Single Spin Measurement Using Cellular Automata Techniques

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We analyze a conceptual approach to single-spin measurement. The method uses techniques from the theory of quantum cellular automata to correlate a large number of ancillary spins to the one to be measured. It has the distinct advantage of being efficient: under ideal conditions, it requires the application of only $O(\sqrt[3]{N})$ steps (each requiring a constant number of rf pulses) to create a system of N correlated spins. Numerical simulations suggest that it is also, to a certain extent, robust against pulse errors, and imperfect initial polarization of the ancilla spin system.

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One of the most interesting challenges in physics today is that of measuring the state of a single (nuclear) spin. Being able to do this would bring us closer to spin based quantum computers [1], and have a myriad of applications, ranging from spintronics to protein analysis. Unfortunately, performing such measurement is not an easy task. Several methods have been proposed [2], and single-spin *detection* has been done [3], and the measurement in some specific cases has also been achieved [4] for electron spins.

Cappellaro *et al.* [5] propose using a system of N independent spins as a measurement system. This system is coupled to the spin being measured, and using entangling operations, creates a large correlated state, one whose signal can be measured with current NMR technology. The methods presented there require $O(N)$ pulse sequences in order to achieve N quanta of polarization. We expand on their ideas to create a scheme which uses $O(\sqrt[3]{N})$ pulses, and is fairly robust against noise and errors, and does not rely on entanglement. The improved running time is the most important advantage, since the whole procedure must finish before decoherence destroys the information being measured.

The method presented here is inspired by quantum cellular automata [6,7] and pulse driven quantum computers [8,9]. It uses a cubic lattice crystal [10] with two nucleus types, which we call A and B. Each species A nucleus is connected only to B nuclei, and *vice versa* in a checkerboard fashion (see Fig. 1).

We will refer to upward and downward z polarizations as $|+1\rangle$ and $|-1\rangle$. We assume, for the time being, that the crystal is initialized to a completely polarized state with all nuclear spins in a downwards z polarization state, $|-1\rangle$. The method then consists of bringing one corner of the crystal into close proximity to the spin we wish to measure, so as to couple the two spins. Once coupled we can use NMR rf pulses to correlate them, or swap the states. Suppose the spin we wish to measure is initially in the state $|\psi\rangle$, being either the eigenstate $|-1\rangle$ or $|+1\rangle$. After the swap the top-left vertex nuclear spin will be in the state $|\psi\rangle$.

What we present now is an efficient method to create a very large correlated state within the crystal. Under ideal conditions, that is complete polarization, perfect pulses, and no decoherence, the method creates the state $|\psi\rangle^{\otimes N}$ using only $O(\sqrt[3]{N})$ steps (each requiring a constant number of rf pulses). When $N \sim 10^6$ the resulting state gives a strong enough magnetic signal to be measured. Achieving this polarization, in the ideal case, requires applying about 200 steps of our algorithm.

In order to more easily illustrate our algorithm it is best to visualize the cube lattice in the following way. We envision slicing the cube into layers, such that the first layer is the corner nuclear spin that contains the state to be measured. Layer two contains all nuclei coupled to layer one. Layer three contains all nuclei coupled to layer two which are not in layer one, and so on. This is illustrated in Fig. 2.

Each layer includes spins of only one species, layer one being all A, layer two all B, layer three all A again and so on. We envision taking only half the cube lattice, so that

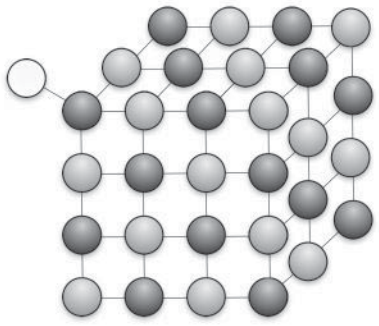

FIG. 1. *Cube lattice:* a crystal with two types of nuclei A and B, one represented as light gray spheres, the other dark gray. Each species A is neighbored by only B type nuclei and vice versa. The lines connecting the spheres represent the nearest-neighbor couplings. The white sphere represents the spin we wish to measure. This spin is coupled to the dark gray nucleus in the top-left vertex.

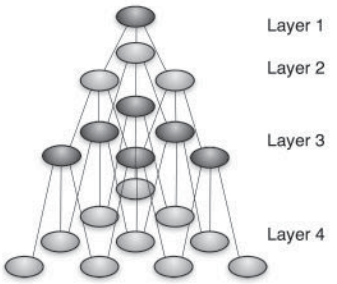

FIG. 2. *Pyramid lattice:* a different view on the same structure as Fig. 1. The top gray sphere is layer 1 and corresponds to the top-left vertex spin in Fig. 1. The three light gray spheres directly below it are layer two, and so on. The lines connecting the spheres represent the nearest-neighbor couplings, and are exactly the same as in Fig. 1.

each layer is larger than the previous one. Layer i has i more spins than layer $i-1$.

For sake of analysis, suppose the crystal's Hamiltonian has nearest-neighbor (Manhattan distance one) couplings only. In such a Hamiltonian, each A spin is coupled only to B spins, and *vice versa*. The resonant frequency of each A (conversely B) spin is affected by the states of its B (conversely A) spin neighbors. Since the neighbors are all indistinguishable spins, only the total *field* value is important, i.e., the number of neighbors pointing up, minus the number of neighbors pointing down.

Using well-known methods, first applied in a scheme similar to the one proposed here by Lloyd [8] [and later used in [9] and others], it is possible to create gates that address species A spins that have a particular neighbor field value. For instance, it is possible to apply a NOT gate (using the language of quantum computation) to all A spins that have neighbor field value 0, *and only* these spins. Later, we will show one way to actually achieve these gates, by using a (constant size) sequence of strongly modulating pulses [11].

Now we show how to use the lattice structure, and the above gates, to *"amplify"* the spin we wish to measure to a detectable signal strength. (We call the set of all species X spins with neighbor field k, X_k.)

The *algorithm* is the following. Repeatedly apply a NOT gate to the following sets of spins: B_{-2}, B_{-1}, B_0, A_{-2}, A_{-2}, A_0.

Suppose that $|\psi\rangle = |-1\rangle$. Then absolutely nothing happens to the lattice (ignoring errors), and so it remains in the all $|-1\rangle$ state. To see this, note that all lattice points have at least three neighbors, all in the $|-1\rangle$ state. Hence the field k of every cell is at most -3. Since we are only doing flips on $k = 0, -1, -2$ this does not affect the lattice at all.

Suppose now that the top cell of the pyramid is initialized to the state $|+1\rangle$. Then, all B neighbors of this vertex (those in layer 2) will have field value -2: -3 from three downward neighbors each in state $|-1\rangle$ and a $+1$ from the upward neighbor in state $|+1\rangle$. Therefore, they will be flipped by the first π pulse. No other spin will be affected. In the next stage, all A spins in layer 3 will be flipped, and so on. In n stages all spins in the first n layers will be flipped to $|+1\rangle$, for a total of $N = \frac{1}{6}(n+1)n(n-1)$ nuclear spins pointing up. Hence, only $O(\sqrt[3]{N})$ stages are required to obtain a total field of N spins.

At the end of such procedure, one can measure the magnetic field of the cube lattice crystal, obtaining the desired measurement result.

Khitrin *et al.* used a similar approach [12] in their scheme for polarizing spin chains. Although their method could potentially be used for spin measurement, the method presented here is cubically more efficient.

In order for the scheme to work it is tantamount for the frequencies of the target spins to be different from the ones we do not wish to affect. In the ideal setting, where the Hamiltonian has only first-neighbor (strictly speaking Manhattan distance 1) couplings, this is the case. In Fig. 3 we see what an ideal spectrum for a second layer spin looks like. It has 5 distinct peaks, one for each of its possible neighbor fields.

We have so far assumed a nearest-neighbor coupling Hamiltonian. A solid crystal, however, is governed by a direct dipole coupling Hamiltonian,

$$\mathcal{H} = \sum_{i<j} d_{i,j}[\sigma_z^i \sigma_z^j - k_{i,j}(\sigma_+^i \sigma_-^j + \sigma_-^i \sigma_+^j)],$$

where $k_{i,j}$ equals one if i, j are of the same species and zero otherwise;

$$d_{i,j} = \frac{g_{i,j}}{r_{i,j}^3}\frac{1}{2}(3\cos^2\Theta_{i,j} - 1) = \omega_d \frac{r_{i,i+1}^3}{r_{i,j}^3},$$

where $r_{i,j}$ is the distance between the two nuclei, $\Theta_{i,j}$ is the angle between the vector connecting the two nuclei and the z axis (determined by the magnetic field), and $g_{i,j}$ is a simple constant that depends only on the nuclear types of i and j.

In order to maximize symmetry, and avoid problems with the *"magic angle"*, we choose a rhombohedral crystal structure, and we orient it so that the top of the pyramid points up in the z direction. The actual Bravais angles of the crystal are unimportant, as long as they are sufficiently far from 90°. We chose 60° for our simulations. With this configuration the angles between every spin and its nearest

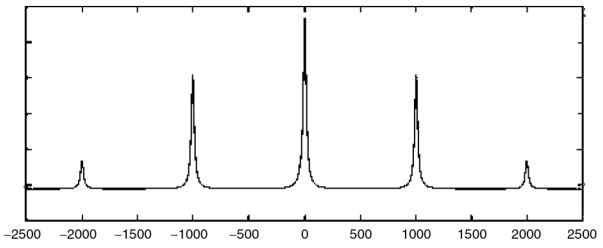

FIG. 3. *Ideal NMR spectrum:* this is the ideal spectrum for a spin on the second layer. There are 5 distinct peaks, one for each of the five neighbor field values.

neighbors is the same, making all these couplings strengths equal.

It has been shown [13] that it is possible to suppress all homonuclear dipolar coupling via the 48 pulse sequence. More recent experiments [14] are using a modified sequence to refocus the homonuclear couplings while just rescaling the heteronuclear dipolar coupling. It is thus within the current NMR practice to create the interaction: $\propto \sigma_z\sigma_z$ limited to heteronuclear spins in a solid.

By suppressing all but the heteronuclear couplings, the Hamiltonian resembles the nearest-neighbor interaction only, albeit with extra "error" terms, that are generally no stronger than roughly $1/30$ the strength of first-neighbor couplings. In Fig. 4 we show the absorption spectrum of a second layer spin (in a hypothetical crystal, where the couplings are set up so that the nearest-neighbor couplings are roughly 1000 Hz). Notice how similar it is to the ideal (nearest-neighbor only coupling) case.

Using these techniques it is possible to tailor a pulse sequence to achieve the gates we require. Consider, for example, a spin of the B species in the interior of the crystal, that is, with six neighbors. Three of these will be in the layer above the spin under consideration and three in the one below. Therefore, the spin should be flipped if, and only if, the spins in the upper layer are in the $|+1\rangle$ state. To perform this transformation, we rotate the heteronuclear Hamiltonian $\mathcal{H} = \sum_k \omega_d^k \sigma_z^B \sigma_z^{A_k}$ to the transverse plane by a $\pi/2$ pulse about y: $\mathcal{H}' = \sum_k \omega_d^k \sigma_x^B \sigma_z^{A_k}$. This Hamiltonian will rotate the spin B at a rate dictated by the number of A spins up and down to which it is interacting with, until we apply another $\pi/2$ pulse about y. If the A spins are all up, then the B spin oscillates between the states (the A spins remain invariant under this evolution): $-i\sin(6\omega_d t)|+1\rangle + \cos(6\omega_d t)|-1\rangle$.

If they are down (and the spin B is down as well, since the algorithm has already rotated these layers) we get the evolution: $-i\sin(6\omega_d t)|-1\rangle - \cos(6\omega_d t)|+1\rangle$, while if three neighbors are up and three down, the spin remains unchanged. Hence, if we apply the second $\pi/2$ pulse about y after $t = \pi/(12\omega_d)$, we can obtain the wanted evolution.

We can use a similar scheme to make the $\mathcal{H}'$ interaction rotate only the B (A) spins with neighbors in the upper layer in the up state and neighbors in the lower layer still in the down state. This simple two-pulse sequence is a zero order example of pulse sequences, where the time during which the spins are let rotate at the spin-state dependent frequencies is further and further subdivided to obtain the desired selectivity in the effective rotation applied (see Fig. 5).

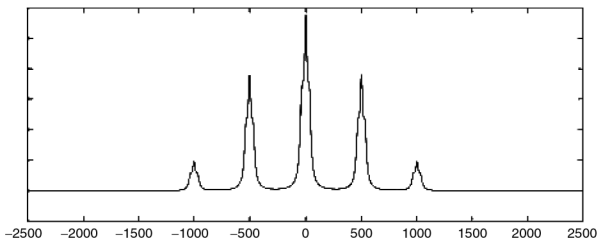

FIG. 4. *Suppressing homonuclear coupling:* this is the spectrum for a spin on the second layer of a rhombohedral lattice with angles $\alpha = \beta = \gamma = \pi/3$, with the homonuclear couplings suppressed. Note the similarity to the ideal case.

As we mentioned, the Hamiltonian we obtain after suppressing the heteronuclear couplings is not *exactly* nearest-neighbor coupling only, but has some small error terms. These error terms, as well as imperfect control, will cause imperfect gates. Also, the crystal lattice may not be perfectly polarized initially. It is important to deal with these issues.

One important fact to notice is that our scheme is impervious to phase-flip errors in the lattice. Effectively, all pulses, and the final output, depend only on the diagonal terms of the density operator ρ of the lattice.

The diagonal elements of ρ must be protected. A single bit-flip error in the cube lattice by itself does not drastically change the overall field. If this bit, however, flips during the running of the algorithm it has the potential to influence all lattice points in a radius around it during the next step of the algorithm, by changing their neighbor fields during the pulse sequence, potentially creating a cascade of errors.

The first fact to notice is that errors inside the pyramid are less critical than errors on the faces, or worse, edges, of the pyramid. The reason is that inside the pyramid all lattice points have exactly 6 neighbors. If one flips erroneously, there are still 5 neighbors in the correct state.

Take an interior lattice point that is in the state $|-1\rangle$ and should be flipped to $|+1\rangle$ in the next stage. Since it is supposed to flip, it should have three positive neighbors and three negative ones. Suppose that an upward neighbor has an error, then it will have two positive and four negative. This is, however, not a problem. The lattice point in question will have a field value $k = -2$, instead of $k = 0$, but will still be flipped correctly.

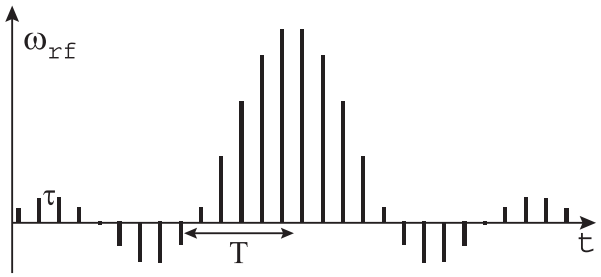

FIG. 5. *Pulse Sequence:* rf power as a function of time. By choosing $\tau = 1/(10\omega_d)$ and $T = 1/(2.1\omega_d)$ the frequency profile of this pulse sequence (obtained by a Fourier transform) is an excitation of the frequencies $\omega_{\pm 6} \rightarrow \omega_{\pm 4}$. By choosing the total rotation angle of these pulses to be π, we can rotate just spins B which have frequencies $\omega_{\pm 3} \rightarrow \omega_0$ as required by the algorithm. This pulse sequence is presented only as an example, as more complex pulse sequence can be designed to improve further these results.

Contrast this to the case where a bit flip occurs along the edge of the pyramid. In this case the field of the lower neighbors to a lattice point with error will go from having a field of -2 to a field of -4 and the spin will no longer be flipped. The error will then propagate downwards.

One way to reduce errors is to extend the flipping operation to spins with neighbor fields of $+1$. This will correct some edge-related errors. Another way to drastically reduce error propagation is to force errors into the inside of the pyramid.

Previously we concluded that we need to suppress the homonuclear coupling during our pulse sequences. In this Hamiltonian, the term $\sigma_+^i \sigma_-^j + \sigma_-^i \sigma_+^j$, often referred to as the *"flip-flop"* term, has the effect of swapping two anti-aligned neighboring spins. Take a horizontal slice of the pyramid and suppose there is a single error among these lattice points. The effect of the flip-flop term on neighboring spins is well known and is called *spin diffusion* [15]. A simple approximation to this dynamics is a quantum walk on the lattice. In this model, an erroneous bit not only becomes diffused over several spins, it also has a much lower probability (averaged over time) of being in non-interior points. This leads us to believe that letting the system evolve under the homonuclear interaction for some time before running the algorithm will have the effect of reducing errors in the edges, and increase overall robustness to errors.

In order to test the reliability of our algorithm in the large scale it would be infeasible to have a full quantum-mechanical simulation. However, since the diagonal part of the density matrix captures most of the interesting dynamics and we neglect the coherences created by pulse errors and unwanted evolution we can use a semiclassical Monte Carlo style simulation. We set up a three-dimensional byte array, each byte representing a nuclear spin. Each byte is set to an initial value of -1. In order to simulate an initial polarization of $1 - \epsilon_0$ we then flip the sign of each byte with probability ϵ_0. Each pulse is simulated in a similar fashion. A gate error ϵ_1 is simulated by failing to flip bytes with probability ϵ_1 [16]. This technique allows to simulate very large systems, of size up to 10^8 nuclear spins.

Our purpose in numerically simulating the system is to inform future engineering studies of single-spin detection. At this time we will explore the scalability and error propagation. There remain serious technical challenges before any realistic experimental study can be attempted.

We calculated the signal strength at the end of our algorithm for different lattice sizes N as well as error rates ϵ_0 and ϵ_1. Although, the contrast C [as defined in [5]] does decrease as either N, ϵ_0, and ϵ_1 increase, we found that an error threshold, a bound on the size of ϵ_0 and ϵ_1, exists such that C decreases slowly enough so that the *total* magnetization gap $G = C \cdot N$ increases with lattice size (for lattice sizes tested, $N \leq 10^8$). The threshold found is roughly $\epsilon_0 = 0.1$ and $\epsilon_1 = 0.01$. As an example, a lattice of size 10^8, with these error rates, will have roughly $C = 0.01$, or $G = 10^6$. This gap should produce a difference in magnetic signal strong enough to be detected by current NMR technology.

In conclusion, moving to a three-dimensional measurement system, as opposed to a $1D$ chain as in [5], gives distinct advantages. The clearest benefit is a cubic speedup in the procedure. Also the algorithm gains substantial robustness to errors. This is an even greater benefit, given the current fidelity of NMR operations. Our numerical simulations suggest that the scheme is highly efficient and moderately robust. However, the nature of our simulations do not allow us to take into account large coherent superpositions or errors throughout the pyramid lattice. Large scale coherent simulations are infeasible. Ultimately we will need an actual physical implementation in order to best understand the capabilities, and limits, of our proposed scheme.

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