Selecting ensembles for rare earth quantum computation

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We discuss the issues surrounding the implementation of quantum computation in rare-earth-ion doped solids. We describe a practical scheme for two qubit gate operations which utilise experimentally available interactions between the qubits. Possibilities for a scalable quantum computer are discussed.

I. INTRODUCTION

Quantum computing promises significant advantages over classical computation for a number of important tasks such as factorising large numbers [1] and searching large databases [2]. Experimental quantum computation is difficult because of two competing requirements. Firstly the qubits must be well isolated from the environment to preserve coherence. Secondly they must have interactions among themselves and with whatever is being used to control and read out their states. In addition to this the power of a quantum computer increases exponentially with its number of qubits. For a quantum computer to outperform a classical one it is more than likely a large number of qubits will be required.

There have been a number of demonstrations of quantum computation to date. The physical systems used include liquid state NMR [3], atoms in high-finesse cavities [4] and ion traps [5]. The problem with all such schemes is that there has been trouble in scaling the system to a large number of qubits. The handful of qubits achieved to date are not sufficient for a technologically useful device.

Great effort has been put into the nano-fabrication of devices that, it is hoped, will enable scalable quantum computation. Recently two interacting qubits have been demonstrated [6] but the coherence times in this system were short (approx 10 ns). Difficulties associated with these very short timescales provide a challenge for further scaling of the approach.

Rare-earth-ions provide another possible path to scalable quantum computation, one where the coherence times are much longer and where coherent effects have been studied for many years [7]. Decoherence effects, perhaps the most important issue in the operation of a quantum computer are generally well understood in such systems.

One can summarise the attractive features of rare-earth-ion dopants for quantum computing as below:

- Optical transitions with long coherence times, up to 2.6 ms, previously observed [8].
- Long coherence times in their ground state nuclear spin transitions, up to 80 ms [9].
- Lifetimes for the nuclear spin states as long as several hours [10].
- Strong coupling between the electronic states and nuclear spin states enabling the optical manipulation and readout of the spin states [11, 12].
- Large inhomogeneous broadening in the optical transitions, typically of the order of gigahertz enables many homogeneously broadened ensembles or even single ions to be addressed individually [13].
- Strong electric dipole-dipole interactions (as large as GHz) enabling coupling between the ions [14].
- Unlike liquid state NMR, using optical pumping there are no problems in preparing the starting state.

In this paper we describe a practical method for achieving a two qubit device using ensembles and discuss possibilities for scalability.
II. RARE EARTH QUANTUM COMPUTATION

The use of rare-earth-ions for quantum computation, and in particular the implementation of two qubit gates using electric dipole-dipole interactions, was first proposed by Sellars and Manson [15]. These interactions are due to the fact that the ground and optically excited states have different permanent dipole moments.

Following this a proposal for a complete architecture was given by Ohlsson et al. [16]. The approach given here has the distinct advantage that it is significantly less sensitive to inhomogeneous broadening. This sensitivity to inhomogeneous broadening has been recognised as the main weakness in attempts to improve the Ohlsson scheme [17].

Each qubit in such a scheme is a packet of ions chosen from the inhomogeneous line based on their optical frequency, all ions that are not part of this packet but have similar resonant frequencies would be optically pumped to an auxiliary hyperfine level. Optical absorption around such an anti-hole is shown schematically in Fig. 1. Ensembles of this type were first realised, and their usefulness to quantum computing recognised by Pryde et al. [18]. A clear demonstration that such systems perform well as qubits is given in [18].

There is a strong analogy between the ensemble quantum computation using rare earth ions and liquid state NMR. In both cases the measurements on ensembles can be made by monitoring the coherent emission. In both cases qubits can be addressed based on their resonant frequency and the interaction between the qubits is weak compared to available driving Rabi frequencies. It should be noted that in the case of rare earth ions this weak interaction is a result of using ensembles and the interaction between the ions can be large.

As already stated, due to optical pumping, rare earth ion quantum computation doesn’t share the initialisation problem of NMR. Further to this the rare earth ions have optically resolvable hyperfine structure allowing the transfer of quantum information from the optical transitions to ground state hyperfine transitions. When the quantum information is stored in this ground state structure it can be stored for long periods of time (80 ms[9]) and it is insensitive to the electric dipole-dipole interaction.

The challenge for rare earth quantum computing is the inhomogeneity in the strengths of the interactions between qubits. This is not a problem in liquid state NMR, since the nuclear spins in a molecule have fixed relative positions whereas the rare earth dopant ions in an ordinary crystal are randomly distributed.

The effect on the frequencies of the ions of one anti-hole upon the excitation of another is shown in Fig. 2. The homogeneous linewidths of rare earth systems can be as small as 100 Hz[3]. Individual homogeneous packets are represented by A, B and C in the top trace. The excitation of a second anti-hole causes a broadening in what would have been homogeneously broadened packets denoted by A’, B’ and C’. How much the frequency of an ion shifts depends on how close it is to an ion in the perturbing anti-hole. Obviously the number density of perturbing ions increases with the spectral width of the perturbing anti-hole. Thus the broadening caused by the interaction increases also with the spectral width of the perturbing anti-hole. A simple analysis [19] shows that this broadening is proportional to the spectral width of the perturbing ions and approximately 20 times smaller. This agrees with measurements made of this interaction [18].

Coherent transient techniques [7] have been used extensively in rare earth systems to probe the rare-earth-ion system with greater resolution than would be allowed by the inhomogeneous broadening using conventional techniques. Here we provide a method for achieving both the ion selection and computation that is based on photon echo sequences. The strength of this technique is that it allows the use of interaction strengths smaller than the inhomogeneous linewidth of anti-holes that are used as qubits. As mentioned above the mean interaction strength between the ions of two anti-holes is a small fraction of their homogeneous width. Earlier proposals [16] are limited to frequency shifts bigger than the inhomogeneous linewidth and are thus forced to work with a very small subset of the ions. A level
FIG. 2: A diagram showing the effect on the frequencies of of the ions of an anti-hole upon the excitation of another. Before the other anti-hole is excited (top) the inhomogeneously broadened feature is made up of a whole lot of homogeneously broadened features (A, B and C). The excitation of another group of ions will cause random shifts in the resonance frequencies of the ions leading to broadening of these ensembles. These are shown in the bottom three plots. The technique described here selects out the shaded areas and uses the resulting deterministic frequency shift for quantum computing operations.

of 0.3% has been estimated by one of the proponents of the scheme. The requirement this puts on the level background ions is a problem in practice.

The pulse sequence to achieve a CNOT operation between the two ions is illustrated in figure and can be understood with the help of the following Hamiltonian. In the appropriate interaction picture the Hamiltonian for two ions in two separate anti-holes is give by.

\[
H = \frac{\delta_1}{2} Z_1 + \frac{\delta_2}{2} Z_2 + \frac{\eta}{2} Z_1 Z_2
\]  

(1)

Here \( \delta_i \) represents the detuning from the center anti-hole and \( Z_i \) is the Pauli-Z operator \( (Z = [1 0; 0 -1]) \) for the ion \( i \). The strength of the interaction between the two ions is described by \( \eta \).

The first pulse puts the target ion on the equator of the Bloch sphere where it then precesses around the equator at a rate given by its detuning from resonance. This detuning is given by the sum of \( \delta_1 \) and the effect of the interaction. Without the \( \pi \) pulse on the control qubit at the middle of the gate operation a \( \pi \) pulse to the target gate would refocus this precession. This would lead to the target ion being at the same position on the equator of the Bloch sphere as when it started. The application of the \( \pi \) pulse to the control ions stops the re-phasing of the precession due to the interaction. If the waiting time is equal to an odd multiple of \( \frac{\pi}{4\eta} \), then the two trajectories on the block sphere corresponding to the control ion being initially in the states \(|0\rangle\) and \(|1\rangle\) end up separated by angle \( \pi \). They can then easily be mapped to the ground and excited states with the appropriate \( \pi/2 \) pulse. Such a pulse sequence would
be useful in liquid state NMR if there were limitations imposed by the inhomogeneity of the DC magnetic field.

The unitary evolution operator describing the gate’s operation can be expressed as the product of seven elementary operations.

\[ U = U_7 U_6 U_5 U_4 U_3 U_2 U_1 \]  

where

\[ U_1 = \exp\left(\frac{-iY_1 \pi}{2}\right) \]  
\[ U_2 = \exp(-iH \Delta t) \]  
\[ U_3 = \exp(\frac{-iY_1 \pi}{2}) \]  
\[ U_4 = \exp(\frac{-iY_2 \pi}{2}) \]  
\[ U_5 = \exp(-iH \Delta t) \]  
\[ U_6 = \exp(\frac{-iX_1 \pi}{2}) \]  
\[ U_7 = \exp(\frac{-iY_2 \pi}{2}) \]

this gives us, independent of \( \delta_{1,2} \)

\[ (-1)^\frac{1}{4} \begin{bmatrix} \sin(\theta) & -i \cos(\theta) & 0 & 0 \\ -\cos(\theta) & i \cos(\theta) & 0 & 0 \\ 0 & 0 & \cos(\theta) & -i \sin(\theta) \\ 0 & 0 & -\sin(\theta) & -i \cos(\theta) \end{bmatrix} \]  

where \( \theta = 2n\Delta t \), for \( \Delta t = \frac{(4n+1)\pi}{4} \) this becomes

\[ (-1)^{\frac{1}{4} + n} \begin{bmatrix} -1 & 0 & 0 & 0 \\ 0 & i & 0 & 0 \\ 0 & 0 & 0 & i \\ 0 & 0 & 1 & 0 \end{bmatrix} \]

The difference between this and the evolution matrix describing the CNOT operation

\[ \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \]
is simply rotations about the $Z$ axes of the Bloch spheres of the qubits. These need not be physical operations but instead changes in the definition of the phases for the qubits $^3$.

In order to create an ensemble with interaction strengths given by $\eta \Delta t = (4n + 1)\pi/4$ the gate operation can be applied repeatedly with both ensembles initially in their ground states with a pause between them of the order of the spontaneous emission time to allow the system to relax. The target ions that see the correct interaction strengths will still be in the ground state at the end of the operation while the others will have some population in the excited state. Repeated application of such sequences swapping the roles of target and control qubits will optically pump all the ions that don’t see the correct interaction strength into an auxiliary hyperfine level in a way analogous to spectral holeburning.

Results of modeling of the interaction-strength-holeburning process are shown in figure 4. The branching ratio for an atom to spontaneously emit back down into the state $|0\rangle$ versus another hyperfine level was taken to be one half.

One problem in this method is achieving high fidelity gate operation in the presence of what is still reasonably large inhomogeneity in the interaction strength. This problem can be overcome using the results of Jones $^{20}$. Jones pointed out that the problem of inhomogeneity in interaction strength for two qubit gates is exactly analogous to the problem of inhomogeneity in Rabi frequency for single qubit operations. This means that methods analogous to the “composite pulses” used to overcome these problems can be used. In the absence of other errors, using such techniques would enable a fidelity better than $10^{-6}$ in the presence of $10\%$ inhomogeneity in the interaction strengths.

This leads us to the conditions that must be satisfied in order to demonstrate the CNOT using this refocusing process. Firstly, the average interaction between the ions must be at least an order of magnitude larger than the spontaneous emission rate. This condition is more easily satisfied when the starting ensembles are wider anti-holes. The second condition is that the spectral width of the ensembles must be small enough compared to the available laser power that the pulses applied have the same effect to the whole ensemble. For the example of Eu:Y$_2$SiO$_5$ if we burn anti-holes of the order of 100kHz wide then we expect to have appreciable numbers of ions with interaction strengths of the order of 10kHz. This is large compared to the $\approx 500$ Hz spontaneous emission rate. With 500 mW of laser power focused with a 10cm lens, Rabi frequencies of the order 1 MHz can be easily achieved.

A second condition is that the laser used to produce the pulses is phase stable for the time of the experiment ($\approx 200\mu s$). While making a laser this stable is non-trivial, a laser with sufficient stability designed specifically for the spectroscopy of rare earth ion systems exists $^{13, 13, 21}$. In conclusion, this suggests that the demonstration of such a two qubit gate is achievable with current technology.

III. THE PROBLEM OF INHOMOGENEITY IN INTERACTION STRENGTH

In a sense the problem of inhomogeneity is the only problem to overcome in rare earth quantum computation. The ions have experimentally verified long coherence times and large interaction strengths. Further to this, for ensembles, measurements akin to those used in liquid state NMR are available. In the approach suggested above ions are selected from a macroscopic collection based on their resonant frequency and interaction strengths. The criteria for which ion groups are acceptable to be part of the ensemble of quantum computers gets increasingly more stringent with the number of qubits. As mentioned above this will lead to exponentially fewer ions fitting the criteria as the number of qubits increases.

In order to make rare-earth quantum computing scalable there is a need for a better way of overcoming this
Inhomogeneity. The possibilities discussed here are the use of single ion spectroscopy either directly or by coupling to other ions, and the use of “solid state molecules”.

In liquid state NMR based quantum computing you are dealing with an ensemble of “computers” just as for the rare earth scheme described above. The problems of inhomogeneity are avoided because each computer is a molecule which is identical to all the others. It should be emphasised that rare-earth quantum computing does not share the initialisation problem which causes NMR quantum computing to become untenable for large numbers of qubits. A material can be imagined where there are large numbers of identical collections of rare earth dopants. All the rare earths are strongly electro-positive with their bonding to other atoms essentially ionic in nature \(^{22}\) and as such incorporating them in a molecular solid would be difficult. One possibility for realising something akin to “solid state molecules” is adding defects to a stoichiometric sample. Crystals containing stoichiometric amounts of europiums can still exhibit relatively long coherence times so long as the inter-europium space is large within the crystal \(^{23}\).

The europiums close to a defect would provide one member of an ensemble of an identical groups of europium ions. The defect would shift the resonant frequencies of the members of this group to differing amounts allowing them to be manipulated based on their optical frequencies. The fact that they are shifted out of resonance with the bulk europiums ions should also increase their coherence times.

Another way of overcoming the inhomogeneity in interaction strength is by abandoning the use of ensembles. In such a situation the computer would consist of a cluster of ions. Because the ions are selected based on their frequency rather than their precise positions and the gate operations can be tailored to given interaction strengths, no complex fabrication would be required. This leaves the problem of detection of single ions. Spectroscopic measurements of single NV centres in diamond has been demonstrated \(^{24}\). While the lower oscillator strengths for rare earth ions would push current detector technology, it may be possible to detect the 1000 photons/sec produced when strongly driving an optical transition. How long this emission lasts depends on the rate at which the population gets optically pumped into other hyperfine levels. For free atoms/ions strong selection rules result in cyclic transitions where the optically excited state only decays into the ground state from which it is being driven. These cyclic transitions are harder to come across in the solid state but one option is using a site with a symmetry axis (for example LaCl\(_3\)). At zero magnetic field the hyperfine structure is described by a pseudo-quadrupole Hamiltonian of the form

\[
H = D(I_x^2 - I_y^2/3) + E(I_z^2 - I_y^2)
\]

For reasons of symmetry the \(z\) axes are the same for each electronic state of the crystal. The eigenvalues for the above Hamiltonian can be broken into two groups one of which consists of linear combinations of the \(I_x\) states \(\{1/2, -3/2, 5/2\}\) and the other linear combinations of the states \(\{-1/2, 3/2, -5/2\}\). These two groups are closed under the operations of driving and spontaneous emission leading to a cyclic transition that can be used to read out the state if RF repumping fields are applied that connect all the other members of the group. One complication is that the hyperfine states are two fold degenerate at zero field with each pair consisting of a member of each group. This degeneracy can be lifted without affecting the closed nature of the groups by applying a magnetic field along the \(z\) direction. This is shown on an energy level diagram in Fig. 4.

\[\text{IV. CONCLUSION}\]

We have described a practical method for two-qubit quantum computing demonstrations using ensembles. However, we conclude that such an approach will not be scalable to a large number of qubits. Various possibilities for scaling were discussed.

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FIG. 5: Energy levels diagram showing cyclic transition. ES denotes the optically excited state and GS denotes the ground state.

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