Anisotropic Stark effect and electric-field noise suppression for phosphorus donor qubits in silicon

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We report the use of novel, capacitively terminated coplanar waveguide (CPW) resonators to measure the quadratic Stark shift of phosphorus donor qubits in Si. We confirm that valley repopulation due to strain in our samples. We show that in the presence of this strain, electric-field sources of decoherence can be non-negligible. Using our measured values for the Stark shift, we predict magnetic fields for which the spin-orbit Stark effect cancels the hyperfine Stark effect, suppressing decoherence from electric-field noise. We discuss the limitations of these noise-suppression points due to random distributions of strain and propose a method for overcoming them.

Quantum computing architectures based on donor qubits in silicon have generated a great deal of interest due to their long coherence times exceeding seconds in isotopically enriched $^{28}$Si, scalability, and their compatibility with fabrication techniques refined by the Si industry. In many donor-based architectures the mechanism for manipulating individual spins relies on the tuning of a donor in and out of resonance with a global microwave magnetic field ($\vec{B}_1$). Donor tuning via the Stark shift of Sb donors and As donors in Si has been studied using electron spin resonance (ESR) techniques. The Stark addressability of Sb donor nuclear spins was demonstrated as was the strong electroelastic tuning of the hyperfine interaction.

In the present work, we measure the Stark shift of phosphorus donors in Si using ESR with novel, capacitively terminated, coplanar waveguide (CPW) resonators. These high-sensitivity resonators allow us to measure small spin ensembles subjected to locally homogeneous electric fields. Our measurements resolve a previously predicted anisotropy in the spin-orbit Stark shift due to valley repopulation.

It is expected that electric-field noise can contribute substantially to decoherence in the presence of strain. Large strains and/or electric fields are present in gated single-donor devices. By measuring the linear Stark effect, we estimate the effective electric field due to strain in our devices and the resulting sensitivity of the donors to electric-field noise. The effect of electric-field noise on the donor spin coherence depends on the field and strain orientation and thus the detailed device configuration. From our results we find magnetic fields and crystal orientations where the spin-orbit and hyperfine components of the Stark shift cancel, such that spins are protected from electric-field noise. These “noise-suppression points” may be important for near-surface donors and quantum devices incorporating electrostatic gates.

Our experiments were conducted using 1/4-wavelength superconducting CPW resonators operating at 7.1 GHz with Q-factors of ~1200. An example is shown in Fig. 1(a). Resonators were patterned from 35 nm thick Nb films deposited on 2 μm, P doped (5 × 10^{15} cm⁻³), $^{28}$Si epilayers (800 ppm $^{29}$Si). One end of a resonator is capacitively coupled to a transmission line which acts as an antenna. The other end is capacitively shorted to ground. This short consists of a 2.9 nF parallel plate capacitor having a plate area of 0.5 mm². The capacitor is filled with a 17 nm thick atomic layer deposition grown Al₂O₃ dielectric and satisfies the design rule for a good capacitive short. The capacitive short allows the center conductor of the CPW to be biased, providing a direct current (DC) electric field between the center pin and the ground plane of the resonator as shown in Fig. 1(b)-(c). This electric field is inhomogeneous, except near the plane of the CPW and in the gap between the center pin and the ground plane. To confine spins to these homogeneous regions, we employed a thin, 2 μm, phosphorus-doped $^{28}$Si epitaxial layer grown on high resistivity p-type Si as our spin ensemble. However, regions producing the ESR signal vary depending on sample orientation because only $\vec{B}_1$ perpendicular to the DC magnetic field ($\vec{B}_0$) drives spin rotations. The relevant components of $\vec{B}_1$ are plotted in the supplementary information. We calculated the sub-ensembles of spins contributing to at least half of the signal and they are shaded red in Fig. 1(b)-(c). The weighted electric-field distribution over the subensembles is shown in Fig. 1(d). The standard deviation of the distribution in the x-component magnitude (the dominant component which is directed from the ground plane to the center pin) is ~ 8% for both orientations.

Two sets of resonators were fabricated with center pins oriented parallel to either the [010] or the [110] crystal axes. These orientations place $\vec{E}$ along either the [100] or [110] axes for spins contributing to the ESR signal. The
resonators were wire bonded to copper printed circuit boards, connected to a low-noise, cryogenic preamplifier, and placed in a DC magnetic field. With $\vec{B}_0$ oriented in the plane of the Nb to avoid trapping magnetic flux vortices, devices were cooled to 1.7 K to conduct pulsed ESR experiments.

A pulsed ESR technique sensitive to small resonance shifts [10] [12] was used to measure the quadratic Stark shift. This technique uses a two-pulse Hahn echo sequence ($\pi/2(x) - \tau - \pi(y) - \tau - \text{echo}$), with an electric-field pulse applied to the spins during the first dephasing period, $\tau$. The electric field detunes the spins relative to the driving microwaves such that they accumulate an additional phase, $d\phi$, in the Hahn echo which is measured using a quadrature detector. This experiment utilized bipolar electric-field pulses (pulse sequence IV in [10]) consisting of a positive pulse immediately followed by a negative pulse of the same amplitude and duration. These pulses refocus linear Stark effects (arising from random strain as discussed below) thus allowing the measurement of the quadratic Stark effect. The phase shift is given by

$$d\phi = \tau df = [\eta_g \beta B_0 + \eta_a M_i] E^2 \tau_E / \hbar$$  \hspace{1cm} (1)$$

where $df$ is the frequency shift of the spins, $\eta_g$ and $\eta_a$ are the spin-orbit and hyperfine Stark fitting parameters, respectively, $g$ is the electron g-factor, $\beta$ is the Bohr magneton, $a$ is the hyperfine coupling constant, $M_i$ is the nuclear spin projection, $\tau_E$ is the duration of the electric-field pulse, and $\hbar$ is the reduced Planck constant [10]. A model was developed to simulate the Stark effect in our device including the inhomogeneity in both $\vec{B}_1$ and $\vec{E}$. Both models were computed using a conformal mapping technique [21], and each spin’s contribution to the echo was calculated as described in [22]. This model also took into account $\vec{B}_1$ inhomogeneity present along the length of the CPW. The total echo phase shift of the spin ensemble, $\Delta \phi$, was determined by taking a weighted average of the Stark shift of each spin:

$$A e^{i \Delta \phi} = \frac{\sum_i e^{-i \phi_i} g_i \sin^3 (g \beta B_1 \tau_p / \hbar)}{\sum_i g_i \sin^3 (g \beta B_1 \tau_p / \hbar)}$$  \hspace{1cm} (2)$$

where the sum is taken over all $i$ spins, $A$ is an amplitude coefficient, $d\phi_i$ is the phase shift of the $i$th spin, $g_i$ is the coupling of the $i$th spin to the resonator, $B_{1i}$ is the microwave magnetic field seen by the $i$th spin, and $\tau_p$ is the duration of the first microwave pulse in the Hahn echo sequence. In this expression, the $\sin^3$ term takes into account signal attenuation due to pulse errors arising from $\vec{B}_1$ inhomogeneity [23]. We note that the phase shift of a single spin, $d\phi_i$, is not affected by these errors [24].

Data for $\vec{E}$ applied along the [100] and [110] axes with bias voltages up to 8 V are shown in Fig. 2. These data were taken with an electric-field pulse length of 38 $\mu$s and microwave $\pi$-pulses of 400 $\mu$s. Eq. (2) was fitted to the data and the fitting parameters are given in Table 1. While the hyperfine Stark parameter remains nearly constant, the spin-orbit Stark parameter changes sign and magnitude depending on the $\vec{E}$ orientation relative to $\vec{B}_0$ and the crystal axis.

This anisotropic Stark shift was predicted by Rahman et al. [10] and is explained using a valley repopulation model [25]. In Si, the g-factor of an electron is related to its effective mass in the direction of $\vec{B}_0$. The non-spherical valleys produce a non-uniform effective mass, such that the g-factor of spins in a single valley depends on the angle $\vec{B}_0$ makes with that valley. In the unperturbed ground state with a symmetric valley combination, the g-factor is equally averaged over all valleys, and no g-factor anisotropy can be resolved. However, when an electric field is oriented along a valley axis (\{100\} for Si), the valley degeneracy is partially lifted, and electrons preferentially fill valleys oriented along the electric field. This changes the effective g-factor and induces an anisotropy in the Stark parameter $\eta_g$. The anisotropy is most pronounced when the electric field is oriented along a valley axis. Moreover, application of an electric field in the \{111\} axes would result in no valley repopulation, since it makes the same angle with all valleys. This ori-
where the primary source of noise (and thus the direction of \( \vec{E} \)) is known, such as in gated donor architectures. For this reason, noise suppression points vary with the direction of \( \vec{E} \), and no single \( \vec{B}_0 \) can cancel all randomly oriented electric-field noise. For this reason, noise suppression points are most effective in situations where the primary source of noise (and thus the direction of \( \vec{E} \)) is known, such as in gated donor architectures.

In the simplest picture, electric-field noise (which is presumably small) should not contribute to decoherence, since the Stark effect is quadratic. However, this changes dramatically when a large DC electric field (present in gate-addressed architectures) or strain is applied. In this work we consider this field coming from strain [26], inducing a shift in the ESR frequency by modulating the hyperfine interaction [15] and causing valley repopulation [25].

The Stark shift in the presence of strain is given as

\[
df = [\eta g \beta B_0 + \eta_t a M_I] (\vec{E}^2 + 2\vec{E} \cdot \vec{E}_{\text{strain}})/\hbar, \tag{3}
\]

where \( \vec{E}_{\text{strain}} \) is the effective electric field due to strain. When electric-field noise, \( \vec{E}_{\text{noise}} \), is small, the \( \vec{E}_{\text{noise}}^2 \) term is negligible whereas the \( \vec{E}_{\text{noise}} \cdot \vec{E}_{\text{strain}} \) term can be large. Using data in [25], we calculate that a strain of \( 10^{-3} \) is equivalent to an effective electric field of \( 10 \, V/\mu m \). We hereafter refer to strain in units of \( V/\mu m \), which corresponds to the strength of \( \vec{E}_{\text{strain}} \).

To investigate strain we use unipolar (positive bias) pulses, instead of the bipolar pulses used to gather the data for Fig. 2. Bipolar pulses cancel the linear term of Eq.(3) whereas unipolar pulses lead to a broadening of the ESR line and loss of signal when internal strains are inhomogeneous across the spin ensemble. Despite this broadening, data were taken using unipolar pulses with amplitudes of up to \( 4 \, V \) (supplemental material). These data indicate that strain is approximately \( 1 \, V/\mu m \) in our wafers, and the signal loss indicates that the strain is primarily random. We compare this to a similar sample (10 \( \mu m \) P doped epitaxial layer of \( \text{Si} \)) reported [27] with an electron nuclear double resonance (ENDOR) linewidth of 100 kHz. Assuming that broadening of the ENDOR line is due primarily to strain, this linewidth corresponds to an \( \vec{E}_{\text{strain}} \) distribution spanning 0.75 \( V/\mu m \), comparable to our results. For these strains, the spins’ sensitivity to electric-field noise, \( df/dE \), can be large. The \( \vec{E}_{\text{noise}} \) limited coherence time \( (T_2) \) is inversely proportional to \( (df/dE)^2 \) [28] so electric-field sources of decoherence can be substantial. While the \( \vec{E}_{\text{noise}} \) contribution to the coherence time will vary from system to system, we calculate (using [28]) that for 10 \( \mu V \) of noise on our CPW center pin, \( T_2 \) would be limited to 70 ms in the devices used in these experiments. Devices with gates more strongly coupled to the donors would have their \( T_2 \) affected more severely. These \( T_2 \) effects are not directly observed in our device geometry, but we were able to apply a [110] oriented electric field, and, as expected, the spin-orbit anisotropy became small as shown in Table 1.

FIG. 2. Measured ESR frequency shift as a function of CPW center pin voltage for \( \vec{B}_0 \) oriented along the [100] (a) and [110] (b) crystal axes. Data are plotted for \( \vec{E} \) either parallel (red diamond) or perpendicular (black square) to \( \vec{B}_0 \). Smooth curves are fits to the data using Eq.(2). Note that the hyperfine Stark shift is symmetric whereas the spin-orbit Stark shift is asymmetric with respect to zero as a function of \( M_I \). The error bars for the data are smaller than the points used in the plot. Data were taken at 1.7 K with a \( B_0 \) of 0.26 \( T \).

| \( \vec{E} \) Orientation | \( \vec{B}_0 \) Orientation | \( \eta_{a} (\mu m^2/V^2) \) | \( \eta_{b} (\mu m^2/V^2) \) | \( \eta_{\text{theory}} (\mu m^2/V^2) \) |
|------------------------|------------------------|------------------|------------------|------------------|
| [100] \( \vec{E} \parallel \vec{B}_0 \) | \( \vec{B}_0 \) | \( -2.6 \pm 0.1 \times 10^{-3} \) | \( -8 \pm 2 \times 10^{-6} \) | \( -12 \times 10^{-6} \) |
| [100] \( \vec{E} \perp \vec{B}_0 \) | \( \vec{B}_0 \) | \( -2.8 \pm 0.1 \times 10^{-3} \) | \( 6 \pm 1.5 \times 10^{-6} \) | \( 14 \times 10^{-6} \) |
| [110] \( \vec{E} \parallel \vec{B}_0 \) | \( \vec{B}_0 \) | \( -2.7 \pm 0.1 \times 10^{-3} \) | \( -3.5 \pm 1.5 \times 10^{-6} \) | - |
| [110] \( \vec{E} \perp \vec{B}_0 \) | \( \vec{B}_0 \) | \( -2.7 \pm 0.1 \times 10^{-3} \) | \( -2.8 \pm 1.5 \times 10^{-6} \) | - |

Theoretical values are obtained from tight binding calculations reported by Rahman et al. in [10].

TABLE I. Stark Shift Fitting Parameters
devices since the coherence time is already limited by instantaneous diffusion to $\sim 2\ ms$. Recent experiments on single-donor devices have reported a Hahn echo $T_2$ of $\sim 1\ ms$ where it was determined that the dominant noise is not electrical in this device configuration\cite{19}. As other noise sources are eliminated and coherence is pushed to longer timescales, electric-field noise may become dominant. 

Internal strains can also lead to errors in measuring $\eta_g$, even when using bipolar pulses. This is because $\eta_g$ depends on the direction of the total electric field which includes $\vec{E}_{\text{strain}}$. Since $\vec{E}_{\text{strain}}$ is random, there is uncertainty in the actual direction of the total electric field relative to $\vec{B}_0$. Care was taken to minimize strain when mounting the devices, but not all strain can be avoided and in our devices we found that $\vec{E}_{\text{strain}}$ was larger than the applied electric fields. The errors arising from strain should become small as $\vec{E}$ becomes large, so data taken at higher bias voltages were weighted more heavily when fitting the model. For our samples we estimate that the magnitude of $\eta_g$ can be underestimated by up to a factor of 2.5 for the [100] data.

Taking into account strain, we quantitatively compute the sensitivity of spins to electric-field noise ($df/dE$). For the simple case, where the strain is uniform and oriented in the same direction as the $\vec{E}_{\text{noise}}$, we plot $|df/dE|$ in Fig. 3(a) (assuming $\vec{E}_{\text{strain}}$ is 1 $V/\mu m$). $\vec{E}$ noise suppression points appear as minima in $|df/dE|$. This case applies to bulk $^{28}\text{Si}$ crystals where the strain distribution can be small ($< 10^{-3} \ V/\mu m$) and single-donor systems.

We recognize that in devices containing ensembles of spins, randomly oriented strain leads to a distribution in $\eta_g$ over the ensemble, washing out noise suppression effects. Assuming random strain of order 1 $V/\mu m$, comparable to the strain in our samples, $df/dE$ should on average decrease by a factor of 5 for one hyperfine line compared to the other. This corresponds to an increase in $T_2$ by a factor of 25 (because $1/T_2 \propto (df/dE)^2$ \cite{28}) as shown in the supplemental information. This implies that, even with the simple approach of choosing the optimal field and hyperfine line, one can substantially suppress $\vec{E}$ noise.

We propose applying a large uniform external strain or DC electric field as a remedy to random strain effects. This external field adds to $\vec{E}_{\text{strain}}$ such that the total field becomes nearly uniform. The overall $\vec{E}$ vector is pinned along the external-field axis and is insensitive to any small variations in $\vec{E}_{\text{strain}}$. External strain fields of up to 10 $V/\mu m$ have been studied \cite{28} and for our samples we calculate that applying a strain of this magnitude would decrease $df/dE$ by a factor of $\sim 25$ (increases $T_2$ by two orders of magnitude). However, one must take care when orientating the external strain. If it is large and oriented perpendicular to the electric-field noise, a slight deviation from perfect alignment can lead to substantial decoherence due to the linear term in Eq.(3). Applying strain perpendicular to the $\vec{E}$ noise will suppress the linear term and protect the donor spin from electric-field induced decoherence. Fig. 3(b) shows the effect of external strain on the magnitude of $|df/dE|$.

While electric-field noise suppression points seemingly undermine the electrostatic addressability of donors, only one of the two hyperfine lines for phosphorus is protected. Global RF pulses can be used to flip the nuclear spins, toggling between electric field protected and sensitive states. Furthermore, applying an external strain or electric field enhances the Stark effect for spins in the sensitive state.

In conclusion, we have measured the quadratic Stark shift for phosphorus donors in silicon using a novel, capacitively-terminated CPW resonator. We resolved both a hyperfine and a highly anisotropic spin-orbit Stark shift. We measured $\vec{E}_{\text{strain}}$ in our samples to be on the order of 1 $V/\mu m$ and showed that this leads to a large linear Stark shift for even small applied electric fields, making spins sensitive to electric-field noise. Using our data, we predict DC magnetic fields where electric-field noise can be suppressed. In the presence of randomly distributed internal strains, the noise suppression is weakened, but by choosing the correct ESR transition, we calculate that one can enhance $T_2$ by a factor of 25. We have proposed the use of large external strains to over-

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig3.png}
\caption{(a) Plot of the electric-field sensitivity of P donors in Si for various orientations of $\vec{E}$ and $\vec{B}_0$ as a function of $B_0$. This plot assumes an internal strain of 1 $V/\mu m$ directed along $\vec{E}$. Dashed lines indicate $M_1 = -1/2$ whereas solid lines indicate $M_1 = +1/2$. $\vec{E}$ noise is suppressed at 19.12 GHz, 27.41 GHz, and 45.32 GHz. Another minima for the [110] oriented $\vec{E} \perp \vec{B}_0$ occurs at 56.65 GHz but is not shown. (b) Plot of the maximum (worst case) $\vec{E}$ sensitivity of spins subject to random strain (with magnitude 1 $V/\mu m$) as a function of externally applied strain. This plot assumes the external strain is oriented perpendicular to the $\vec{E}$ noise.}
\end{figure}
come this limitation such that $T_2$ can then be extended by two orders of magnitude. While the noise suppression techniques described in this paper use phosphorus donors in Si as an example, they should extend to other donor qubits as well.

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