Quantum computer using a trapped-ion spin molecule and microwave radiation

D. Mc Hugh and J. Twamley*

Department of Mathematical Physics, National University of Ireland Maynooth, Maynooth, County Kildare, Ireland

(Received 16 October 2003; revised manuscript received 15 July 2004; published 12 January 2005)

We propose a design for a quantum-information processor where qubits are encoded into hyperfine states of ions held in a linear array of individually tailored linear microtraps and sitting in a spatially varying magnetic field. The magnetic field gradient introduces spatially dependent qubit transition frequencies and a type of spin-spin interaction between qubits. Single- and multiqubit manipulation is achieved via resonant microwave pulses as in liquid-NMR quantum computation while the qubit readout and reset is achieved through trapped-ion fluorescence shelving techniques. By adjusting the microtrap configurations we can tailor, in hardware, the qubit resonance frequencies and coupling strengths. We show that the system possesses a sideband transition structure which does not scale with the size of the processor, allowing scalable frequency discrimination between qubits. By using large magnetic field gradients, one can reset individual qubits in the ion chain via frequency selective optical pulses to implement quantum-error correction, thus avoiding the need for many tightly focused laser beams.

DOI: 10.1103/PhysRevA.71.012315 PACS number(s): 03.67.–a

A quantum computer requires well-characterized quantum bits (qubits), sufficient control to perform a universal set of quantum gates, long decoherence times compared to gate times, and a means of performing qubit readout [1]. To be of practical use, any design must scale to a large number of qubits. Current ion-trap and nuclear magnetic resonance (NMR) implementations are capable of satisfying many of these criteria to varying degrees. Liquid-state NMR quantum computing has demonstrated very precise control in the manipulation of qubits with microwave and radio frequency pulses and the execution of a number of quantum algorithms.

The main drawback of liquid-NMR quantum computing is the extreme difficulty, due to tiny spin polarization and weak measurements, in scaling up to a large number of qubits. Ion-trap quantum computing has recently shown progress in implementing quantum algorithms [2] and a controlled interaction between two qubits [3]. Here the initialization and readout of qubits are particularly good, and while there are difficulties due to ion heating, the attainment of very precise laser focusing, and stability problems of operating at optical frequencies, these obstacles have been steadily tackled through very significant efforts, and recent experiments look very promising [4,5].

The tools and techniques needed to currently surmount these difficulties are complex and only a few groups around the world have mastered such advances. Moreover, as the field moves toward smaller devices with more qubits, these difficulties may compound and hinder the ability to scale optically addressed ion-trap technologies to large numbers of ions although a number of potentially scalable designs involving moving and stationary optically manipulated trapped ions have been proposed [6,7,8,11,12,13].

In this article we describe an alternative design for a potentially scalable quantum-information processor which combines the trapped-ion and NMR technologies in a manner that retains the advantages of both and which might be technologically more available to a larger number of researchers, at least for small-scale test quantum processors.

We assume that two hyperfine levels in each ion serve as the qubit. As demonstrated by Wunderlich et al. [14–16], one can induce a coupling between the qubits through the application of a magnetic field gradient along a string of ions. This, together with the Coulomb force, couples the qubits together in a way analogous to the spin-spin coupling observed between nuclear spins in a molecule. Obviously then, similar techniques to those used in NMR, and the related field of electron spin resonance (ESR), can be utilized to realize two- and multiqubit quantum gates. Further, due to the absence of any motional coupling between the ions and the internal spin Hamiltonian at lowest order, the spin state of the ions is quite robust and less stringent cooling techniques are required for coherent spin operations [16].

The work presented by Wunderlich et al., though possessing obvious benefits for the precise manipulation of quantum information, displays, however, a number of serious obstacles with respect to scalability. In that design we will find that the spin-spin coupling varies in strength throughout the ion chain, thus leading to varying quantum gate durations between qubits depending on their location in the ion chain. This itself poses a serious difficulty in that a scalable device will require device-wide parallel quantum-information processing and quantum-error correction and this will need careful synchronization of logical operations throughout the device. More problematic is the existence in the Wunderlich design of an upper limit to the number of qubits which can be cleanly frequency differentiated for a given size of magnetic field gradient. Finally, the technical difficulty and potential added source of decoherence introduced by the focusing of individual laser beams on each ion in the chain for individual qubit initialization, readout, and reset may also be problematic for scalability [16]. Here we show that by considering a design where the ions are stored in a linear array of individually tailored linear microtraps [12], we can sur-

*Email address: Jason.Twamley@may.ie
mount all of the above mentioned difficulties and achieve significant gains in scalability. In particular we find that the resulting system is, as before, analogous to an $N$-atom molecule with spin-spin couplings, but now these couplings can be tailored very precisely, and quite robustly, through altering the individual microtrap parameters. Our design is also exactly analogous to a true ion crystal where each ion is harmonically bound to a periodic spatial lattice. The resulting qubit resonance frequencies together with the vibrational side transitions form a band structure (as in condensed matter systems), where a band’s extent now depends only on the interior spacing and end trap strength and does not grow with the number of ions in the chain. Finally, as previously shown by Wunderlich [15], the magnetic field gradient allows the qubits to be individually frequency addressed in the microwave (MW) via Zeeman splitting of the hyperfine structure. We further show that for large magnetic field gradients one can engineer for frequency-addressed optical resetting of an individual hyperfine qubit via Zeeman splitting of the optical transitions. This capability allows for scalable quantum-error correction and relaxes the need for focusing of individual laser beams on each ion through the use of frequency multiplexed laser sources. Previous difficulties predicted in liquid-NMR quantum-information processing related to the saturation of the available rf bandwidth with a moderate number of frequency differentiated qubits is no longer an issue here as the qubit manipulation in the MW (or readout in the optical) has available radiation sources which are tunable over many MHz (GHz). Further, our design uses the highly developed and relatively widespread technology of microwave pulse synthesis to precisely manipulate the qubits. This avoids the need to develop and maintain ultrastable narrowband laser systems as used in in [2,3], although high-frequency optical systems will still be required for the qubit initialization, reset, and readout processes. Our model differs fundamentally from other quantum-computer designs based on trapped ions. In [17], a two-qubit gate is realized through the exchange of a phonon through collective vibrational motion of the ions while in [13] the ions are also stored in an array of microtraps and qubit gates are realized through a state-dependent displacement of the motional wave packet of the ions. In the scheme of Wunderlich and in our scheme, the spin-spin coupling is achieved via virtual excitation of the ion’s motion and thus gate operations should be more robust against decoherence arising from the motion of the ions than in the schemes presented in [11,18,19].

We first explain qualitatively how the model operates and follow this with a quantitative analysis. We consider $N$ ions, with each ion occupying a separate harmonic oscillator potential well, arranged in a linear array. We assume we can independently fix (1) the strength of the each potential well and (2) the separation between each well. Each ion stores a qubit in two hyperfine states and taken together constitutes a quantum register. The initialization of the qubits is performed as usual via fluorescence shelving and repumping [20]. A magnetic field gradient is applied along the ion string and results in frequency differentiated qubits in the string due to the Zeeman shifting of each ion’s hyperfine levels. Single-qubit operations on a given ion are performed by illuminating the ion string with a pulse of microwave radiation of the appropriate frequency. The spin-spin coupling between the ions is achieved through a combination of the Coloumb force and the qubit-dependent Zeeman energy which is spatially modulated by the magnetic field gradient [15]. The resulting spin-spin coupling is thus “on” all the time and gates are achieved via a combination of single-qubit operations and free evolution as in liquid-NMR quantum computation. Thus one can use the considerable knowledge of NMR refocusing and averaging techniques [21] to tailor the system Hamiltonian and perform quantum-information processing. However, quantum computing using liquid-state NMR and an ion spin molecule sitting in a single trapping potential as proposed by Wunderlich differ in that the latter allows one to control (although in a very rough manner), in hardware, the interqubit coupling strengths. For the latter the resulting interqubit couplings vary in strength throughout the ion chain no matter how one alters the single-trap parameters (see Fig. 3). This lack of homogeneity represents a significant barrier for the scalability of [15]. In addition, using a single linear trap to contain the ion string yields limits on the number of ions in the string that can be cleanly frequency differentiated for a given size of magnetic field gradient. By introducing linear microtraps and individually tailoring their strengths and locations we can surmount both of the above problems to yield a design with high scalability. We can precisely engineer the interqubit couplings to be homogeneous throughout the chain while maintaining uniform separation between the ions and consequently well-differentiated qubit resonant frequencies irrespective of the size of the device. Having a homogeneous system enormously boosts the scalability of the device as the alternative would imply that all gate operations (pulse sequences) would be highly dependent on the location of the ions in the chain that are involved in the gate. In addition by varying the ion separation and microtrap strengths we also have some control over the relative sizes of non-nearest-neighbor to nearest-neighbor spin-spin coupling strengths. In [15], and in our model, the ions in the string are spatially separated on length scales varying from 2 to 10 $\mu$m, and although the individual focusing of lasers on each ion is possible, such a readout scheme may yield too
much decoherence due to laser pointing fluctuations, amplitude noise, etc. Also in [15] one can read out the entire qubit register at once at the completion of a quantum algorithm. However, to execute quantum-error correction, intermediate measurements are usually desired. As shown in [22], though, quantum-error correction requires only the capability of supplying fresh ancilla qubits, or in the present case, the resetting of any individual qubit to a preset quantum state. We show that in the case of large constant magnetic field gradients, the resulting spatial dependence of the energies of both the qubit hyperfine levels and the optically excited “readout” level allows one to achieved optical frequency differentiated reset through optical pumping or through engineered decoherence processes, with little disturbance of neighboring qubits. This yields another boost for the scalability of the resulting design.

We now look at the model more quantitatively. Consider $N$ ions each of mass $m$ confined in $N$ individual harmonic potential wells. The $i$th linear trap has frequency $\omega_i$ and is located at position $k_i$ along the $x$ axis. A spatially varying magnetic field $B= (B_0 + bx)\hat{z}$ is applied across the line of ions. The resulting Hamiltonian, to second order in the ions’ vibrational motion, is given by [15]

$$H = \frac{\hbar}{2} \sum_{n=1}^{N} \omega_n (x_{0,n}) \sigma_{z,n} + \frac{\hbar}{2} \sum_{i=1}^{N} v_i a_i^\dagger a_i - \frac{\hbar}{2} \sum_{n<m} J_{nm} \sigma_{z,n} \sigma_{z,m}. \tag{1}$$

The first term represents the electronic Hamiltonian of the qubits, now with separated qubit resonances $\omega_n(x_{0,n})$, and where $x_{0,n}$ is the equilibrium location of the $n$th ion in the string sitting in the trapping potential. The second term describes the collective quantized vibrational motion of the ions. Even though the ions are now in individual linear traps, this term describes the quadratic interactions between the ions and is essentially identical to the case of a single harmonic trap. The last term expresses the pairwise coupling between qubits analogous to the well-known spin-spin coupling in molecules used for NMR quantum computing. In [15], it is then proposed that this last term can be used to implement quantum gates.

One can show that the spin-spin coupling between ions $n$ and $m$ can be expressed in the relatively simple form

$$J_{nm} = \frac{\hbar}{4 \pi m} \sum_{j=1}^{N} \frac{1}{v_j} \frac{\partial \omega_n}{\partial x_{0,n}} \frac{\partial \omega_m}{\partial x_{0,m}} D_{nj} D_{mj}$$

$$= \frac{\hbar}{4 \pi} \frac{\partial \omega}{\partial x} \frac{\partial \omega}{\partial x} (A^{-1})_{nm}, \tag{2}$$

where $(\partial \omega/\partial x)|_0$ is the gradient of the qubit transition resonant frequency for ion $k$, at equilibrium location $x_{0,k}$; $A$ is the Hessian of the potential in which the ions sit; $D$ is the unitary transformation matrix that diagonalizes $A$; and $nv_j^2$ are the eigenvalues of $A$.

In the high-field or Paschen-Bach limit ($B_0 \sim 1$ T), the frequency gradients are independent of $x$ and thus $n$, and so $J \propto A^{-1}$. To achieve uniform off-diagonal values for $J \sim A^{-1}$, i.e., $J_{ij} \sim J_{|i-j|}$, we now tailor the values of the Hessian $A$.

First the off-diagonal elements of $A$ are functions only of the interior spatial separations. We can fix the positions of the individual microtraps, $k_i$, to achieve a uniform ion separation $h$, thus enormously simplifying the structure of $A$. The diagonal elements of $A$ are functions of both the interior separation $h$ and the individual trap strengths. Letting $g_{i} = \frac{\omega_{i}}{\omega_{0}}$, be a measure of the $i$th trap strength, $\epsilon_{i} = (e^2 / 4 \pi e \hbar) / (\frac{1}{2} g_{i} \hbar^2)$ [13], and assuming only nearest-neighbor coupling, one can analytically show that for uniform off-diagonal $J$’s one must have

$$g_1 = g_N, \quad g_i = \frac{g_1}{1 + \epsilon_i}, \quad 1 < i < N, \tag{3}$$

with all interior traps being weaker in strength than the end traps. Resorting to numerics to include non-nearest-neighbor terms in the Hessian, one can determine the interior microtrap strengths for any given length of ion string with a uniform spatial ion separation. As one might expect both $k_i$ and $g_i$ are symmetrically valued about the midpoint of the ion chain. As an example, for Yb$^+$ ions, where the qubit is encoded in the hyperfine states $|0\rangle = |6S_{1/2}, M_J = \frac{1}{2}, M_s = \frac{1}{2}\rangle$, $|1\rangle = |6S_{1/2}, M_J = \frac{1}{2}, M_s = \frac{1}{2}\rangle$ of each ion we can obtain the microtrap strengths in Fig. 2. Once suitable values for $g_i$ are obtained, the resulting microtrap positions $k_i$, which yield the specified uniform ion separation, can be separately computed numerically. As expected, the microtrap separation decreases slightly toward the edges of the ion string to compensate for the larger outward Coulomb forces experienced by ions in these regions. From Fig. 3, the resulting improvement in the uniformity of the $J$ couplings throughout the ion string is quite striking. In addition, however, we have also succeeded in significantly reducing the non-nearest-neighbor $J$ couplings, thus reducing these potential sources of error in the performance of nearest-neighbor quantum gates. Further, by varying both the interior separation $h$ and end-trap strength...
mum vibrational frequency of the collective motion of $N$ which can be cleanly discriminated. In our model, the max-
ions, early with field gradient i.e., the gap between the asymptotic value of the maximum frequency extent independent of $N$. Empiri-
cally, we also can find the scaling of this convergence with ion separation $h$ to be $\Delta v(N,h,g) \sim \Delta v(N',h',g_1) \times (h/h')^{-3}$ so the further apart the ions are the faster this gap goes to zero, for a given $N$.

It is necessary to discuss in more detail how it is proposed that the qubits can be individually manipulated, read out, and reset. First, we will talk about manipulation. Since we are proposing to use two hyperfine levels for the qubit, long wavelength radiation is involved and so we will have to man-
ipulate the qubits via frequency selection rather than by attempting to focus laser light on the ions individually. As an example, we again identify the $|S_{1/2},M_f=\frac{1}{2},M_I=\frac{1}{2}\rangle$ and $|S_{1/2},M_f=\frac{1}{2},M_I=\frac{1}{2}\rangle$, states of $^{171}$Yb$^+$ as the qubits $|0\rangle$ and $|1\rangle$. The Zeeman splitting of the hyperfine levels lies in the Paschen-Back region when $g_f \mu_B B(\zeta)/E_{HFS} > 1$, where $E_{HFS}$ is the hyperfine splitting constant, $g_f$ the g factor, and $B(\zeta)$ the strength of the magnetic field. For Yb$^+$, this gives $B > 1$ T. If we are in this region then the difference between the manipulation frequencies of neighboring qubits is given by $\Delta v_{\text{manipulate}} = g_f \mu_B B(\zeta)/h$, where $b = dB(\zeta)/\zeta$ and $\zeta$ is the separation between the ions. Choosing a field gradient of 1000 T/m and a typical ion separation distance of 10 $\mu$m we can realize a neighboring qubit frequency difference of 280 MHz, irrespective of the length of the ion string. This separation is easily differentiated by current ESR microwave pulse spectrometers.

The final readout of the state of the qubits can be per-
formed, as usual, by spatially resolved resonance fluores-
cence. However, scalability will require the capability to per-
form quantum-error correction. This capability will require indi-
vidual ion readout and/or reset. However, as the spatial sepa-
ration between ions is $\sim 1 \mu$m, readout and reset of in-
dividual ions through individual laser focusing may be diffi-
cult. Instead, one can use frequency addressing of the optical trans-
itions to achieve individual ion readout and reset. For $B > 1$ T, both readout levels $|6S_{1/2},M_f=\frac{1}{2},M_I=\frac{1}{2}\rangle$ and $|6P_{1/2},M_f=\frac{1}{2},M_I=-\frac{1}{2}\rangle$ are in the Paschen-Back region and the resulting frequency separation between the optical trans-
itions of neighboring qubits is $\Delta v_{\text{readout}} = \frac{3}{2} \mu_B B(\zeta)/h$. This gives an optical frequency difference of 187 MHz for the above situation, which is far in excess of the excited state lifetime $\sim 10$ MHz, and thus cleanly discriminated between neighboring ions. Quantum-error correction (QEC) typically involves the measurement of an individual qubit state but to use fluorescence detection in a manner which leaves the spectator qubits undisturbed requires the additional correction of considerable ac Stark shifts suffered by neighboring ions during the illumination and acquisition of $\sim 10^4$ fluorescent photons from the target ion. Techniques to perform this correction have been demonstrated [24], but such invasive detection may not be necessary as only the capability to per-
form a qubit specific reset is required for quantum error cor-
rection [22]. Resetting the hyperfine qubit to a known quan-
tum state should only require the scattering of far fewer fluorescent photons (number of photons $\sim M = 10^0 \cdots 10^3$) via optical pumping, and the resulting phase acquired by a neighboring ion off resonant by $L \sim 19$ radiative linewidths will be $\phi \sim M/L \sim 1/5$ rad. The correction of such phases is
TABLE I. Relevant parameters for ten Yb+ ions, with \( B_0 = 1 \) T, \( b = 1000 \) T/m, \( \nu_1 = 1 \) MHz, and \( h = 10 \) \( \mu \)m, held in individually tailored microtraps for uniform separation and \( J \) couplings.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mean qubit resonance frequency (GHz)</td>
<td>34.3</td>
</tr>
<tr>
<td>Neighboring-qubit resonance frequency separation (MHz)</td>
<td>280</td>
</tr>
<tr>
<td>Motional sideband extent (MHz)</td>
<td>3</td>
</tr>
<tr>
<td>Neighboring-qubit optical readout frequency separation (MHz)</td>
<td>187</td>
</tr>
</tbody>
</table>

well within the capabilities of the techniques demonstrated in [24]. Alternatively, a technique to reset an individual hyperfine qubit by simultaneously resonantly irradiating the qubit and optical transitions with strong MW and extremely weak optical radiation at 369 nm (with a laser power of nanowatts) has previously been demonstrated in [25]. This process of \textit{engineered decoherence} may also be used as a qubit reset and can be used to achieve either transverse or longitudinal relaxation. This reset-based QEC leads to a significant amount of extra overhead, so that it would be preferable to use quantum measurement followed by recovery operations. Theoretically feasible methods for improving the fluorescence photon detection by two orders of magnitude suggest this might be possible.

Recent applications of narrowband ultraviolet diode lasers to ytterbium trapping might be adapted for the frequency selective optical addressing [26]. By using electro-optic modulators and external cavity tuning elements, tuning ranges of several gigahertz are currently possible at these wavelengths. Through illumination of the entire ion chain by a frequency multiplexed laser source one can achieve individual qubit readout and reset in a highly scalable manner. Achieving in-trap magnetic field gradients of 1000 T/m over several micrometers can be achieved through methods similar to those presented in [27]. Also, engineering linear ion traps on the micrometer scale is currently being investigated by experimental groups, such as described in [28], but at this point in time they are not fully suited to the requirements of this proposal.

However, by decreasing \( h \), we increase the qubit coupling strengths while decreasing the frequency separation between the qubit manipulation and readout frequencies. As a final example, in Table I, we have computed the parameters for ten Yb+ ions, with \( B_0 = 1 \) T, \( b = 1000 \) T/m, \( \nu_1 = 1 \) MHz, and \( h = 10 \) \( \mu \)m, held in individually tailored microtraps for uniform separation and \( J \) couplings. Here the uniform nearest-neighbor coupling strength \( J_{i,i+1} \approx 850 \) Hz. The tabulated parameters are within current microwave source capabilities and clearly indicate scalable frequency discrimination for the manipulation, readout, and reset of neighboring qubits.

We now discuss possible architectures for the scaling up of such a processor to \( 10^4 \)–\( 10^5 \) qubits, a size where useful quantum algorithmic tasks might be implementable. In alternate designs [6,12,13], scalability is not proposed via the construction of a single very large processor containing the entire computational quantum register. Instead, isolated computational subprocessor units are connected either photонically [9], or via physical motion [7], or by other means [10]. These connected architectures can also be utilized with the trapped-ion spin molecule as the fundamental subprocessor unit. Moreover the use of a spin-molecule subprocessor, with several hundred ions in each subprocessor, (a) allows the execution of many simultaneous two-qubit gates between pairs of neighboring qubits in an individual subprocessor unit, (b) avoids the use of very large magnetic field strengths as each subprocessor unit will contain a large, but fixed number of ions, and (c) when the microtrap configurations are arranged so as not to depress non-nearest-neighbor couplings, as in Fig. 1 in the spin molecule, allows one to engineer true multiqubit gates such as three-qubit Fredkin or Toffili gates. Multiqubit gates can improve significantly the “gate depth” of quantum algorithms [29], and thus counter the obvious deficiency of quantum-computer architectures possessing only nearest-neighbor interactions (such as the significant computational resources expended in shuffling information around the processor). These capabilities may be difficult to attain in other proposals for a scalable trapped-ion processor and thus these additionalities may outweigh the relatively slow gate frequencies of \( \sim \)kHz exhibited by the spin-molecule processor. Further, in our example above, we choose the microtrap configuration so as to demonstrate a large microwave frequency separation between adjacent qu-bits \( \sim 280 \) MHz. This large a separation is not ultimately necessary as by reducing the interior separation one can theoretically obtain frequency separations of 5 MHz (with correspondingly larger coupling strengths for a set magnetic field gradient). Microwave sources and composite pulses can differentiate frequencies separated by as little as 5 MHz [30], thus greatly reducing the bandwidth required for the addressing of a 1000-ion spin molecule subprocessor unit.

In conclusion, we have presented here a design for a trapped-ion spin-molecule quantum-information processor which we feel should be highly scalable. Our design surmounts the difficulties in scalability faced by the scheme of Wunderlich \textit{et al.} By storing the ions in individually tailored linear microtraps we can engineer homogeneous coupling strengths throughout the chain while simultaneously achieving a constant frequency separation between neighboring qu-bits, irrespective of the length of the ion chain. This enormously simplifies the microwave pulse sequences required to manipulate the quantum information in the ion chain. At the same time we have removed the limit on ion numbers which can now be cleanly frequency discriminated in a fully scalable manner. Finally, we can utilize the spatial dependence of the energy level structure of the optical transitions to achieve qubit frequency selective reset and initialization, tasks that

\[ \frac{f}{g} \]
are essential for the ultimate fault tolerant operation of a scalable device.

D. Mc HUGH AND J. TWAMLEY

PHYSICAL REVIEW A 71, 012315 (2005)

D. McH. kindly acknowledges support from Enterprise-Ireland Basic Research Grant No. SC/1999/080.