We propose an implementation for quantum logic and computing using trapped atomic spins of two different species, interacting via direct magnetic spin-spin interaction. In this scheme, the spins (electronic or nuclear) of distantly spaced trapped neutral atoms serve as the qubit arrays for quantum information processing and storage, and the controlled interaction between two spins, as required for universal quantum computing, is implemented in a three step process that involves state swapping with a movable auxiliary spin.

The field of quantum computing has advanced remarkably in the few years since Shor [1] presented his quantum algorithm for efficient prime factorization of very large numbers, potentially providing an exponential speed up over the fastest known classical algorithm. Because much of today’s cryptography [2] relies on the presumed difficulty of factoring large numbers, Shor’s discovery has important implications to data encryption technology and has stimulated much work in the field of quantum information.

Motivated by this and other theoretical developments, there is much interest in identifying and realizing experimental systems capable of generating large-scale quantum entanglements. In atomic systems, there have been several recent proposals using trapped ions/atoms and cavity QED systems [3–7]. Indeed, atomic systems capable of entangling two qubits have already been realized in some of these systems [8,9]. A common element in most of these proposals is that the qubits are stored in distinguishably trapped atoms/ions. The proposals differ principally in the nature of the atom-atom interaction (either phonons, photons, collisional, and induced electric-dipole moments) and in the way that these interactions are controlled.

In this paper, we propose an implementation of a quantum logic scheme utilizing the direct magnetic spin-spin interaction between individually trapped neutral atoms. The qubits of this system are stored in the long-lived hyperfine ground states of atoms, and coherent control of the spin-spin interactions is accomplished by controlling inter-atomic spacings. Our proposal is distinctive in that (1) the magnetic spin-spin interaction used to create the inter-atom entanglements is virtually decoherence-free and (2) atom-atom interactions are mediated via a movable ‘header’ atom which serves to transfer quantum information from one qubit to another (see Fig. 1). The header atom can in fact be a different species, and hence, in contrast to [5,7,10], the atom trapping potentials are not required to be spin-dependent in order to maintain trap distinguishability for small atom separations and can be realized with far-detuned laser beams. This latter distinction is important because near-resonant laser traps are a significant source of decoherence.

We begin by considering in detail the inter-atomic potential between two neutral atoms separated by an inter-nuclear distance $\vec{R}$. For We assume two spin 1/2 alkali atoms and momentarily neglect the hyperfine interactions. The potential can be written as the sum of three terms [11].

$$V(\vec{R}) = V_T(\vec{R})P_T + V_S(\vec{R})P_S + V_D,$$

$V_T$ and $V_S$ are the (electronic) spin triplet and singlet potentials, respectively. $V_D$ represents the long range direct magnetic dipole interaction between two atoms. $P_T$ and $P_S$ are the projection operators into the total electronic subspace 1 (triplet) and 0 (singlet). The difference between $V_T$ and $V_S$ represents the exchange interaction, which is typically most important when $\vec{R}$ is less than the LeRoy radius $R_0$ ($\lesssim 40a_0$ for alkali atoms). In the long range limit both $V_T$ and $V_S$ are dominated by the van de Waals term $-C_6/R^6$ [12].

At low energies, we can re-express the first two terms of the potential by writing the spin triplet and singlet potentials in terms of the scattering lengths, $a_T$ and $a_S$

$$V_{\nu}(\vec{R}) = \frac{4\pi\hbar^2}{M}a_{\nu}\delta(\vec{R}), \quad \nu = T, S,$$

and explicitly evaluating the projection operators to yield

$$V(\vec{R}) = \frac{4\pi\hbar^2}{M}\left(\frac{3}{4}a_T + \frac{1}{4}a_S\right)I\delta(\vec{R})$$

$$+ \frac{4\pi\hbar^2}{M}(a_T - a_S)\frac{1}{4}\vec{\sigma}_1 \cdot \vec{\sigma}_2 \delta(\vec{R}) + V_D. \quad (1)$$

where $\vec{\sigma}_{\nu}$ is electron Pauli spin operators [13].

At this juncture, we point out that the recent Innsbruck proposal [10] employs the close-range part of the potential represented in the first line of Eq. (1) in a type of “controlled collision”. In our scheme we will use the spin-dependent interaction, i.e. the long range atomic magnetic interaction represented in the last term of Eq. (1). The proposal of Brennen et. al. [7] relies on the near-resonant electric dipole interaction (not present here in the ground state Hamiltonian).
It is convenient to re-express the second term of Eq. (1) by assuming that the two interacting atoms (denoted by subscripts q and h) are harmonically bound in cylindrically symmetric traps with characteristic radial and axial sizes: \(a_{qr}, a_{hr}, a_{qz}, \) and \(a_{hr}\) and furthermore that the atoms occupy the ground states of their respective traps \(|0\rangle_q |0\rangle_h\). In this case, we obtain

\[
J_E = \frac{4\sqrt{2}\hbar}{M} (a_T - a_S) \delta (\vec{r}_q - \vec{r}_h - z_0 \hat{z})(0)
\]

\[
= \frac{4}{\sqrt{2\pi} a_T^2 a_z} e^{-\frac{2a_z^2}{a_T^2} (\hbar\omega)}
\]

for a reference harmonic trap frequency \((\hbar \omega)\) with ground state size \(a\). We have used \(\vec{r}_q\) and \(\vec{r}_h\) for the nuclear coordinates of the atoms with respect to their own trap centers, which are displaced by \(\vec{d} = (0, 0, z_0)\), and we have defined \(a_\nu = \sqrt{a_{q\nu}^2 + a_{h\nu}^2}\), \((\nu = r, z)\). It’s important to recognize that \(J_E\) decays exponentially with the nominal atom-atom separation, \(z_0\).

The last term in Eq. (1), \(V_D\), contains three separate terms corresponding to electron-electron, electron-nuclear, and nuclear-nuclear magnetic dipole interactions. Between alkali atoms, the strongest is the electron dipole interaction

\[
V_{ee}^{rc} = \frac{\mu_e^2}{R^3} \langle \sigma_q \cdot \sigma_h - 3(\hat{R} \cdot \sigma_q)(\sigma_h \cdot \hat{R}) \rangle,
\]

where \(\mu_e\) is the Bohr magneton. The strength of this interaction is

\[
\gamma_e(R) = \frac{\mu_e^2}{R^3} \approx 5 \times 10^{-11} \left(\frac{a_0}{R}\right)^3 \text{(Hz)},
\]

while \(\gamma_{en}(R)\) (electron-nuclear) and \(\gamma_n(R)\) (nuclear-nuclear) are about 10^{-3} and 10^{-6} times smaller respectively. Therefore at \(R > R_0\) one may effectively write the spin-dependent interaction Hamiltonian as

\[
\mathcal{H} = J_E(z_0) \sigma_q \cdot \sigma_h + \gamma_e(R) \sigma_q \cdot \sigma_h - 3(\hat{R} \cdot \sigma_q)(\sigma_h \cdot \hat{R})
\]

Typically, we will have \(\gamma_e(R) > J_E(z_0)\) for \(R > 1000a_0\).

We will now discuss how this interaction Hamiltonian can be used for logic gates. We first point out that this interaction resembles the quantum gate implementation using the Heisenberg spin (exchange) interaction [15] \(H_J = J(t) \sigma_1 \cdot \sigma_2\), which is known to be universal. For \(\int_0^T dt (J/q) = \pi/4 (\text{mod}2\pi)\), its unitary evolution operator creates a swap gate

\[
U_{\text{swap}}(T)|i\rangle_1 |j\rangle_2 = \exp(-i\pi/4) |j\rangle_1 |i\rangle_2.
\]

which in turn can be use to generate XOR (controlled-NOT) gates by incorporating single bit operations [15]. However, our interaction Hamiltonian includes an anisotropic term. Fortunately, we can borrow a decoupling technique developed in NMR [16] to effect the conversion of \(\sigma_q \cdot \sigma_h \rightarrow \sigma_{qz} \cdot \sigma_{hz}\), which is also universal. In fact, the phase gate [15] in terms of these operators is simply

\[
U_{\text{phase}} = e^{i(\pi/4)\sigma_z} \times e^{i(\pi/4)\sigma_z} \times e^{i(\pi/4)\sigma_z},
\]

from which \(U_{\text{XOR}}\) can be easily made [9,17]. Furthermore, the swap gate, which we will require, can be made according to

\[
U_{\text{swap}}(1\rightarrow 2) = U_{\text{XOR}}(1, 2)U_{\text{XOR}}(2, 1)U_{\text{XOR}}(1, 2),
\]

where \(U_{\text{XOR}}(i, j)\) denotes a C-NOT with \(i\) as control operating on \(j\). The necessary de-coupling is achieved through a “stirring” radio frequency field acting on the \(h\)-atom [16], and is most easily discussed in the context of the following model hamiltonian

\[
H_S(t) = \hbar \omega_1 \sigma_{1z} + \hbar \omega_2 \sigma_{2z} + \Omega_S (\sigma_{2+} e^{-i\omega_S t} + \h.c.)
\]

\[
+ \gamma_e(R) \sigma_1 \cdot \sigma_2 - 3 \sigma_1 \cdot \sigma_2 (\hat{R} \cdot \hat{z})^2,
\]

(2)

where \(\omega_S\) is the frequency of the stirring field, and \(\Omega_S\) is the Rabi frequency of the stirring field. By analyzing this system in the rotating frame defined by \(U_R = e^{i\omega_S t} \sigma_{2z}\), we obtain [16] \(U_R \sigma_{2z} U_R^\dagger = \sigma_{2z} + e^{i\omega_S t} \sigma_{2z}\), and invoking a rotating wave approximation, the desired result is obtained,

\[
H_S^{\text{eff}} \approx \gamma_e(R)[1 - 3(\hat{R} \cdot \hat{z})^2] \sigma_{1z} \sigma_{2z},
\]

\[
+ \hbar \omega_1 \sigma_{1z} + \hbar \omega_2 - \omega_S \sigma_{2z} + \Omega_S (\sigma_{2+} + \sigma_{2-}).
\]

(3)

Although there are unwanted single atom terms in the second line of this Hamiltonian, they can be easily compensated with one-bit rotations. For our system, a similar procedure yield the following effective Hamiltonian,

\[
\mathcal{H}_{\text{eff}}(\hat{R}) \approx \{ J_E(z_0) + \gamma_e(R) - 3 \gamma_e(R) (\hat{R} \cdot \hat{z})^2 \} \sigma_{qz} \sigma_{hz}.
\]

(4)

Interestingly, we note that the spin and effecting spatial dependence of the operators factorizes. This implies that coherent spin-spin interactions only requires that the motional states of the atoms remain unchanged—the atoms are not necessarily required to be in the ground state \(|0\rangle\) of their respective trapping potential. This particular feature of our proposal will be discussed in detail elsewhere. At \(z_0 > R_0\), the effective spin-spin interaction strength is

\[
J_E(z_0) \approx (\gamma_e(R)[1 - 3(\hat{z} \cdot \hat{R})^2]),
\]

which for atoms in the ground states \(|0\rangle\) previously described is readily evaluated to be

\[
\frac{1}{R^3} [1 - 3(\hat{z} \cdot \hat{R})^2] = \frac{1}{\sqrt{2\pi} a_{z}^2} \frac{1}{2 a_z^2} \int_{-\infty}^\infty dz \exp \left[ -\left(\frac{z - z_0}{a_z}\right)^2 \right]
\]

\[
\left[ 2|z| - (a_z^2 + z^2)^{\frac{3}{2}} \frac{2\pi}{a_z^2} \exp \left( \frac{z^2}{2a_z^2} \right) \text{erfc} \left( \frac{|z|}{\sqrt{2a_z}} \right) \right],
\]

2
where \( \text{erfc}(\cdot) \) is the complementary error function. The geometry of the system of two interacting spins are illustrated in Fig. 2. The result of the effective interaction is shown in Figure 3, we note that \( J_E(\omega) \) is in the kHz range for a distance of 1000\( a_0 \) (\( \sim 50 \) nm), which will be more than adequate for gate operations for atoms trapped in far off-resonant optical lattices.

The principle challenge in implementing this scheme is in providing the appropriate confining potentials for the atoms. On one hand, the trapping potentials for the individual atoms need always be distinguishable in order to maintain identifiable qubits. On the other hand, as we can see from Figure 2, the atoms need to be in close proximity (\( \sim 50 \) nm) in order for an appreciable interaction rate even for this ‘long-range’ potential. Previous proposals also requiring small inter-atomic spacings have suggested spin-dependent traps created by optical lattices with polarization gradients [5,7,10]. Because of the nature of these types of traps, the types of atomic manipulations are rather restricted, and hence scalability is difficult.

To circumvent this complication, we will use two different atomic species, one for the (stationary) quantum register, and one for the quantum header atom. Each species of atom will be separately trapped by different laser fields. By appropriate choice of atom and frequency of the trapping fields, we can make these traps essentially independent. For a concrete example, consider a quantum register consisting of an array of single atoms (type \( q \) for qubit) trapped in 3D standing wave formed by interfering laser field of a CO\(_2\) lasers (wavelength \( \lambda_{\text{CO}_2} \approx 10.6 \) \( \mu \)m) [18]. The qubits will be separated by \( \lambda_{\text{CO}_2}/2 \) which is more than enough to allow individual addressing, and at this separation, the long range Casimir-Polder interaction is negligible [12]. The trapping details are discussed in the appendix, but we point out that the potential \( V \) is very well approximated by the dc-polarizability (0) and the laser electric field amplitude \( E \) as \( V = -\alpha(0)E^2/2 \). The relevant parameters are tabulated for alkali atoms in I.

A separate laser field provides confinement for the header atom (of a different type atom, \( h \) ). By choosing a different species, we can, by choosing a trapping wavelength somewhat closer to the atomic resonance of \( h \) (and detuned to the blue of the resonance), provide a potential which acts principally on the \( h \) atom. The potential for this trap is given by \( V_{\text{max}} = \Omega_L^2/4\delta_L \), with \( \Omega_L \) the Rabi frequency of the laser, and \( \delta_L = \omega_L - \omega_0 \) the detuning. The \( h \) atom is also affected by the far off-resonant CO\(_2\) laser field of course, but we can easily arrange for the off-resonant blue detuned field to dominate the far off-resonant CO\(_2\) laser potential. Trapping parameters in this case are listed in Table II. The quantum register atoms (type \( q \)) will also be affected, at some level, by the blue lattice, but the detuning between the blue field and the \( q \) atoms will be much larger, so the \( q \) atoms potential will be dominated by the CO\(_2\) laser field.

Gate operations in this system can be achieved in a three step process requiring quantum state swapping between the quantum bits and the header atom. To execute a gate operation between two qubits \( q_i \) and \( q_j \), we first translate the header atom \( h \) to the location of \( q_i \) and perform a state swap \( q_i \leftrightarrow h \). The header atom is then translated to site \( q_j \) and the gate operation between \( h(q_i) \) and \( q_j \) is performed. Finally the header atom is translated back to \( q_i \) to and the state swap is repeated. The header atom effectively acts as an quantum bus between the qubits, and in this sense our scheme shares certain features with the quantum gear machine proposed by Di-Vincenzo [14].

Single-bit operations can be realized either by directly addressing the individual qubits \( q_i \), or, alternatively, we can use the header atom as a mediator. This is easier in some cases than the direct spatial selection of \( q_i \) because the \( h \) atoms can be sparsely distributed and have different resonance levels. The single bit operation will again be a three step process: 1) perform a state swap between \( q_i \) and \( h \), 2) perform the arbitrary qubit operation on \( h \), 3) repeat the state swap between \( h \) and \( q_i \).

Decoherence-free quantum information processing will require that the transport of the \( h \)-type atom be adiabatic. This is in addition to the requirement that the total transport duration be less than the available coherence time. The adiabatic condition limits the transportation speed, which we estimate using canonical perturbation theory. Consider the Hamiltonian for a one dimensional harmonically trapped particle with mass \( M \) and trap frequency \( \omega_0 \),

\[
H = \frac{p^2}{2M} + \frac{1}{2} M \omega_0^2 (q - q_0)^2, \tag{5}
\]

with \( q_0 \) the trap center. For a constant trap center \( q_0 \), the Hamilton-Jacobian formulation gives the set of action and angle variables \( \{ J_0, \omega_0 \} \); with a moving center \( q_0(t) \), the corresponding dynamic equation is then given by

\[
\frac{dJ_0}{dt} = \dot{q}_0(t) \sqrt{M \omega_0 J_0(2\pi) \sin(2\pi \omega_0)},
\]

\[
\frac{d\omega_0}{dt} = \frac{\omega_1}{2\pi} + \dot{q}_0(t) \sqrt{M \frac{\omega_1}{J_0} - \frac{1}{2} \cos(2\pi \omega_0)}. \tag{6}
\]

When \( \dot{q}_0(t) = dq_0(t)/dt = 0 \), we have the adiabatic invariant action \( J_0^{(0)} \) = const. and the cyclic angle variable \( \omega_0 = \omega_1 t/2\pi \). For adiabatic motion with small \( \dot{q}_0(t) \), we can find corrections to the above solution in terms of successive higher orders of \( \dot{q}_0(t) \). We can show that the time averaged (over a period \( \tau = 2\pi/\omega_1 \)) dynamic equations of Eq. (6) give \( \langle J_0 \rangle_{\omega_1} = J_0^{(0)} + O(\dot{q}_0^2) \), which is a form of an adiabatic limit provided \( \dot{q}_0(t) \) is small. A conservative estimate for adiabaticity would be to simply require

\[
|\dot{q}_0(t)| \sqrt{\frac{M \omega_1}{J_0^{(0)}}} \lesssim \frac{\omega_1}{2\pi}. \tag{7}
\]
such that the perturbation on the angle variable remains negligible. This is equivalent to \( \dot{q}_0(t) \gg \omega_t a_t \), with \( a_t = \sqrt{\frac{\hbar}{2M\omega}} \) being the ground state size in the trap, (we have taken the smallest allowed action \( J_0^{(0)} = \hbar/2 \)). Since \( \omega_t a_t \) is the amplitude of classical velocity for the trapped particle, this is a limiting condition on the velocity for trap translation \( \dot{q}_0 \). It is in fact the same strong condition as obtained in [19]. Physically this is equivalent to the condition that the motion of trap center be small compared to the size of the atomic center of mass wavefunction during a complete oscillation period of the trap. For our problem, assuming a coherence time \( \sim 1/\gamma_{\text{eff}} \) of one second, a trap frequency of 100 (kHz), and a ground state size of 50 (nm), we obtain a adiabatic transport distance of 5 (mm), which is many times the inter-qubit spacings.

Our discussion thus far has been limited to atoms with no nuclear spin (e.g. \(^{78}\text{Rb} \)). When the nuclear spin \( I \) is nonzero, the atomic spin takes on values \( f = I \pm 1/2 \) and we must include the hyperfine interaction \( V_{hf} \sim \alpha_{hf} \vec{s} \cdot \vec{\sigma}^n \). The spin-spin interaction becomes considerably richer in detail. However, if a strong Zeeman interaction is applied using a uniform magnetic field, the resulting two manifold structure of \( I;S;I \) parallel processing of information can be implemented using \( I = 10^6 \) (watts/cm\(^2\)). For the ‘red’ \(^{87}\text{Rb} \) lattice, the maximum level shift is \( V_{\text{max}} = \alpha(0)E_R^0/4 \). At an intensity of \( \sim 10^6 \) (watts/cm\(^2\)), the single photon scattering rate can provide decoherence times of many minutes. Assuming a harmonic approximation, the oscillation frequency \( \nu_{osc} \) inside the \(^{87}\text{Rb} \) trap is \( \nu_{osc} = 2\sqrt{V_{\text{max}} E_R^{CO_2}} \) with \( E_R^{CO_2} = \hbar/(2M\lambda_{CO_2}^2) \) the recoil energy (in Hz) for emitting/absorbing a CO\(_2\)-photon. The Lamb-Dicke parameter \( \eta_0 = \hbar a_{osc}/(E_R) \) measures the trap ground state size \( a_{osc} \) in terms of the resonant wavelength \( \lambda_0 \) (CO\(_2\) laser \( \lambda_{CO_2} \)).

### Table I. Parameters for different alkali-metal atoms inside a CO\(_2\) lattice with intensity \( I = 10^6 \) (watts/cm\(^2\)).

<table>
<thead>
<tr>
<th>( M )</th>
<th>Li</th>
<th>Na</th>
<th>K</th>
<th>Rb</th>
<th>Cs</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \alpha(0) ) (( a_0^0 ))</td>
<td>159.2</td>
<td>162</td>
<td>292.8</td>
<td>319.2</td>
<td>402.2</td>
</tr>
<tr>
<td>( V_{\text{max}} ) (MHz)</td>
<td>181</td>
<td>185</td>
<td>334</td>
<td>364</td>
<td>458</td>
</tr>
<tr>
<td>( \nu_{osc} ) (kHz)</td>
<td>432</td>
<td>239</td>
<td>247</td>
<td>172</td>
<td>156</td>
</tr>
<tr>
<td>( \alpha_{osc} ) (( a_0 ))</td>
<td>778</td>
<td>573</td>
<td>433</td>
<td>347</td>
<td>295</td>
</tr>
<tr>
<td>( \lambda_0 ) (nm)</td>
<td>670</td>
<td>589</td>
<td>766</td>
<td>780</td>
<td>852</td>
</tr>
<tr>
<td>( E_R ) (kHz)</td>
<td>64</td>
<td>25</td>
<td>8.7</td>
<td>3.7</td>
<td>2</td>
</tr>
<tr>
<td>( \eta_0 )</td>
<td>0.39</td>
<td>0.32</td>
<td>0.19</td>
<td>0.15</td>
<td>0.11</td>
</tr>
<tr>
<td>( \eta_{CO_2} )</td>
<td>0.025</td>
<td>0.018</td>
<td>0.014</td>
<td>0.011</td>
<td>0.009</td>
</tr>
</tbody>
</table>

### Table II. Parameters for a ‘blue’ lattice with \( \Omega_L \sim 1.6 \times 10^{16} \) (Hz) (\( \gamma \) laser power of 10 kw/cm\(^2\)), \( \gamma = 10^7 \) (Hz), and \( \delta_L = 2 \times 10^{12} \) (Hz). For the near resonant ‘blue’ lattice on the \( h \)-type atoms, the effective single photon scattering rate is approximately \( \gamma_{\text{eff}} \sim \eta^2 \Omega_L^2 / \delta_L \).

We see as indicated in Table I the confining frequency \( \nu_{osc} \) is indeed much larger than that of CO\(_2\) laser (on \( q \)-type atoms).

<table>
<thead>
<tr>
<th>( M )</th>
<th>Li</th>
<th>Na</th>
<th>K</th>
<th>Rb</th>
<th>Cs</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \nu_{osc} ) (kHz)</td>
<td>4061</td>
<td>2530</td>
<td>1494</td>
<td>982</td>
<td>727</td>
</tr>
<tr>
<td>( a_{osc} ) (( a_0 ))</td>
<td>254</td>
<td>176</td>
<td>176</td>
<td>145</td>
<td>137</td>
</tr>
<tr>
<td>( \eta )</td>
<td>0.13</td>
<td>0.1</td>
<td>0.076</td>
<td>0.06</td>
<td>0.05</td>
</tr>
<tr>
<td>( \gamma_{\text{eff}} ) (Hz)</td>
<td>2.5</td>
<td>1.6</td>
<td>0.9</td>
<td>0.6</td>
<td>0.5</td>
</tr>
</tbody>
</table>


FIG. 1. A one dimensional illustration. The q−type atom array are trapped in a red periodic CO$_2$ laser lattice. The movable header atom is trapped in a blue lattice.

FIG. 2. The geometry of interacting header atom and qubit atom pair. The large ellipses denote trap ground states with trap centers crossed and separated by $z_0$. Solid circles with arrow heads denote electron spins separated by $\vec{R}$.

FIG. 3. The solid line denotes $J_E$, while the dots are numerical results of the averaged spin dipole interaction strength $J_E$ for $a_{q\tau} = a_{qz} = 400a_0$ and $a_{h\tau} = a_{hz} = 100a_0$. The dotted line represents the simple $1/z_0^3$ dependence.