Eliminating Leakage Errors in Hyperfine Qubits

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Population leakage outside the qubit subspace presents a particularly harmful source of error that cannot be handled by standard error correction methods. Using a trapped $^{171}$Yb$^+$ ion, we demonstrate an optical pumping scheme to suppress leakage errors in atomic hyperfine qubits. The selection rules and narrow linewidth of a quadrupole transition are used to selectively pump population out of leakage states and back into the qubit subspace. Each pumping cycle reduces the leakage population by a factor of ~3, allowing for an exponential suppression in the number of cycles. We use interleaved randomized benchmarking on the qubit subspace to show that this pumping procedure has negligible side-effects on un-leaked qubits, bounding the induced qubit memory error by $\leq 2.0(8) \times 10^{-5}$ per cycle, and qubit population decay to $\leq 1.4(3) \times 10^{-7}$ per cycle. These results clear a major obstacle for implementations of quantum error correction and error mitigation protocols.

Qubits are the starting point in most quantum computing architectures. The idealized two-level systems are ubiquitous in theoretical proposals and analysis, but are commonly only approximately realized in experiments by restricting the relevant dynamics to just two levels. This paradigm has been the cornerstone of demonstrations of high fidelity qubit initialization, quantum memories, single-qubit and two-qubit gates, state-detection[1−7], and algorithms of increasing complexity[8−11]. Deviations from these idealized two-level system models are known as leakage errors, which are quantum processes that drive population from a qubit subspace to other levels supported by the physical medium. While the experimental progress in quantum information processing is evident, the ultimate noise sensitivity of these machines is notoriously difficult to predict, and leakage errors are perhaps amongst the most worrisome.

Powerful algorithms require large circuit depths, necessitating the use of error correction and mitigation techniques. One technique of particular importance is quantum error correction, which allows for the efficient suppression of errors to an arbitrary level, thereby allowing for the possibility of universal quantum computation[12]. However, proofs of fault tolerance via quantum error correcting codes commonly assume the errors and subsequent corrections act within the qubit space and studies have shown that leakage can have a devastating effect on these codes[13]. Other error mitigation techniques circumvent active feedback and are more akin to open-loop control; including random sampling of noisy circuits[14], quantum subspace expansion[15], and stabilizer based error mitigation[16]. These methods are attractive for near-term use since they do not require large qubit overheads, but they too assume noise models that act on qubits and may be ineffective on systems with significant leakage errors.

Researchers have recognized this issue and constructed various leakage reducing units[17], but they typically require extra qubit resources and circuitry, and lower the physical error rate threshold. This additional overhead on top of the already formidable overhead of quantum error correction has even led some researchers to consider abandoning hyperfine clock-qubits and their magnetic field insensitivity in favor of a leakage-free qubit[18].

In this work, we propose a scheme to correct leakage errors in hyperfine clock-qubits without introducing additional qubit or gate overheads. Namely, we propose and demonstrate an optical pumping scheme that drives leaked population incoherently back into the qubit subspace, thereby converting leakage errors into conventional qubit errors, which can be handled by the aforementioned error correction and mitigation techniques. Each leakage repump pulse succeeds probabilistically, resulting in an exponential reduction of leakage population with pulse number. Utilizing atomic selection rules and pulse shaping techniques, we ensure that this pumping has a negligible impact on un-leaked qubits. These results bring trapped-ion platforms in line with the assumptions of error-correction and mitigation techniques.

We analyze and demonstrate our leakage suppression scheme in $^{171}$Yb+. This system admits a relatively simple hyperfine structure that provides a low-field clock-qubit in the $^2S_{1/2}$ manifold, $\{|F = 0, m_F = 0\}, |F = 1, m_F = 0\} \equiv \{\{0\},\{1\}\}$, and can be controlled using stimulated Raman transitions through an excited meta-stable state[19]. Spontaneous scattering during these gates is a fundamental error that is partially leakage inducing[20]. In the case of $^{171}$Yb+, these scattering events drive population into two leakage states denoted as $|L_z\rangle \equiv ^2S_{1/2}|F = 1, m_F = \pm 1\rangle$. In principle, population in these states can be optically pumped back into the qubit space through the dipole transition $|L_z\rangle \leftrightarrow ^2P_{1/2}|F = 0, m_F = 0\rangle$ using $\sigma_+$ light. However, this scheme’s usefulness is limited by the off-resonant transition $|1\rangle \leftrightarrow ^2P_{1/2}|F = 1, |m_F = 1\rangle$. Moreover, impure polarization would drive the $|1\rangle \leftrightarrow ^2P_{1/2}|F = 0, m_F = 0\rangle$ transition and damage the un-leaked qubit population. Instead, we propose a much more robust scheme that
takes advantage of the narrow linewidth and selection rules of the $^2S_{1/2} \leftrightarrow ^2D_{3/2}$ quadrupole transition.

The quadrupole transition Rabi frequency between angular momentum states with z-components $m_{j_{1}}, m_{j_{2}}$ is proportional to a geometric factor $g(\Delta m_{j})$ [21], given by,

$$g^{(0)}(\theta, \phi) = \frac{1}{2} |\cos \theta \sin 2\phi|$$

$$g^{(1)}(\theta, \phi) = \frac{1}{\sqrt{6}} |\cos \theta \cos 2\phi + i \sin \theta \cos \phi|$$

$$g^{(2)}(\theta, \phi) = \frac{1}{\sqrt{6}} |\cos \theta \sin 2\phi + i \sin \theta \sin \phi|,$$

where $\theta$ and $\phi$ are the respective polarization and k-vector angles relative to the quantization axis defined by the local magnetic field. When the polarization and k-vector are both orthogonal to the quantization axis, $g^{(0)}(\pi/2, \pi/2) = g^{(1)}(\pi/2, \pi/2) = 0$ and $g^{(2)}(\pi/2, \pi/2) = 1/\sqrt{6}$, meaning that only $|\Delta m_{j}| = 2$ transitions will occur as illustrated in Fig. 1. When the laser is tuned into resonance with the $^2S_{1/2} |F = 1\rangle \leftrightarrow ^2D_{3/2} |F = 1\rangle$ transitions, the selection rules and $^2D_{3/2}$ hyperfine splitting ensure that only the leakage states will be transferred to the $^2D_{3/2}$ manifold, leaving the qubit states unperturbed. After the leakage population has been transferred to the $^2D_{3/2}$ state, we apply $\pi$-polarized 935nm light that is resonant with the $^2D_{3/2} |F = 1 \rangle \leftrightarrow ^3[3/2]_{1/2} |F = 1 \rangle$ transition[2], which returns the ion to $^2S_{1/2}$ with a 98% branching ratio. Assuming perfect transfer pulses on the quadrupole transition and ignoring the 2% chance of decaying back into the $^2D_{3/2}$ manifold, this cycle will reduce the population in the leaked states as $P_{0} \rightarrow P_{0}/3$ per cycle. We note that the 2% chance of decaying to the $^2D_{3/2} |F = 2 \rangle$ manifold can be mitigated by adding a second frequency or by power broadening. After n cycles, the leaked population would ideally be reduced as $P_{0} \rightarrow P_{0}/3^{n}$ and we note that polarization errors in the 935nm light would, at worst, lead to a $P_{0} \rightarrow P_{0}(2/3)^{n}$ reduction.

We demonstrate this exponential decrease in leaked population using a single $^{171}$Yb+ ion in an RF Paul trap and employ the standard Doppler cooling, state initialization and read-out schemes outlined in Ref.[2]. The measurement is made by preparing one of the leakage states, applying n cycles of the leakage repump protocol, and then reading out the populations of the four different states in the $^2S_{1/2}$ manifold. The state initialization is performed by optically pumping to the $|0\rangle$ state followed by a 20$\mu$s microwave $\pi$-pulse at $\nu_{0} \pm \nu_{Z}$, where $\nu_{0} \approx 12.643$GHz is the qubit splitting in a magnetic field of 5.6G and $\nu_{Z} = 7.8$MHz is the associated Zeeman splitting of the $|m_{j}| = 1$ states. The quadrupole transition is driven with 8mW of 435nm light, focused to a beam diameter of 50$\mu$m resulting in a 1$\mu$s $\pi$-time. The $|L_{+}\rangle \rightarrow ^2D_{3/2} |F = 1, m_{f} = \pm 1\rangle$ transfer pulses are done sequentially for convenience, but could in principle be done simultaneously. Before measurement, we apply an additional 935nm pulse with 870MHz sidebands to depopulate the $^2D_{3/2} |F = 2\rangle$ manifold. This population accrual stems from the 2% branching ratio from $^3[3/2]_{1/2}$ back down to $^2D_{3/2}$ as well as off-resonant coupling during the quadrupole transition. However, this population accrual should be small as it is already mitigated during the sequence due to power broadening of the $^2D_{3/2} \leftrightarrow ^3[3/2]_{1/2}$ transition. The standard state-dependent fluorescence read-out of the $^{171}$Yb+ qubit mixes the three states in the $F = 1$ manifold[2], and therefore provides an estimate of the population in $F = 0$ and a sum of the populations in $F = 1$. We measure the population in only one of the $F = 1$ states by applying a final microwave pulse to swap $|0\rangle$ with the population we want to measure. As shown in Fig. 2, we observe an exponential decay in the leakage population with a slight deviation from the ideal decay of $1/3^{n}$ due to imperfect transfer pulses caused by Debye-Waller effects[22], laser imperfections and magnetic field fluctuations, and imperfect 935nm polarization that drives population to $^3[3/2]_{1/2} |F = 1, m_{f} = 0\rangle$ which decays into the qubit subspace with probability 1/3.

Deviations from the ideal pumping scheme are quantified by fitting the observed data with a simple model. Ignoring any coherent effects, each repumping cycle will change the population distribution according to a linear operator $R$, such that the population after the $n^{th}$ cycle is $P(n) = RP(n-1)$. We order the populations so that
respectively and the leakage state populations, respectively back into the qubit subspace. The qubit state populations, \( P_0 \) and \( P_1 \), are shown in red squares and black triangles respectively. The standard error on the data is at the 1\% level. The solid lines show fitted curves using the theory described in the main text.

The narrow linewidth of the quadrupole transition allows the presence of polarization impurities in the 935nm beam. An important requirement of the leakage repump is that it leave unlocked qubits unperturbed. The quadrupole transfer pulses can cause decoherence in the qubit subspace by one of two means: 1) off-resonant coupling from \( |1\rangle \) to \( ^2D_{3/2} |F = 2, m_f = \pm 2\rangle \) transition, or \( k \)-vector misalignment driving \( |\Delta m_f| = 0, 1 \) transitions. The narrow linewidth of the quadrupole pulse allows these errors to be controlled via pulse shaping or longer \( \pi \)-times. For a square pulse, the first mechanism results in an induced error per cycle given by (\( \Omega_f/2\pi = 860\text{MHz} \) is the hyperfine splitting of \(^2D_{3/2}\) and \( \Omega_c \) is the on-resonance Rabi frequency for the \([1] \leftrightarrow ^2D_{3/2} |F = 2, |m_f| = 2\rangle \) transition. We relate this to the \( \pi \)-time of the transfer pulse \( \tau_\pi = \pi/\Omega_0 \) by noting that \( |\Omega_0/\Omega_c| = 3/2\sqrt{2} \), so that the induced error per cycle is approximately \( 8\pi^2/(3\delta_{hf} \tau_\pi)^2 \), which induces an error of less than \( 10^{-6} \) per cycle when a 1\( \mu \)s \( \pi \)-time is used. Assuming the polarization and \( k \)-vector can be aligned with the fit parameters being \( \{ \rho, \delta_{hf}, \tau_\pi \} \) and \( R_{ij} \) is equal to the probability of state \( j \) getting pumped to state \( i \) in a single cycle. Observing that the qubit states are approximately steady states, we set \( R_{1,1} = \delta_{1,1} \) and \( R_{1,3} = \delta_{1,3} \). We also assume a symmetry in the leakage states so that \( R_{2,2} = R_{4,4} \), \( R_{2,1} = R_{4,1} \), and \( R_{2,3} = R_{4,3} \). These assumptions and the normalization \( \sum_j R_{ij} = 1 \) reduce the model to three free parameters, \( R_{2,1} \), \( R_{2,2} \), and \( R_{2,3} \) allowing for a straightforward calculation of the populations after \( n \) pulses as \( P^{(n)} = AR^n P^{(0)} + B \). We’ve included two additional fitting constants, \( A \) and \( B \), to account for state-initialization and measurement errors with their ideal values being 1 and 0 respectively. As shown in Fig. 2, the data is in relatively good agreement with the fit parameters being \( \{ R_{2,1}, R_{2,2}, R_{2,3}, A, B \} = \{ 0.323, 0.272, 0.225, 0.951, 0.025 \} \). Ideally \( R_{2,1} = R_{2,2} = R_{2,3} = 1/3 \) and our measurement showing an asymmetry in the pumping rates into the two qubit states and the transient transfer of population from \( |L_-\rangle \) to \( |L_+\rangle \) implies the presence of polarization impurities in the 935nm beam.

Errors induced by the leakage repump protocol on unlocked qubits can be quantified via interleaved randomized benchmarking (IRB) experiments [23]. IRB is a protocol constructed so as to quantify an error rate for a particular gate of interest. The basic idea of IRB is that a particular gate’s error can be quantified by repeatedly inserting it into randomized gate sequences and subtracting off the error ascribed to the truly random component. Presuming that the leakage repump protocol would be implemented during idle times, (during the identity gate), we benchmark the identity gate both with and without the leakage repump protocol being simultaneously performed. Our IRB measurement consists of two experiments: first, standard randomized benchmarking, which acts as a reference, and second, standard randomized benchmarking plus an \( n = 10 \) leakage repump sequence applied after each gate. We also ran IRB with a similar delay time interleaved in the second experiment to measure the memory errors (similar to Ref. [24]). For each IRB run, we measure the survival probability of ten random sequences for three different sequence lengths. The results of each experiment are plotted in Fig. 3 along with fits to the standard decay equation. The decay rate of each experiment is then used to estimate the interleaved gate’s average error, \( \epsilon_g = \frac{1}{2} (1 - p_{1/2}/p_1) \), where \( p_{1/2} \) are the decay rates from the first and second experiments for each IRB run. From IRB, we estimated the average \( n = 10 \) leakage repump error is \( \epsilon_{\text{repump}} = 2.0(8) \times 10^{-4} \) and the average memory error is \( \epsilon_{\text{memory}} = 1.5(6) \times 10^{-4} \) with the uncertainties estimated from confidence intervals obtained by semi-parametric bootstrap resampling [25]. These measurements imply that the effects of leakage repump are dominated by the idling memory errors of the system and

![Figure 2](image-url)
we are, therefore, only able to establish an upper bound for the error per cycle as $\epsilon_{\text{repump}}^{n+1} \leq 2.0(8) \times 10^{-5}$.

Since our IRB measurements are limited by the intrinsic memory errors of the system, we also performed a measurement of the population decay out of $|1\rangle$ as a function of the number of leakage repump cycles. As shown in Fig. 4, we observe a decay in population at the 1% level after $5 \times 10^4$ cycles. Fitting the data to a decaying exponential results in a decay per cycle constant of $1.4(3) \times 10^{-7}$.

A rough analysis of the practical limits of the protocol can be made by assuming a qubit initialization with an error dominated by leakage occurring with probability $\epsilon_0$. We then imagine applying the leakage repump protocol and define the probabilities of errors induced by each cycle as $\epsilon_i$ and $\epsilon_q$ where the subscripts respectively denote leakage-inducing and non-leakage-inducing errors. Assuming the ideal pumping rate of $1/3^n$, the leakage population after $n$ cycles is $\epsilon_0 (1/3)^n + 3\epsilon_i (1 - 1/3^n)/2$ and the total error is $\epsilon_0 + n(\epsilon_i + \epsilon_l)$. If, for example, a trapped-ion quantum computer’s error rate is dominated by a $10^{-3}$ two-qubit gate error$^{26}$ and it is assumed to be dominated by leakage channels, we can use our lower bound for the leakage repump induced error $\epsilon_0 + \epsilon_l = 2.0(8) \times 10^{-5}$ and examine the protocol in two different limits. In the limit where $\epsilon_i = 0$, we find that an $n = 5$ sequence would only increase the total error by $10^{-4}$, yet would reduce the leakage error to $4 \times 10^{-6}$. In the limit where $\epsilon_q = 0$, we can reduce the leakage error to $3.4 \times 10^{-5}$. This sequence would take approximately 50 $\mu$s, which is small compared to the typical times needed for sub-Doppler cooling plus gating operations and could be reduced through further optimizations. Additionally, we note that being able to remove leakage errors to a certain level is superior to designing a gate with an equivalent level of inherent leakage since, in the latter case, it will continue to accumulate in long gate sequences.

Our protocol can be generalized for use in atoms with more complicated hyperfine structures. The spin-1/2 nucleus in $^{171}$Yb+ simplifies the scheme by ensuring that there are no $|\Delta m_f| = 2$ transitions for the qubit states in the $^2D_{3/2}|F = 1\rangle$ manifold, meaning that systems with larger nuclear spins will need to rely on spectroscopic resolution to suppress excitations out of the qubit space. On the other hand, systems with larger nuclear spins admit clock qubits at higher fields, resulting in larger energy splittings and looser spectroscopic resolution requirements.

In conclusion, our protocol can reduce leakage populations by orders of magnitude with a negligible induced error in the qubit space. Since this protocol works at the physical level instead of the circuit level, it can also be orders of magnitude faster than algorithmic leakage reduction units. This work removes a significant obstacle to implementing the error mitigation techniques that will be crucial to both near term and long term development of trapped-ion quantum computers.

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