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14. ABSTRACT
We devised a novel scheme for electron-nuclear quantum information processing that exploits the anisotropic hyperfine coupling. This scheme enables universal control over a 1-electron, N-nuclear spin system, addressing only a single electron spin transition. Not having to address the nuclear spins directly significantly speeds up the control. We designed and fabricated a pulsed electron spin resonance spectrometer, along with a cryogenic probe which we used to experimentally implement this scheme on a single crystal sample of irradiated malonic acid.

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Electron-nuclear quantum information processing

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List of papers submitted or published that acknowledge ARO support during this reporting period. List the papers, including journal references, in the following categories:

(a) Papers published in peer-reviewed journals (N/A for none)

Universal control of nuclear spins via anisotropic hyperfine interactions,
J. S. Hodges, J. C. Yang, C. Ramanathan, D. G. Cory,
Physical Review A, 78, 010303(R), 2008

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(b) Papers published in non-peer-reviewed journals or in conference proceedings (N/A for none)

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Number of Manuscripts: 0.00

Number of Inventions:

Graduate Students

NAME	PERCENT_SUPPORTED
Jamie Yang	0.68
FTE Equivalent:	**0.68**
Total Number:	**1**

Names of Post Doctorates

NAME	PERCENT_SUPPORTED

FTE Equivalent:
Total Number:

Names of Faculty Supported

NAME	PERCENT_SUPPORTED

FTE Equivalent:
Total Number:

Names of Under Graduate students supported

NAME	PERCENT_SUPPORTED

FTE Equivalent:
Total Number:

Student Metrics

This section only applies to graduating undergraduates supported by this agreement in this reporting period

The number of undergraduates funded by this agreement who graduated during this period: 0.00

The number of undergraduates funded by this agreement who graduated during this period with a degree in science, mathematics, engineering, or technology fields:...... 0.00

The number of undergraduates funded by your agreement who graduated during this period and will continue to pursue a graduate or Ph.D. degree in science, mathematics, engineering, or technology fields:...... 0.00

Number of graduating undergraduates who achieved a 3.5 GPA to 4.0 (4.0 max scale):...... 0.00

Number of graduating undergraduates funded by a DoD funded Center of Excellence grant for Education, Research and Engineering:...... 0.00

The number of undergraduates funded by your agreement who graduated during this period and intend to work for the Department of Defense 0.00

The number of undergraduates funded by your agreement who graduated during this period and will receive scholarships or fellowships for further studies in science, mathematics, engineering or technology fields:...... 0.00

Names of Personnel receiving masters degrees

NAME

Total Number:

Names of personnel receiving PHDs

NAME
Jamie Yang

Total Number: 1

Names of other research staff

NAME	PERCENT_SUPPORTED
FTE Equivalent:	
Total Number:	

Sub Contractors (DD882)

Inventions (DD882)

Scientific Progress (46263PHQC)

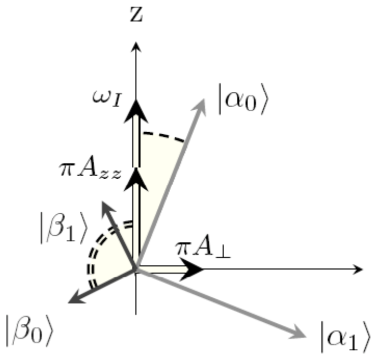
We devised a novel scheme for electron-nuclear quantum information processing that exploits the anisotropic hyperfine coupling. This scheme enables universal control over a 1-electron, N-nuclear spin system, addressing only a single electron spin transition. Not having to address the nuclear spins directly significantly speeds up the control. We designed and fabricated a pulsed electron spin resonance spectrometer, along with a cryogenic probe which we used to experimentally implement this scheme on a single crystal sample of irradiated malonic acid.

Electron-nuclear hypefine couplings

We have proposed a new approach to solid-state quantum computing, the key feature of which is to use an electron/nuclear spin system and to take the best from each. Nuclear spins make great qubits since they have long coherence times, but they are difficult to prepare and readout. Furthermore nuclear/nuclear spin interactions are typically slow, being generally a few kHz. Electron spins have the advantages that they can be prepared in well-defined computational states and individual electron spin readout has been demonstrated. However, electron spins have relatively short coherence times making them difficult to employ for qubits. Fortunately the electron/nuclear spin interaction, the hyperfine coupling, can be quite large, up to a few 100 MHz, and this provides a means for rapid information exchange between electron and nuclear spin systems. So the proposal employs electron spins for state preparation and readout, but the qubits are nuclear spins. The novel element and what makes this approach viable is the mediation of nuclear/nuclear spin gates via the *anisotropic* hyperfine interaction. We have devised a scheme for controlling many nuclear spin states local to a single electron spin where the overall hyperfine coupling of each nuclear spin has an anisotropic form. In such a system, any unitary operation over the nuclear spin system can be created by modulating transitions between the electron spin eigenstates.

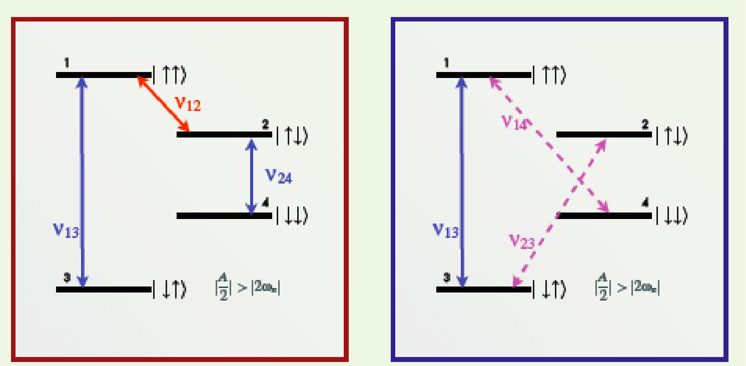
Consider an coupled electron-nuclear spin system. In an external magnetic field about a few hundred Gauss, the electron spins are strongly quantized along this external field. The quantization axis of the nuclear spins depends on the relative magnitudes of the nuclear Zeeman energy and the hyperfine coupling strength. At low magnetic fields, the nuclear spins are quantized along the local hyperfine fields, while at high fields the nuclei are quantized along the external field. For moderate field strengths, the nuclear Zeeman energy is comparable to the hyperfine coupling strength and the effective quantization axis lies between the two cases discussed above. Note that in general the hyperfine interaction is a tensorial coupling. If the external field B_0 is along a canonical axis of the hyperfine interaction, the eigenfunctions are product states of $|e,n>$. The transition frequency for an electron spin, is just $\nu_s \pm A/2$. The transition frequency for the nuclear spin is just $\nu_I \pm A/2$.

If B_0 is not along a canonical axis of the hyperfine interaction, the eigenfunctions are mixed in the nuclear manifolds. The electron frequencies and nuclear frequencies are geometric means of A,B and ν_I, and forbidden transitions of two spin flips now become allowed. In the presence of anisotropic hyperfine interactions, flipping the electron spin changes the quantization axis of the nuclear spins, as can be seen in the figure alongside for a single nuclear spin. As the two quantization axes are not co-linear, this sequence of evolutions under non-commuting axes permits arbitrary nuclear rotations. For the 1e-N nuclear spin system, distinct Larmor frequencies and hyperfine couplings for each nuclear spin guarantee the non-degeneracy of the eigenstates. The hyperfine couplings and the Zeeman frequencies must also be chosen such that $\omega_{jk}/\omega_{j'k'} \neq 1$.



The above two situations are compared in the figure below. We can examine the controllability of the coupled system in the two cases. A system of N spin-1/2 nuclear spins coupled to a single spin-1/2 electron is completely controllable, or universal, when the nested commutators of the internal Hamiltonian and each of the control Hamiltonians generate a closed Lie Group SU(2^{N+1}). For this system we achieve universal control by adding just one control field, a microwave driven transition at any one electron transition. The figure also shows the control Hamiltonians that permit universal control in these two systems. While we need to address three of four transitions if the hyperfine coupling has the form I_zS_z, we only need to address a single transition if the coupling has the form $S_z \otimes (AI_z + BI_x)$. We can therefore control the nuclear spin system via the electron spins.

In a magnetic field of 0.4 T, the electron and nuclear spin Larmor frequencies are ω_S = 11.2 GHz, and ω_I = 17 MHz (protons). The typical strength of the hyperfine interaction can range from about 2-100 MHz. The typical RF field strengths achievable to rotate the nuclear spins is 200 kHz while the RF field strengths for the electron spins is in the 10 MHz range. The need to apply pulses of the form $E_+^S I_y$ directly to the nuclear spins for the isotropic case on the left of the figure, significantly slows down the overall gate speed. The scheme utilizing the anisotropic interaction does not require the application of nuclear spin pulses, and is significantly faster.



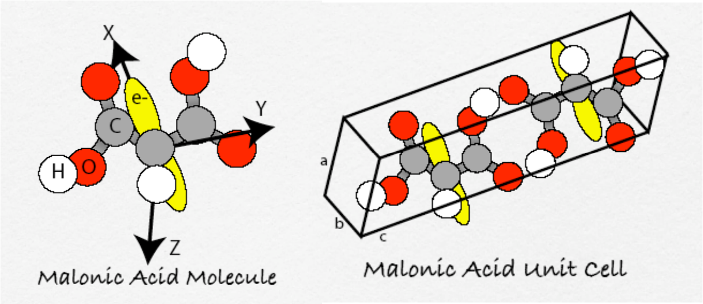
$$\frac{H_0}{\hbar} = \omega_e S_z + \omega_n I_z + A S_z I_z$$
$$\{H_c\} = \{S_x E_+^I, E_+^S I_x, S_y E_+^I, E_+^S I_y\}$$

Orientation along the PAS requires excitation of 3/4 transitions for universal control.

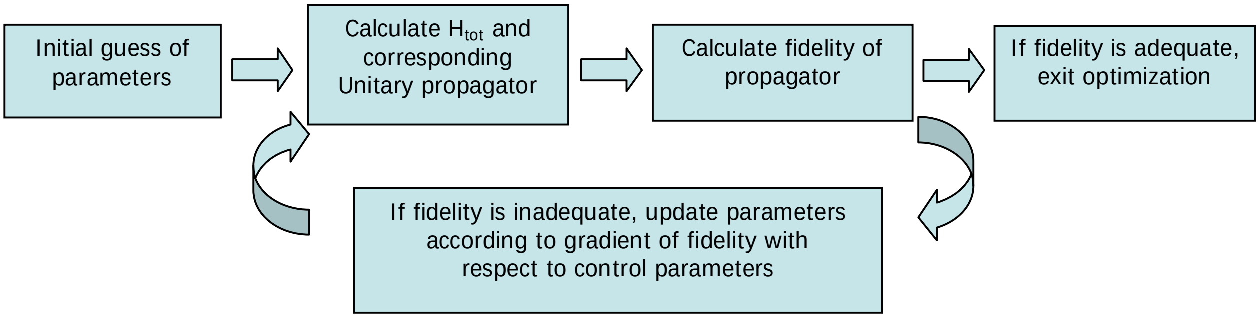
$$\frac{H_0}{\hbar} = \omega_e S_z + \omega_n I_z + A S_z I_z + B S_z I_x$$
$$\{H_c\} = \{S_x E_+\}$$

Introducing a HF anisotropy allows for universal control with only 1 transition.

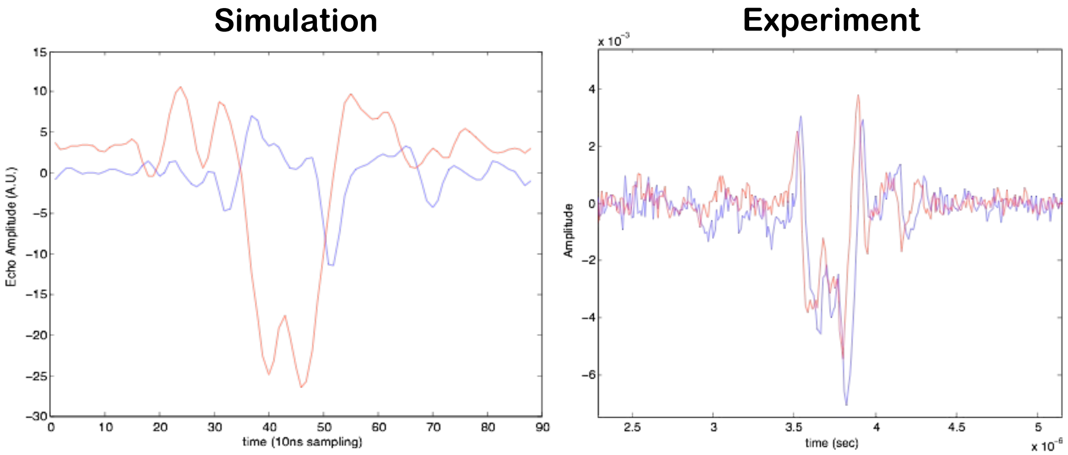
Consider the malonic acid system (shown below) that has previously been used to show entanglement between an electron and a nuclear spins. Malonic acid is a three-carbon backbone organic molecule that can be grown into a single crystal via evaporative methods. Irradiation of the crystal with 75 keV x-rays produces a unpaired electrons which is highly localized on the middle carbon. The Zeeman splitting of the electron (S=1/2) spin is split due to an anisotropic hyperfine interaction with the neighboring proton (I=1/2). At low defect densities, the electron-electron dipole interaction can be neglected; the system is thus an ensemble of isolated two-qubit systems. The hyperfine tensor in the principal axis system is (30, 60, 90) MHz.



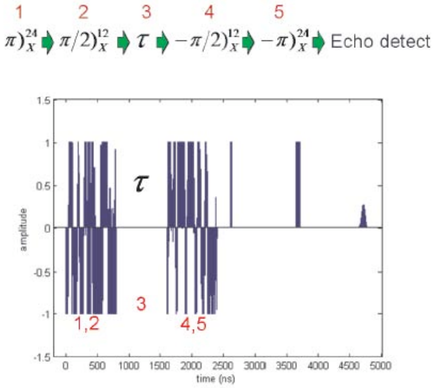
We can use numerical optimal control methods to engineer arbitrary unitary operations. By limiting the control fields of the electron-nuclear system to only the electron spin flip transitions we achieve quantum gates whose operation times are faster than if we had relied upon nuclear spin nutation rate alone, and faster than any relaxation process in the system, including the electron spin T_2. The gradient ascent pulse engineering (GRAPE) algorithm can be used to design a classical control waveform that achieves either a particular state transformation or a particular unitary operation and is shown below. The scheme subdivides the control waveform into a set of piece-wise constant intervals, and then uses a gradient algorithm to update the control parameters at every step to maximize the fidelity of the desired transformation.

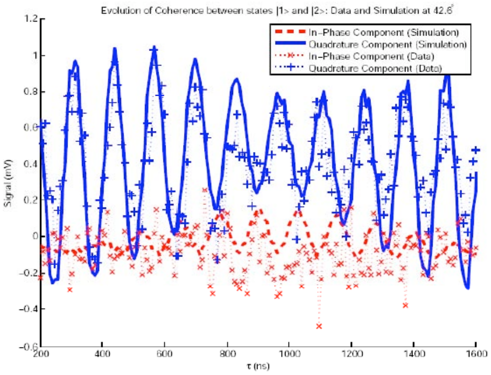


In our experiments the orientation of the crystal in the external field resulted in ESR frequencies of 12.01 GHz and 11.96 GHz and ENDOR frequencies of 8 MHz and 40 MHz. The figure below shows the experimental echo obtained using a GRAPE pulse to perform the π/2 S_x rotations in a spin echo experiment, in excellent agreement with numerical simulations of the expected echo.



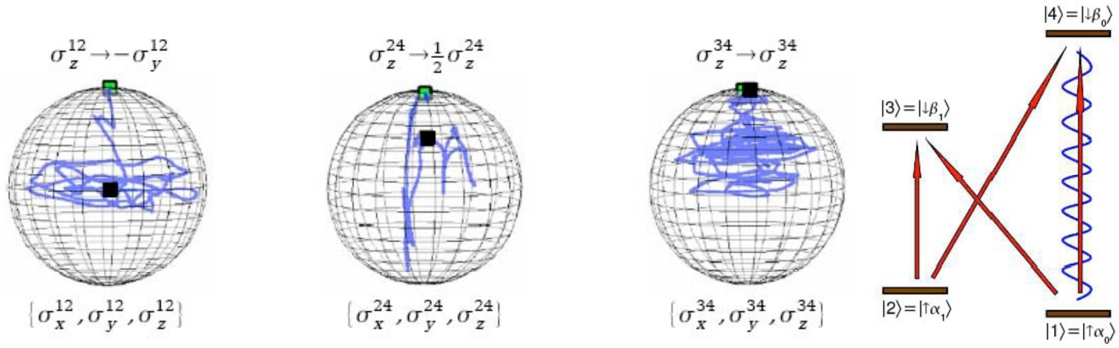
The figure below shows a Ramsey fringe experiment on a 1e-1n system, an irradiated single crystal of malonic acid. The figure on the left shows the sequence with the optimized GRAPE waveforms, while the figure on the right shows a comparison of the experimental data and theoretical simulations.





In the above experiment the detection of the nuclear spin coherence is performed by first transferring this to a population difference on the nuclear spins, and then transferring this to the electron spin where it is finally measured. The final detection is always performed on the electron spin.

The GRAPE waveforms realize a particular state transformation or unitary operation over the entire pulse, though the intermediate trajectories may be complicated. The figure below shows the Bloch sphere plots for different pairs of eigenstates, during a π/2$)_x$ pulse applied to the nuclear 1-2 transition. It is seen that though the 2-4 and 3-4 transitions are modulated, their final state is unchanged from the intial state. Though the microwaves are applied at the frequency of the 1-4 transition, all ESR transitions are allowed.

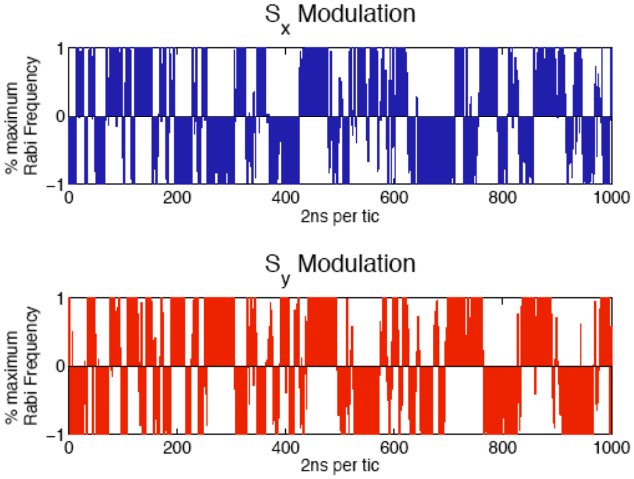


We have recently improved on the above implementation by modifying the GRAPE algorithm to take into account the bandwidth limitations of the control system. For any physical implementations of a set of time-varying controls the system bandwidth of the control electronics limits how well it can respond to an impulsive change of the controls. This bandwidth limitation implies that in searching for optimal controls for implementing a target unitary transformation, one must also include the impulse response function for the system. The actual control parameters $\{v_k\}$ seen by the quantum system are related to the ideal control parameters $\{u_k\}$ by a convolution:

$$v_j^k = u_j^k * \kappa^k = \sum_l \kappa_{l-j}^k u_j^k$$

where κ^k is the time-domain linear response kernel of the control electronics for the k-th parameter. We can now incorporate either a real or complex kernel into the GRAPE algorithm to find control sequences that are optimized to the bandwidth of the control electronics. For the case of multiple quadrature controls the scheme can be extended in P pairs of derivatives for a total of 2P controls.

Examples of GRAPE



Nuclear-Nuclear CNOT Modulation for ^{13}C-labeled irradiated malonic acid. We can implement this proton-carbon gate in 2μs, with maximum electron Rabi frequency of 15MHz. The time for performing the gate using nuclear-nuclear dipole couplings (tens of kHz) in the absence of an electron spin would be much longer.

In the presence of multiple nuclear spins it is possible to find subspaces of the nuclear spin system that are protected against electron spin flips. This would allow us to achieve coherence times in the nuclear spin system that are longer than the electron spin T_1.