B} \sigma_z - g_n \mu_n B \sigma_n^z] + A \sigma^e \cdot \sigma^n
\]

where \(\mu_B\) and \(\mu_n\) are the Bohr and nuclear magnetons, \(g_e\) (\(g_n\)) is the electron (nuclear) \(g\)-factor, and \(A\) characterizes the strength of the hyperfine interaction between the two spins\(^1\) (we set \(\hbar = 1\) throughout the paper). For moderate and large values of \(B\), the \(\sigma_z\) terms dominate and we can make the secular approximation, to arrive at:

\[
H \approx 1/2 [g_e \mu_B \mathbf{B} \sigma_z - g_n \mu_n B \sigma_n^z] + A \sigma^e_z \sigma^n_z.
\]

The energy levels and eigenstates of this Hamiltonian are shown in Fig.\(^4\). Note that we have ignored the coupling of both spins to uncontrolled degrees of freedom such as paramagnetic defects and phonons (coupling to lattice spins can be mitigated by the use of a \(^{28}\)Si substrate). These environmental couplings will contribute to decoherence of the nuclear and electron spin states (e.g. \(5\)), and we will simply assume that this results in some effective relaxation and dephasing of the electron and nuclear spins.

The use of electrical conductivity properties of semiconductors to investigate spin properties of (bulk-doped) impurities has a long history\(^1\), including studies of donor polarization using a 2DEG probe\(^2\). The basic principle exploited in these studies is the role of the
The spinor components of the conduction and impurity electrons. We write this transformation as $\rho_{\text{out}}(\Omega) = T \rho_{\text{in}} T^\dagger / \text{tr}(T \rho_{\text{in}} T^\dagger)$, where $\rho_{\text{in/out}}$ are the density operators for the spin state of the combined two-electron system, and: $T = F_0 + F_x \sigma_z \cdot \sigma_1$. Here $F_0$ ($F_x$) is the amplitude for un-exchanged (exchanged) conduction and impurity electron scattering. Note that the spatial aspects of the problem only enter into the amplitudes: $F_{0/x} \equiv F_{d/x} \Omega$. We are not aware of any calculations of these in the quasi two-dimensional situation relevant here and will therefore leave them as free parameters. The differential cross section for scattering into all final spin states, $d \Sigma(\Omega)/d\Omega$ is the trace of $T \rho_{\text{in}} T^\dagger$.

Now, assume an initial state $\rho_{\text{in}} = (p | \uparrow \rangle_c \langle \downarrow | + (1 - p) | \downarrow \rangle_c \langle \uparrow |) \otimes \rho_i$, where the first term in the tensor product is the state of the conduction electron (the conduction band is assumed to be polarized to the degree $P_0 = 2p - 1, 0 \leq p \leq 1$), and the second term is the general state of the donor electron given above. After applying the scattering transformation and tracing out the conduction electron (because we have no access to its spin after the scattering event in this experimental scheme) we get a map that represents the transformation of the impurity electron state due to one scattering event:

$$\rho_i \rightarrow \rho_i' = \frac{(1 - p)}{N} [(F_0 + F_x \sigma_z) \rho_i (F_0 + F_x \sigma_z) + |F_x|^2 \sigma_-, \rho_i \sigma_+]$$

$$+ \frac{p}{N} [(F_0 - F_x \sigma_z) \rho_i (F_0 - F_x \sigma_z) + |F_x|^2 \sigma_+ \rho_i \sigma_-]$$

where $N$ is a normalization constant to ensure $\text{tr}(\rho_i') = 1$. In order for the measurement to be faithful, the diagonal elements of the impurity spin state (the population probabilities) must be preserved under the interaction — that is, the measurement interaction can induce dephasing (in the measurement basis), but no other decoherence. However, the terms proportional to $|F_x|^2$ in Eq. (2) suggest that there will be population mixing. This can be quantified by iterating the recursion to simulate the effects of the repeated scattering events that contribute to the current. An appropriate quantification of measurement quality is the measurement fidelity [12]:

$$F_n = 2\left[ \left( \sqrt{a^{\langle n \rangle}} \sqrt{a^{\langle 0 \rangle}} + \sqrt{b^{\langle n \rangle}} \sqrt{b^{\langle 0 \rangle}} \right)^2 - 0.5 \right],$$

where $a^{\langle n \rangle}$ and $b^{\langle n \rangle}$ are the diagonal elements of $\rho_i$ after $n$ scattering events. An ideal measurement has $F_n = 1$, while $F_n = 0$ indicates a measurement that yields no information — i.e. no correlation between the original qubit state and the meter variables. Since the measurement should work for all initial states, we consider the worst-case measurement fidelity: $F_n^w = \min_{a^{\langle 0 \rangle}, b^{\langle 0 \rangle}} F_n$. By extrapolating from present experiments [7], factoring in improved 2DEG mobility [13] and increased conduction electron polarization, we show below that an optimistic estimate for the shot-noise-limited measurement time is $\tau_m \sim 10^{-3}$ s, within which there will be $\sim 10^6$ scattering events [14]. Although we do not have explicit knowledge
of the scattering amplitudes, we find from iterating the above recursion for a broad range of values $F_2/F_3$ that $\mathcal{F}_n^w$ after $\sim 10^8$ scattering events is $\ll 1$ for any non-zero exchange amplitude $|F_2|$ and any polarization, $P_n^0$. In fact, $\mathcal{F}_n^w$ typically drops to near zero already after $\sim 10 - 100$ scattering events. Thus the measurement induced population mixing time is $T_{\text{mix}} \sim 1 - 10$ ps, which is drastically smaller than $\tau_n$ [21]. This makes it impossible to faithfully map the electron spin state onto the meter variables, and hence impossible to perform a single electron spin state measurement using the 2DEG current directly. However, as we will now show, it is possible to make use of the nuclear spin degree of freedom in order to utilize EDMR for projective and QND measurement of single spin states. Note that the state of the nuclear spin affects the Zeeman splitting of the electron spin and is acting as the control. However, the complete exchange of qubit states is unnecessary, since the spin relaxation is not well characterized under these conditions but we expect that in large magnetic fields the donor electron dynamics contributes primarily to dephasing of the nuclear state. This can be made precise by performing perturbation theory on Eq. (1) in the parameter $A/\Delta$, where $\Delta \equiv \omega_n - \omega_e = B(g_e \mu_B - g_n \mu_n)$. In the $\Delta \ll 1$ regime where $A/\Delta \ll 1$, the effective Hamiltonian describing the coupled systems is $H \approx H_{\text{eff}} = \frac{1}{2} \omega_e \sigma_z^e - \frac{1}{2} \omega_n \sigma_z^n + A \sigma_z^e \sigma_z^n + \frac{A^2}{\Delta} (\sigma_z^e - \sigma_z^n)$ [17]. Therefore we see that to first order in $A/\Delta$ the donor electron can only dephase the nuclear spin, and direct contributions to nuclear spin $T_1$ through the hyperfine interaction are small. Other mechanisms such as phonon-assisted nuclear spin relaxation can contribute to the nuclear $T_1$, but these will be small effects. Considering that the nuclear spin $T_1$ is on the order of hours in a static electron environment at low temperatures [16, 18], as long as these effects do not reduce this $T_1$ more than five orders of magnitude, – an unlikely scenario – the nuclear $T_1$ in the presence of electron driving will be comfortably larger than $\tau_n \sim 10^{-3}$ s. This implies that once the measurement collapses onto a nuclear basis state, the nuclear spin state effectively remains there and therefore the EDMR measurement satisfies the QND requirement on the qubit state [21].

Now we address the issue of the sensitivity of the differential EDMR current in the limit of single donor scattering. As detailed above, the spin state of the donor electron is continually changing due to the scattering interaction, and hence it is time-dependent. However, ignoring the transient, we can approximate it with a time independent value given by the steady state solution of the recursion relation, Eq. (2). This approximation can be thought of as taking the equilibrium spin value, where the “spin temperature” of the impurity has equilibrated with that of conduction electrons via the scattering interaction. Our analysis above indicates that this equilibrium happens on a much faster time scale than the observable time scales of the experiment. Solving for the steady-state ($\rho_i^{(n)} = \rho_i^{(n-1)} \equiv \rho_i^{\text{ss}}$), gives us a time-independent, non-resonant single donor “polarization”,
\begin{equation}
\langle \sigma_z \rangle_i^{ss} \equiv \text{tr} (\sigma_z \rho_i^{ss}) \text{ equal to}
\end{equation}

\begin{equation}
|F_x|^2 - 2\sqrt{4(P_0)^2\text{Re}(F_d F_x^*)^2 + \frac{1}{2}(1 - (P_0)^2)|F_x|^4},
\end{equation}

\begin{equation}
P_c^0 (|F_x|^2 - 4\text{Re}(F_d F_x^*)) \end{equation}

This steady state “polarization” is zero only in the singular case when $|F_x|^2 = 4\text{Re}(F_d F_x^*)$ and $P_0 = 1/\sqrt{2}$. We will assume that this singular condition is not met and take $\langle \sigma_z \rangle_i^{ss} \neq 0$. We can then follow the analysis of Ref. [2], using donor “polarization” $\langle \sigma_z \rangle_i^{ss}$, to estimate the on-resonant ($I$) and off-resonant ($I_0$) current differential (normalized) as:

\begin{equation}
\frac{\Delta I}{I_0} \equiv \frac{I - I_0}{I_0} \approx -\alpha' s \langle \sigma_z \rangle_i^{ss} P_0 \frac{1}{\tau_n} \frac{1}{\tau_i}.
\end{equation}

Here $\alpha' \equiv \langle \Sigma_s - \Sigma_i \rangle_{z=z_i}/(\langle \Sigma_s + 3\Sigma_i \rangle)_{z=z_i}$, $\Sigma_s$ and $\Sigma_i$ are single and triplet scattering cross sections, respectively, and $\langle \cdot \rangle_{z=z_i}$ denotes an average over the scattering region with the donor location in $z$ held fixed. $s = 1 - (1 - s_i)(1 - s_c)$, and $s_i$ and $s_c$ (both between 0 and 1) are saturation parameters which characterize how much of the microwave power is absorbed by the impurity and conduction electrons, respectively [2]. $s_i$ is a function of the broadening at the single donor electron resonance frequency: if we work in a regime where this broadening is minimal (as required to perform the quantum state transfer described above), $s_i \approx 1$ and thus $s \approx 1$. The final term in Eq. (3) represents the ratio between impurity scattering ($1/\tau_n$) and total scattering ($1/\tau_i$) rates. We assume $1/\tau_i = 1/\tau_0 + 1/\tau_n$, where $1/\tau_0$ is the scattering rate due to all other processes (such as surface roughness scattering and Coulomb scattering by charged defects).

To estimate the expected magnitude of this current differential, we begin by considering present state of the art 2DEG mediated EDMR experiments where this current differential is $\sim 10^{-7}$ (with $T \sim 5K, B \sim 0.37T$, a 2DEG channel area of $160 \times 20\mu m^2$, and a donor density of $2 \times 10^{13}$donors/cm$^2$) [2]. We assume that $\alpha'$ will be similar for the single donor device as in current experiments. Then in scaling down to a single donor, the first aspect to consider is the scattering rate ratio: $\rho \equiv \frac{1/\tau_n}{1/\tau_i}$. This ratio can be kept constant if we scale the 2DEG area concomitantly with the donor number. From the channel area and density of current experiments, we extrapolate that a 2DEG area of $\sim 30 \times 30 nm^2$ – well within the realm of current technology – would keep $\rho$ unchanged. Furthermore, the mobility of the 2DEG channel can be improved – e.g., by using hydrogen passivation to mitigate surface roughness at the oxide interface [13] – to increase $\rho$. We conservatively estimate a factor of 10 increase in $\Delta I/I_0$ from such improvements. The saturation parameter $s \sim 1$ for large enough microwave powers in the recent measurements [3] and so does not present an area for improvement. Finally, an avenue for significant improvement in signal is to increase the conduction electron polarization, $P_c^0$, which is currently $\sim 0.1%$. This polarization is roughly proportional to the applied static magnetic field, and therefore a factor of 10 improvement is possible by operating at $B = 3T$. Additionally, spin injection techniques can be employed to achieve $P_c^0 > 10\%$ (e.g., [15]), resulting in a 100-fold improvement in $\Delta I/I_0$. Hence, by improvements in device scaling and channel mobility, and by incorporating spin injection, we estimate a realistic current differential of $\Delta I/I_0 \sim 10^{-4}$. With shot-noise limited detection and $I_0 \sim 1 \mu A$ it will require an integration time of $\tau_m \sim 10^{-3}$ s to achieve an SNR of 10. This is well within the expected nuclear $T_1$ time in this environment.

In conclusion, by utilizing resonant pulse gates and 2DEG-mediated-EDMR readout, we have proposed a realistic scheme for measuring the spin state of a single donor electron in silicon. By making use of the hyperfine coupled donor nuclear spin, the readout scheme provides a single shot measurement that is both projective and QND. The QND aspect also makes this technique an effective method for initializing the state of the nuclear spin. The fact that the measurement is facilitated by the nucleus of the donor atom intimates a hybrid donor qubit where quantum operations are carried out on the electron spin and the state is transferred to the nucleus for measurement and storage (advantageous due to the longer relaxation times). Finally, although the above analysis was done with the example of a phosphorous donor, it applies equally well to other donors, such as antimony [3, 4], and some paramagnetic centers. One merely has to isolate two (dipole-transition allowed) nuclear spin levels to serve as qubit basis states and transfer the electron state to these nuclear states with resonant pulses.

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**APPENDIX 1: TECHNICAL DETAILS OF THE PROPOSED EXPERIMENT**

Figure 2 shows a cross section of the EDMR based single donor spin readout device (e.g. Ref. [2]).

In detail, the single qubit spin readout proceeds as follows. After completion of operations on a selected qubit the electron is in a state $|\psi\rangle_e = \alpha |\uparrow\rangle_e + \beta |\downarrow\rangle_e$. Following state transfer to the nuclear spin, one of the two hyperfine split electron spin resonance lines that corresponds to a given nuclear spin projection is addressed by dialing in the corresponding microwave frequency for resonant excitation of electron spin transitions. At the same time, the transistor is turned on and the channel current is monitored. Now, assume that the magnetic fields...
FIG. 2: A cross section of the field-effect transistor (FET) used to create the 2DEG. In order to reduce qubit decoherence, it is beneficial to implant into isotopically purified silicon.

have been tuned to address the $|\uparrow\rangle_n$ nuclear state projection. Then with probability $|\alpha|^2$ the transistor current will differ from the off-resonant current value and with probability $|\beta|^2$ it will be just equal to the off-resonant channel current. In either case, monitoring the current at one hyperfine resonance for the $\tau_m$ measurement duration constitutes a readout of the nuclear spin. For this to work, the measurement time $\tau_m$ has to be shorter then the nuclear spin flip time $T_1$. Typical channel currents in readout transistors are of order $1\mu A$. For readout devices with optimized conduction electron polarization and channel mobilities, resonance current differences can be $\geq 10^{-4}$, leading to signal-to-noise ratios greater than $10:1$ for measurement times of $\sim 1$ ms. Nuclear spin flip times under these readout conditions are not known, but nuclear spin relaxation times under static conditions are several hours $[16, 18]$, making it a realistic expectation that the donor nuclear spin will be stable during readout timescales. We note that a similar conclusion, that electron driving will not affect nuclear spin $T_1$ dramatically, was arrived at in the recent article by Jiang et. al. $[22]$, for a similar physical system.

FIG. 3: Illustration of single spin readout. In experiments with large ensembles of donor spin qubits, lines from all nuclear spin projections are present in EDMR measurements (left). In measurements with single donors (right), only single lines are present for measurement times shorter then the nuclear spin relaxation time. Monitoring the current at a given resonant field measures the spin state of the donor nucleus with the correct statistics.

APPENDIX 2: SIMULATIONS OF DONOR ELECTRON SPIN RELAXATION DUE TO 2DEG INTERACTION

Here we show sample results from simulations of scattering dynamics derived in the main text of the article. The aim of these simulations is to show that the worst-case measurement fidelity:

$$F_w = \min_{a(0), b(0)} 2|\sqrt{a(n)}\sqrt{a(0)} + \sqrt{b(n)}\sqrt{b(0)}|^2 - 0.5|$$  \hspace{1cm} (4)

(worst-case taken over all possible initial state populations, $a_0, b_0$) approaches zero rapidly as a function of the number of scattering events, $n$, for almost all values of the exchange and direct scattering amplitudes ($F_d$ and $F_x$ respectively). In Eq. (4) $a^{(n)}$ and $b^{(n)}$ are the diagonal elements of the electron state density matrix after $n$ scattering events. A measurement fidelity of zero indicates a measurement that yields no information – i.e. there is no correlation between the original qubit state and the final measurement meter variables.

Figure 4 shows worst-case fidelity decay as a function of scattering amplitude parameters for various values of 2DEG polarization $P_{0c}^d$. These simulations clearly show that the relaxation of a general electron spin state is rapid across virtually all reasonable parameter ranges.
For $P_0 > 0.1$, we see that there are fairly large regions in the $F_x/F_d$ parameter space for which the worst-case measurement fidelity is non-zero: however, (i) $F_{wn}^w$ peaks at $\sim 0.25$, a value that is too small for a high-quality measurement, and (ii) $F_{wn}^w$ is highly sensitive to the precise value of $F_x/F_d$ and $P_0$ in these regions.

These simulations show conclusively that under realistic experimental conditions, the electron spin relaxation induced by the scattering interaction makes the 2DEG current an ineffective measurement of the electron spin state.

FIG. 4: Evolution of worst-case measurement fidelity, $F_{wn}^w$, during 2DEG scattering dynamics as a function of the number of scattering events $n$, for a range of values of the ratio of direct and exchange scattering amplitudes and of 2DEG equilibrium polarization. The independent (base plane) axes on the plots parametrize the complex scattering amplitude ratio $F_x/F_d \equiv |F_x/F_d|e^{i\chi}$: one axis is the magnitude, $|F_x/F_d|$ (shown for $0 < |F_x/F_d| < 4$), and the other is the phase, $\chi$ (shown for $0 < \chi < 2\pi$). The number of scattering events, $n$, varies across the columns, with values $n = 10, 10^2$ and $10^4$ shown here. The 2DEG equilibrium polarization, $P_0^c$, varies across the rows, with values $P_0^c = 0, 0.1$ and 1 shown here.

[14] Here we have used an estimate of the scattering cross section from Ref. 9 to appropriately scale the total number of electrons passing through the channel within $\tau_m$.
[17] This effective Hamiltonian is of course also the justifica-
tion for the secular approximation made above.


