

Quantum Logic with Spin $1/2$ Neutral Atoms in
Double Gaussian Wells
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Abstract:

In this study we investigate the possibility of implementing two-qubit quantum logic gates in double Gaussian well traps based on ultra-cold collisions of spin 1/2 neutral atoms. In our model, two identical particles are initially trapped in wells that are sufficiently far apart to prevent tunneling. The traps are then brought together adiabatically and allowed to interact for a time and are finally separated again to the original distance. Using the quantum mechanics governing identical particles we calculate the adiabatic potential curves, which govern the dynamics. Under the assumption of adiabatic evolution, we explicitly solve for the conditional parameters, namely the speed at which the traps are brought together and the time they are allowed to interact, in terms of energy eigenvalue integrals and zero separation energy ratios that we have found numerically. We have also laid the groundwork for the path toward an exact solution that takes into account the non-adiabatic effects that arise in systems described by time-dependent Hamiltonians.

Introduction:

For a little over 10 years physicists have been seriously exploring the possible computing power of quantum systems and how one would build a capable instrument. Computing power has been instrumental for the scientific community for a long time now and has indeed brought forth great advances in almost every field, yet many answers remain out of reach because of the limitations of our current capabilities. Many problems simply would take too much time, or space for a classical computer. Many experts believe that some of these problems would be no match for a quantum computer, one of

the most famous examples being Shor's factoring algorithm that would render most of today's encryption schemes obsolete, [1].

Classical computers process information fundamentally in binary code, zeros and ones, yes or no, something or nothing, or at least can always be thought of as doing so. A bit can be a mechanical switch, possibly a voltage, where the two distinguishable states would ideally never spontaneously switch values. A quantum computer was naturally designed in the language of zeros and ones as well, but a quantum object that allows two possible states can only be properly described generally as a superposition. It is superposition that allows two or more quantum particles to become entangled, a property that seems to play a pivotal role in quantum computing.

While the classical bit is either 0 or 1, the qubit is generally a superposition given by,

$$\alpha|0\rangle + \beta|1\rangle \text{ where, } |\alpha|^2 + |\beta|^2 = 1 \quad (1)$$

With the logical zero and one being represented by orthonormal state vectors meaning, $\langle 0|1\rangle = \langle 1|0\rangle = 0$ and $\langle 0|0\rangle = \langle 1|1\rangle = 1$. In order to process bits of information, a classical computer uses what is referred to as logic gates, a deterministic operation where the output of bits is only dependent on the input of bits. While a computer might use a multitude of different types of gates, all the operations that a classical computer is capable of can be simulated by combinations of one, so-called *universal*, gate called the *nand* gate, assuming that copies of bits can be made, [1]. A *nand* gate takes two bits as an input and first applies the *and* gate, which returns a one if and only if the two inputs are both one, and then switches the value of the *and* output. A quantum computer maps states in Hilbert space to others according to the Schrödinger equation. This map is a

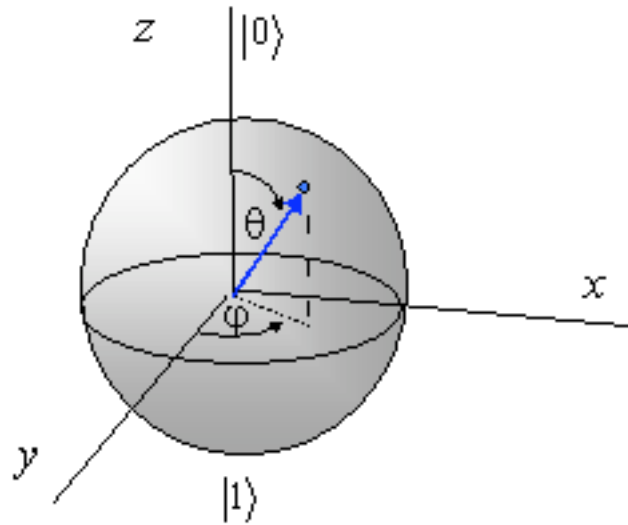
unitary matrix. Like classical computation, a combination of single qubit operations and one of the universal entangling logic gates can simulate any unitary operation used in a quantum-computing scheme. The classical *NOT* operation acting on the logical basis states $|0\rangle \rightarrow |1\rangle$, $|1\rangle \rightarrow |0\rangle$, generalizes for quantum superpositions, $\alpha|0\rangle + \beta|1\rangle \rightarrow \beta|0\rangle + \alpha|1\rangle$. This unitary map is represented in the logical basis by the matrix,

$$\hat{U}_{NOT} = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} = \hat{\sigma}_x, \quad (2)$$

where $\hat{\sigma}_x$ is a Pauli spin matrix. The most single general single-qubit unitary map can be written as,

$$\hat{U}(\theta, \phi) = \begin{bmatrix} \cos(\theta/2) & -e^{-i\phi} \sin(\theta/2) \\ e^{i\phi} \sin(\theta/2) & \cos(\theta/2) \end{bmatrix}, \quad (3)$$

which can be viewed as a rotation on the Bloch sphere, figure 1.



$$\psi = \psi_0|0\rangle + \psi_1|1\rangle \equiv \cos\frac{\theta}{2}|0\rangle + e^{i\varphi}\sin\frac{\theta}{2}|1\rangle$$

Figure 1. The Bloch sphere

Image courtesy [4]

A two-qubit logic gate is a unitary operation where the evolution of one qubit is dependent on another qubit, [1]. One simple example of one these universal gates is the *cnot* gate which flips the value of one qubit, (target), if the other, (control), is set to one.

$$\begin{array}{l} |00\rangle \rightarrow |00\rangle \\ |01\rangle \rightarrow |01\rangle \\ |10\rangle \rightarrow |11\rangle \\ |11\rangle \rightarrow |10\rangle \end{array} \quad \text{so that, } \quad \text{cnot} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \quad (4)$$

This gate can easily be shown to be entangling by taking the input state of

$$|\psi\rangle = \frac{|00\rangle + |10\rangle}{\sqrt{2}}, \text{ a state that can be written as a product, } |\psi\rangle = \frac{|0\rangle + |1\rangle}{\sqrt{2}} \otimes |0\rangle; \text{ that is to}$$

say that we have maximal knowledge of the individual qubits.

$$\text{cnot}|\psi\rangle = \frac{|00\rangle + |11\rangle}{\sqrt{2}} \neq |\varphi\rangle \otimes |\phi\rangle \quad (5)$$

The output state cannot be written as a product of two states and is thus an entangled state. Since the state of each individual qubit, having traced out the state of the other, must be described by completely mixed states, this is the maximally entangled state.

Paths toward a QC

There are many different design proposals currently being researched with varying degrees of progress toward a reliable machine. For example, cavity QED along with trapped ion experiments have both been demonstrated to be capable of providing the platform on which quantum computation is possible using two-level systems coupled to a quantum oscillator, [2]. Experiments exploiting the properties NMR (nuclear magnetic resonance) and quantum dots in order to demonstrate quantum computation are also progressing. There has been some work done studying the possibility of doing quantum computation with neutral atoms in optical dipole traps using ultra-cold collisions as an entangling gate where the qubits are encoded in the motional states of the atom [3], in contrast to our model where qubits will be encoded in the spin states of the atoms. Most of the work in quantum computing with neutral atoms is contemplated in optical lattices, [11], using spin dependent trapping. Researchers have proposed encoding qubits in the hyperfine ground manifold and achieving entanglement via optical dipole-dipole coupling, [12], ground state collisions, [13], or magnetic spin-spin interactions, [14]. There have already been some experiments carried out investigating the possibility of quantum information processing using arrays of optical tweezer traps, [15],[16].

Quantum logic with trapped atoms:

One of the major difficulties in quantum computing is the delicacy of the apparatus; an uphill battle of sorts must be fought where on the one hand interaction between different qubits is necessary to form an entangling gate but we don't want interaction with the environment which usually introduces error. This problem of the environmental perturbation is one reason quantum computing with neutral atoms is an attractive idea. The quantum computer requires the information carriers to be isolated and mobile, reasons that motivate us to study how computing can be achieved with laser tweezers, an environment that has already been studied by [4]. When an external electric field, $\vec{E}(\vec{0}, t) = E_o \cos \omega_l t$, is applied to a neutral two-level atom a dipole moment is induced, given by $\vec{d}_{ab} = \langle a | \hat{d} | b \rangle$ [5]. The force on a dipole with linear polarizability α is given classically by $(\vec{d} \cdot \nabla) \vec{E} = \alpha (\vec{E} \cdot \nabla) \vec{E} = \frac{\alpha}{2} \nabla (E^2)$ showing that the polarizable atom can be trapped in regions where the intensity is at a local maximum [6]. The quantum mechanical two level atom feels a reactive force given by

$$F_{\text{reac}} = -\frac{\hbar(\omega_l - \omega_o)}{4} \frac{\nabla(\Omega^2)}{(\omega_l - \omega_o)^2 + \frac{\Gamma^2}{4} + \frac{\Omega^2}{2}} \quad (6)$$

Where ω_o is the transition frequency between the two atomic levels and Γ is the spontaneous emission rate and Ω , the Rabi frequency, is defined by $\hbar\Omega = \vec{d}_{ab} \cdot \vec{E}_o$ [5]. We can see that the force changes sign with $\omega_l - \omega_o$, so that when $\omega_l < \omega_o$, red detuning, the atom will be attracted to regions of high intensity because of the gradient term, giving us a restoring force that has a maximum value on the order of $|F_{\text{max}}| \approx \hbar |\nabla \Omega|$ [5]. Laser

tweezers can use this principle to trap neutral atoms by focusing a collimated beam creating a small region of high intensity coherent light and are able to translate atoms over distances far greater than the scale of our problem, [7]. The potential created by an optical dipole-force trap has a depth $V_o(\Omega, \Delta) = \frac{\hbar\Omega^2}{4\Delta}$ where Δ is the detuning. The rate at which photons are spontaneously scattered, which leads to heating of the trapped atoms, is given by $\gamma_s(\Omega, \Delta) = \frac{\Gamma\Omega^2}{4\Delta^2}$, [8]. Looking at the depth and scattering expressions tells us that by increasing the Rabi frequency, which is done by increasing the intensity, and increasing the detuning accordingly so that the potential does not change, we should be able to achieve low scattering rates and therefore we will assume that the laser tweezers are operating far-off resonance from any transition frequencies. We will also assume that we can get very tight confinement in two of the three spatial dimensions. This effectively reduces the potential the atom sees due to the laser to a one-dimensional Gaussian profile of the form,

$$V(x) = -V_o \exp\left(-\frac{x^2}{2\sigma^2}\right) \quad (7)$$

The time-dependent Hamiltonian that describes two trapped atoms being brought together and allowed to interact for some time before being separated again takes the form

$$\hat{H}(x_1, x_2, \alpha(t)) = \frac{-\hbar^2}{2m} \left(\frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2} \right) + V(x_1, \alpha(t)) + V(x_2, \alpha(t)) + \hat{P}_s a \delta(x_1 - x_2) \quad (8)$$

where,

$$V(x, \alpha) = -V_o \left(\exp\left\{-\frac{(x - (\alpha_o - \alpha(t)))^2}{2\sigma^2}\right\} + \exp\left\{-\frac{(x + (\alpha_o - \alpha(t)))^2}{2\sigma^2}\right\} \right). \quad (9)$$

$2\alpha_0$ being the initial separation of the traps and $2\alpha(t)$ is the change in separation as a function of time. We have used a Dirac delta function to describe the atom-atom interaction since they are neutral and is valid as long as the atom stays in the vibrational ground states in the dimensions that we are ignoring, [3]. This “contact interaction” describes the s-wave scattering of neutral atoms, valid when the de Broglie wavelength of the atomic motion is large compared to the range of the interaction forces [3]. Since the atoms are neutral, these forces act only over angstrom scales, much smaller than the size of the trapped atomic wave packet. The quantity a is the interaction strength and is proportional to the scattering length, [3]. We have used the operator \hat{P}_s , a projector onto the singlet state, to describe the collisions in S-wave scattering because, in the case of fermionic spin 1/2 atoms, only the singlet states will collide since two atoms with anti-symmetrical motional wave-functions will never be found at the same place at the same time. The interaction operator can be expressed as a unitary time evolution matrix, \hat{T} in the following way,

$$\hat{T} = \begin{pmatrix} e^{-\frac{i}{\hbar}E(a)t} & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} |\chi_0^s\rangle \\ |\chi_{+1}^T\rangle \\ |\chi_0^T\rangle \\ |\chi_{-1}^T\rangle \end{pmatrix} \quad (10)$$

If we use the standard singlet/triplet definitions given by

$$\begin{aligned}
|\chi_{+1}^T\rangle &= |\uparrow\uparrow\rangle \\
|\chi_0^T\rangle &= \frac{|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle}{\sqrt{2}} \\
|\chi_{-1}^T\rangle &= |\downarrow\downarrow\rangle \\
|\chi_0^S\rangle &= \frac{|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle}{\sqrt{2}}
\end{aligned} \tag{11}$$

And define spin up to be logical zero and spin down to be logical one, arriving at a logical basis given by

$$\begin{aligned}
|00\rangle &= |\uparrow\uparrow\rangle = |\chi_{+1}^T\rangle \\
|01\rangle &= |\uparrow\downarrow\rangle = \frac{|\chi_0^T\rangle + |\chi_0^S\rangle}{\sqrt{2}} \\
|10\rangle &= |\downarrow\uparrow\rangle = \frac{|\chi_0^T\rangle - |\chi_0^S\rangle}{\sqrt{2}} \\
|11\rangle &= |\downarrow\downarrow\rangle = |\chi_{-1}^T\rangle
\end{aligned} \tag{12}$$

We can use these definitions to express the operator in Eq. (10) in the logical basis. We seek a unitary operator, \hat{U} that will map an arbitrary vector expressed in the logical basis to the corresponding vector expressed in the single/triplet basis, so that $\hat{U}|\psi_l\rangle = |\psi_{s/T}\rangle$ with the subscript denoting in which basis the vectors are expressed. We can make the following vector assignments to help us find the map:

$$\begin{aligned}
\hat{U}|00\rangle &= \hat{U} \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix} = |\chi_{+1}^T\rangle & \hat{U}|10\rangle &= \hat{U} \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix} = \frac{1}{\sqrt{2}} \begin{bmatrix} -1 \\ 0 \\ 1 \\ 0 \end{bmatrix} = \frac{|\chi_0^T\rangle - |\chi_0^S\rangle}{\sqrt{2}} \\
\hat{U}|01\rangle &= \hat{U} \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 0 \\ 1 \\ 0 \end{bmatrix} = \frac{|\chi_0^T\rangle + |\chi_0^S\rangle}{\sqrt{2}} & \hat{U}|11\rangle &= \hat{U} \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix} = |\chi_{-1}^T\rangle
\end{aligned} \tag{13}$$

The following matrix can easily be shown to satisfy the requirements;

$$\hat{U} = \begin{pmatrix} 0 & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & 0 \\ 1 & 0 & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \quad (14)$$

If the unitary time-evolution operator acting on an arbitrary state expressed in the singlet/triplet basis is described by $\hat{T}_{S/T}|\psi_{S/T}\rangle = |\psi'_{S/T}\rangle$ and the evolution operator expressed in the logical basis acting on an arbitrary state in the logical basis is described by $\hat{T}_l|\psi_l\rangle = |\psi'_l\rangle$, then we can say that the two operators expressed in the different basis vectors are related through the unitary map in the following way,

$$\hat{U}^\dagger \hat{T}_{S/T} \hat{U} = \hat{T}_l = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \frac{e^{-\frac{iE(a)t}{\hbar}} + 1}{2} & \frac{-e^{-\frac{iE(a)t}{\hbar}} + 1}{2} & 0 \\ 0 & \frac{-e^{-\frac{iE(a)t}{\hbar}} + 1}{2} & \frac{e^{-\frac{iE(a)t}{\hbar}} + 1}{2} & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \rightarrow \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} = \text{swap} \quad (15)$$

And if we set $\frac{E(a)t}{\hbar} = \pi$ then we see that the exchange interaction is the generator of the *swap* gate, which acts to switch the values of any two qubits.

Protocol for two-qubit quantum logic:

We define a qubit to be a spin 1/2 neutral atom cooled down to the ground state of a potential of the form given in Eq. (7), using the definition already given for the two logical states. Single qubit operations can easily be done on these qubits by the application of external E/M fields. When two traps are brought into close proximity of

one another, an atom that is definitely localized in one of the wells is only in a stationary-state of the full Hamiltonian, Eq. (8), when the traps are infinitely far apart; but if the traps are far enough apart that the tunneling frequency is large compared to the time scale of the gate operation then these can essentially be thought of as stationary states. To correctly describe a particle localized in one trap, the state must be described in terms of the actual eigenstates of the double-well configuration. The ground state of the double well configuration will be symmetric and denoted as $|S\rangle$, figure 2, while the first excited state will be anti-symmetric and denoted as $|A\rangle$, figure 3.

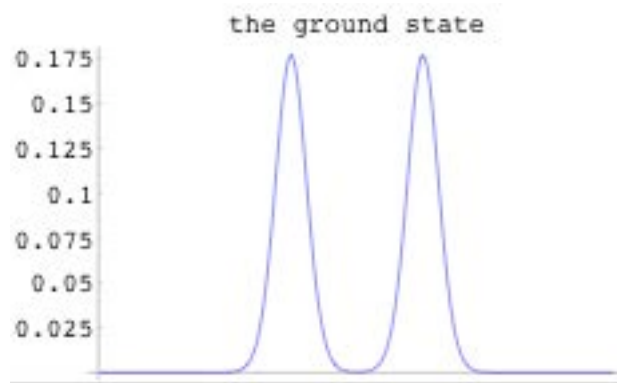


Figure 2

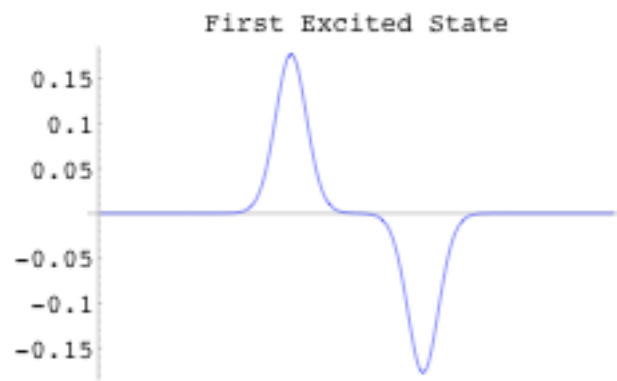


Figure 3

These states allow us to define a particle on the left, figure 4, as

$$|L\rangle = \frac{|S\rangle + |A\rangle}{\sqrt{2}} \quad (16)$$

And a particle on the right, figure 5, as

$$|R\rangle = \frac{|S\rangle - |A\rangle}{\sqrt{2}} \quad (17)$$

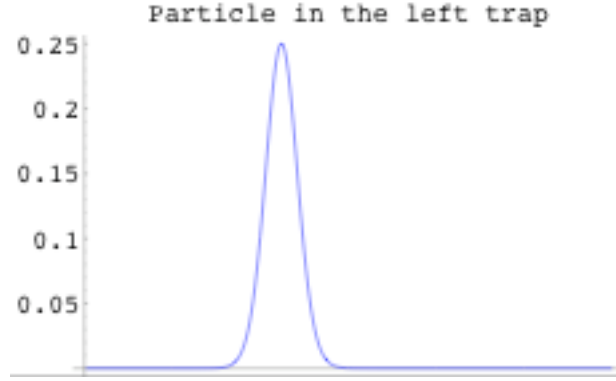


Figure 4

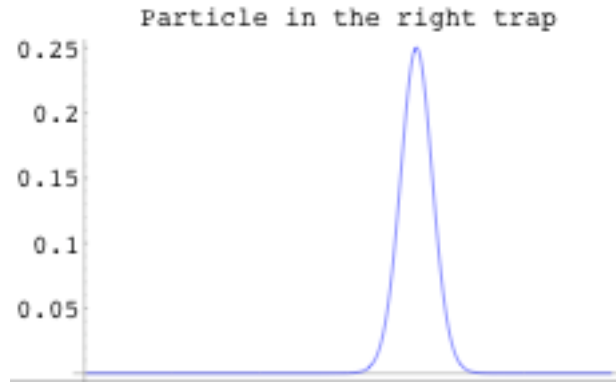


Figure 5

As the separation of the traps increases the $|S\rangle$ and $|A\rangle$ states become degenerate, sending the tunneling period toward infinity. An initial separation of 4σ was chosen for this study, but larger initial separations should be investigated for reasons that will be alluded to later. If we say that our first qubit is the particle in the trap on the left and our second qubit is the particle on the right and spin up is logical zero and spin down is

logical one, then these definitions allow us to ascribed the following properly symmetrized wave functions to our logical basis,

$$\begin{aligned}
|00\rangle &= \frac{|L\uparrow\rangle_1 \otimes |R\uparrow\rangle_2 - |R\uparrow\rangle_1 \otimes |L\uparrow\rangle_2}{\sqrt{2}} = \left(\frac{|AS\rangle - |SA\rangle}{\sqrt{2}} \right) \chi_{+1}^T \rangle \\
|01\rangle &= \frac{|L\uparrow\rangle_1 \otimes |R\downarrow\rangle_2 - |R\downarrow\rangle_1 \otimes |L\uparrow\rangle_2}{\sqrt{2}} = \left(\frac{|AS\rangle - |SA\rangle}{2} \right) \chi_0^T \rangle + \left(\frac{|SS\rangle - |AA\rangle}{2} \right) \chi_0^S \rangle \\
|10\rangle &= \frac{|L\downarrow\rangle_1 \otimes |R\uparrow\rangle_2 - |R\uparrow\rangle_1 \otimes |L\downarrow\rangle_2}{\sqrt{2}} = \left(\frac{|AS\rangle - |SA\rangle}{2} \right) \chi_0^T \rangle - \left(\frac{|SS\rangle - |AA\rangle}{2} \right) \chi_0^S \rangle \\
|11\rangle &= \frac{|L\downarrow\rangle_1 \otimes |R\downarrow\rangle_2 - |R\downarrow\rangle_1 \otimes |L\downarrow\rangle_2}{\sqrt{2}} = \left(\frac{|AS\rangle - |SA\rangle}{\sqrt{2}} \right) \chi_{-1}^T \rangle
\end{aligned} \tag{18}$$

where the tensor product is written for particles 1 and 2 respectively.

It is clear that the $|01\rangle$ and $|10\rangle$ states differ only by a relative phase between the singlet and triplet states that appear in the superpositions. More specifically, if a relative phase of -1 is accumulated then the qubits will have undergone a swap operation. Recalling the difference in s-wave collisions for the different spin states suggests an accumulation of this relative phase should in fact be entirely possible. The swap gate, however, is not an entangling gate and therefore we should be interested in the entangling square root of swap gate which leaves the $|00\rangle$ and $|11\rangle$ states unchanged but evolves the $|01\rangle$ and $|10\rangle$ into maximally entangled states. The $\sqrt{\text{swap}}$ gate is another universal gate and is related to the *cnot* gate through single qubit operations as $\text{cnot} = H_A \sigma_A^{-1} \sigma_B \sqrt{\text{swap}} \sigma_A^2 \sqrt{\text{swap}} H_A$ where H_A and $\sigma_{A,B}$ are the single qubit operators,

[3]. This gate is also generated from the exchange interaction by setting $\frac{E(a)t}{\hbar} = \frac{3\pi}{2}$ in

Eq. (15).

$$\sqrt{\text{swap}} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \frac{1+i}{2} & \frac{1-i}{2} & 0 \\ 0 & \frac{1-i}{2} & \frac{1+i}{2} & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \quad (19)$$

$$\sqrt{\text{swap}}|01\rangle = \frac{e^{i\pi/4}}{\sqrt{2}} (|01\rangle - i|10\rangle) = \left(\frac{|AS\rangle - |SA\rangle}{2} \right) \chi_0^T + i \left(\frac{|SS\rangle - |AA\rangle}{2} \right) \chi_0^S \quad (20)$$

This shows that a singlet-triplet relative phase of i will implement a square root of swap gate, which won't surprise the experienced reader since we've already said that a relative phase of -1 is needed for the full swap.

To calculate the phase evolution we solve the time-dependent Schrödinger equation, $i\hbar|\dot{\psi}\rangle = \hat{H}|\psi\rangle$ where the time dependent Hamiltonian is given in Eq. (8). The solution can be expanded in terms of the time dependent instantaneous energy eigenstates of the Hamiltonian,

$$\text{Expansion: } |\psi\rangle = \sum_n C_n(t) |\Omega_n(t)\rangle \quad (21)$$

$$\text{giving: } i\hbar \left(\sum_n (\dot{C}_n(t) |\Omega_n(\alpha(t))\rangle + \frac{\partial \alpha}{\partial t} C_n(t) \frac{\partial}{\partial \alpha} |\Omega_n(\alpha)\rangle) \right) = \sum_n C_n(t) E_n(t) |\Omega_n(t)\rangle. \quad (22)$$

This means that the phase evolution will be governed by coupled differential equations of the form,

$$\dot{C}_m(t) + \frac{\partial \alpha}{\partial t} \sum_n C_n \langle \Omega_m | \frac{\partial}{\partial \alpha} | \Omega_n \rangle = \frac{-i}{\hbar} E_m(t) C_m(t) \quad (23)$$

The square root of swap operation produces states that are spanned by the $|SS\rangle, \frac{|AS\rangle - |SA\rangle}{\sqrt{2}}, |AA\rangle$ basis vectors and therefore we desire the diabatic coupling term in

Eq. (23) to be negligible, leaving us with an adiabatic evolution given by,

$$C_n(t) = C_n(0) \text{Exp}\left[\frac{-i}{\hbar} \int_0^t E_n(t') dt'\right] \quad (24)$$

This is the adiabatic theorem of quantum mechanics and is valid when $v \ll v_c$, that is to say the velocity describing the movement of the traps is slow compared to some characteristic velocity that can be defined as $v_c \sim \sigma\omega$ where the characteristic frequency of the trap, ω , is estimated by expanding the Gaussian potential in a power series and taking the quadratic coefficient as the spring constant and sigma represents a reasonable estimation of the extent of the ground state wavelength.

In order to evolve the logical basis adiabatically, the wave functions must be expressed in terms of the eigenstates of the full Hamiltonian, a description that does not apply to the singlet states that appear in Eq. (18). If we decompose the singlet states into the true eigenstates by introducing resolutions of the identity of the form,

$\hat{1} = \sum_k |\Omega_k\rangle\langle\Omega_k|$ then we get another form of Eq. (18) appearing as,

$$\begin{aligned} |00\rangle &= \frac{|AS\rangle - |SA\rangle}{\sqrt{2}} |\chi_{+1}^T\rangle \\ |01\rangle &= \frac{|AS\rangle - |SA\rangle}{2} |\chi_0^T\rangle + \frac{\sum_k \langle\Omega_k|SS\rangle|\Omega_k\rangle - \sum_{k'} \langle\Omega_{k'}|AA\rangle|\Omega_{k'}\rangle}{2} |\chi_0^S\rangle \\ |10\rangle &= \frac{|AS\rangle - |SA\rangle}{2} |\chi_0^T\rangle - \frac{\sum_k \langle\Omega_k|SS\rangle|\Omega_k\rangle - \sum_{k'} \langle\Omega_{k'}|AA\rangle|\Omega_{k'}\rangle}{2} |\chi_0^S\rangle \\ |11\rangle &= \frac{|AS\rangle - |SA\rangle}{\sqrt{2}} |\chi_{-1}^T\rangle \end{aligned} \quad (25)$$

If we define $|\tilde{S}\tilde{S}\rangle$ and $|\tilde{A}\tilde{A}\rangle$ as the eigenstates of the full Hamiltonian that map onto the states $|SS\rangle$ and $|AA\rangle$ in the limit where the strength of the interaction goes to zero, then we can re-express Eq. (25) as,

$$\begin{aligned}
|00\rangle &= \frac{|AS\rangle - |SA\rangle}{\sqrt{2}} |\chi_{+1}^T\rangle \\
|01\rangle &= \frac{|AS\rangle - |SA\rangle}{2} |\chi_0^T\rangle + \frac{\langle \tilde{S}\tilde{S} | SS \rangle |\tilde{S}\tilde{S}\rangle + \sum_{k \neq \tilde{S}\tilde{S}} \langle \Omega_k | SS \rangle |\Omega_k\rangle - \langle \tilde{A}\tilde{A} | AA \rangle |\tilde{A}\tilde{A}\rangle - \sum_{k' \neq \tilde{A}\tilde{A}} \langle \Omega_{k'} | AA \rangle |\Omega_{k'}\rangle}{2} |\chi_0^S\rangle \\
|10\rangle &= \frac{|AS\rangle - |SA\rangle}{2} |\chi_0^T\rangle - \frac{\langle \tilde{S}\tilde{S} | SS \rangle |\tilde{S}\tilde{S}\rangle + \sum_{k \neq \tilde{S}\tilde{S}} \langle \Omega_k | SS \rangle |\Omega_k\rangle - \langle \tilde{A}\tilde{A} | AA \rangle |\tilde{A}\tilde{A}\rangle - \sum_{k' \neq \tilde{A}\tilde{A}} \langle \Omega_{k'} | AA \rangle |\Omega_{k'}\rangle}{2} |\chi_0^S\rangle \\
|11\rangle &= \frac{|AS\rangle - |SA\rangle}{\sqrt{2}} |\chi_{-1}^T\rangle
\end{aligned} \tag{26}$$

If we are working with a weak interaction then we can say that $\langle \tilde{S}\tilde{S} | SS \rangle \approx \langle \tilde{A}\tilde{A} | AA \rangle \approx 1$ and the summation terms that appear in Eq. (26) will be negligible, leaving us with,

$$\begin{aligned}
|00\rangle &= \frac{|AS\rangle - |SA\rangle}{\sqrt{2}} |\chi_{+1}^T\rangle \\
|01\rangle &\approx \frac{|AS\rangle - |SA\rangle}{2} |\chi_0^T\rangle + \frac{|\tilde{S}\tilde{S}\rangle - |\tilde{A}\tilde{A}\rangle}{2} |\chi_0^S\rangle \\
|10\rangle &\approx \frac{|AS\rangle - |SA\rangle}{2} |\chi_0^T\rangle - \frac{|\tilde{S}\tilde{S}\rangle - |\tilde{A}\tilde{A}\rangle}{2} |\chi_0^S\rangle \\
|11\rangle &= \frac{|AS\rangle - |SA\rangle}{\sqrt{2}} |\chi_{-1}^T\rangle
\end{aligned} \tag{27}$$

These states will adiabatically evolve to give the following general states,

$$\begin{aligned}
|00\rangle &= C_{AS} \frac{|AS\rangle - |SA\rangle}{\sqrt{2}} |\chi_{+1}^T\rangle \\
|01\rangle &= C_{AS} \frac{|AS\rangle - |SA\rangle}{\sqrt{2}} |\chi_0^T\rangle + (C_{\tilde{S}\tilde{S}} |\tilde{S}\tilde{S}\rangle + C_{\tilde{A}\tilde{A}} |\tilde{A}\tilde{A}\rangle) |\chi_0^S\rangle \\
|10\rangle &= C_{AS} \frac{|AS\rangle - |SA\rangle}{\sqrt{2}} |\chi_0^T\rangle - (C_{\tilde{S}\tilde{S}} |\tilde{S}\tilde{S}\rangle + C_{\tilde{A}\tilde{A}} |\tilde{A}\tilde{A}\rangle) |\chi_0^S\rangle \\
|11\rangle &= C_{AS} \frac{|AS\rangle - |SA\rangle}{\sqrt{2}} |\chi_{-1}^T\rangle
\end{aligned} \tag{28}$$

With this final form, we can solve for the required phase ratios that implement the swap or square root of swap gate by recognizing C_{AS} as a global phase and factoring it out of the logical basis leaving us with,

$$\begin{aligned}
|00\rangle &= \frac{|AS\rangle - |SA\rangle}{\sqrt{2}} |\chi_{+1}^T\rangle \\
|01\rangle &= \frac{|AS\rangle - |SA\rangle}{2} |\chi_0^T\rangle + \frac{C_{\tilde{S}\tilde{S}}}{C_{\tilde{A}\tilde{S}} \sqrt{2}} (|\tilde{S}\tilde{S}\rangle + \frac{C_{\tilde{A}\tilde{A}}}{C_{\tilde{S}\tilde{S}}} |\tilde{A}\tilde{A}\rangle) |\chi_0^S\rangle \\
|10\rangle &= \frac{|AS\rangle - |SA\rangle}{2} |\chi_0^T\rangle - \frac{C_{\tilde{S}\tilde{S}}}{C_{\tilde{A}\tilde{S}} \sqrt{2}} (|\tilde{S}\tilde{S}\rangle + \frac{C_{\tilde{A}\tilde{A}}}{C_{\tilde{S}\tilde{S}}} |\tilde{A}\tilde{A}\rangle) |\chi_0^S\rangle \\
|11\rangle &= \frac{|AS\rangle - |SA\rangle}{\sqrt{2}} |\chi_{-1}^T\rangle
\end{aligned} \tag{29}$$

This shows that there are two requirements for the swap gate, namely $\frac{C_{\tilde{S}\tilde{S}}}{C_{\tilde{A}\tilde{S}}} = -\frac{1}{\sqrt{2}}$

and $\frac{C_{\tilde{A}\tilde{A}}}{C_{\tilde{S}\tilde{S}}} = -1$, and Eq. (20) tells us that the requirements for the square root of swap gate

are given by (i) $\frac{C_{\tilde{S}\tilde{S}}}{C_{\tilde{A}\tilde{S}}} = \frac{i}{\sqrt{2}}$ and (ii) $\frac{C_{\tilde{A}\tilde{A}}}{C_{\tilde{S}\tilde{S}}} = -1$. It is worth noting that one can avoid the

problem of double occupancy within a well by controlling the phase of the ratio $\frac{C_{\tilde{A}\tilde{A}}}{C_{\tilde{S}\tilde{S}}}$. In

fact, if the ratio happens to be positive one rather than negative one, the atoms will definitely be found in the same trap at the completion of the operation, which can be

verified by referring back to Eq. (16),(17).

The fact that we have two conditions that must be met dictates that we need two “control knobs” in order to guarantee the necessary control. The two natural knobs to choose are the velocity at which the traps are brought together and the time that is allowed elapse while the traps are directly overlapped. If we assume a constant velocity then the above phase ratios can be solved exactly for the acceptable velocities and interaction times as long as they meet the previously stated adiabaticity requirements. We combine the phase ratios with the adiabatic evolution from Eq. (24) to arrive at;

$$C_n \rightarrow C_n(0) \text{Exp} \left[\frac{-i}{\hbar v} \int_{2\sigma}^0 E_n(\alpha') d\alpha' - \frac{i}{\hbar} E_n(0)t - \frac{i}{\hbar v} \int_0^{-2\sigma} E_n(\alpha') d\alpha' \right] \quad (30)$$

$$(i) \frac{C_{\bar{s}\bar{s}}(0) \text{Exp} \left[\frac{-i}{\hbar v} \int_{2\sigma}^0 E_{\bar{s}\bar{s}}(\alpha') d\alpha' - \frac{i}{\hbar} E_{\bar{s}\bar{s}}(0)t - \frac{i}{\hbar v} \int_0^{-2\sigma} E_{\bar{s}\bar{s}}(\alpha') d\alpha' \right]}{C_{\bar{A}\bar{S}}(0) \text{Exp} \left[\frac{-i}{\hbar v} \int_{2\sigma}^0 E_{\bar{A}\bar{S}}(\alpha') d\alpha' - \frac{i}{\hbar} E_{\bar{A}\bar{S}}(0)t - \frac{i}{\hbar v} \int_0^{-2\sigma} E_{\bar{A}\bar{S}}(\alpha') d\alpha' \right]} = \frac{e^{i(\frac{\pi}{2} + 2\pi m)}}{\sqrt{2}} \quad (31)$$

$$(ii) \frac{C_{\bar{A}\bar{A}}(0) \text{Exp} \left[\frac{-i}{\hbar v} \int_{2\sigma}^0 E_{\bar{A}\bar{A}}(\alpha') d\alpha' - \frac{i}{\hbar} E_{\bar{A}\bar{A}}(0)t - \frac{i}{\hbar v} \int_0^{-2\sigma} E_{\bar{A}\bar{A}}(\alpha') d\alpha' \right]}{C_{\bar{s}\bar{s}}(0) \text{Exp} \left[\frac{-i}{\hbar v} \int_{2\sigma}^0 E_{\bar{s}\bar{s}}(\alpha') d\alpha' - \frac{i}{\hbar} E_{\bar{s}\bar{s}}(0)t - \frac{i}{\hbar v} \int_0^{-2\sigma} E_{\bar{s}\bar{s}}(\alpha') d\alpha' \right]} = e^{in2\pi} \quad (32)$$

Where n and m must be integers. These equations can be solved for the acceptable

$$v_{\sqrt{\text{swap}}} = (\hbar\pi)^{-1} \left(\frac{\int_{2\sigma}^{-2\sigma} (E_{\bar{A}\bar{A}}(\alpha) - E_{\bar{s}\bar{s}}(\alpha)) d\alpha + \left(\frac{E_{\bar{A}\bar{A}} - E_{\bar{s}\bar{s}}}{E_{\bar{A}\bar{S}} - E_{\bar{s}\bar{s}}} \right) \int_0^{-2\sigma} (E_{\bar{s}\bar{s}}(\alpha') - E_{\bar{A}\bar{S}}(\alpha')) d\alpha'}{2n + \left(\frac{E_{\bar{A}\bar{A}} - E_{\bar{s}\bar{s}}}{E_{\bar{s}\bar{s}} - E_{\bar{A}\bar{S}}} \right) (1/2 + 2m)} \right)$$

velocity and interaction time giving

$$(33)$$

$$t_{\sqrt{swap}} = \frac{\left(\pi\hbar(1/2 + 2m) + v^{-1} \int_{-2\sigma}^{2\sigma} (E_{\bar{S}\bar{S}}(\alpha') - E_{AS}(\alpha')) d\alpha' \right)}{(E_{AS} - E_{\bar{S}\bar{S}})|_0} \quad (34)$$

giving a countably infinite number of suitable velocities and times below the adiabatic threshold. It must be true that the time it takes to successfully produce the entangled states should go to infinity as the strength of the interaction goes to zero. These equations can be used to show that by noting that when the interaction is turned off, $E_{\bar{S}\bar{S}}(\alpha) = 2E_S(\alpha)$, $E_{\bar{A}\bar{A}}(\alpha) = 2E_A(\alpha)$ and $E_{AS}(\alpha) = E_A(\alpha) + E_S(\alpha)$, and when these relations are plugged into Eq. (33),(34), the result is $v_{\sqrt{swap}} = 0$ and $t_{\sqrt{swap}} = \infty$. Shown below are graphs of the relevant energy curves, with figure 6 showing a case of very weak interaction and figure 7 showing a case of very strong interaction to illustrate the energy splitting where in the case of no interaction there would be a threefold degeneracy.

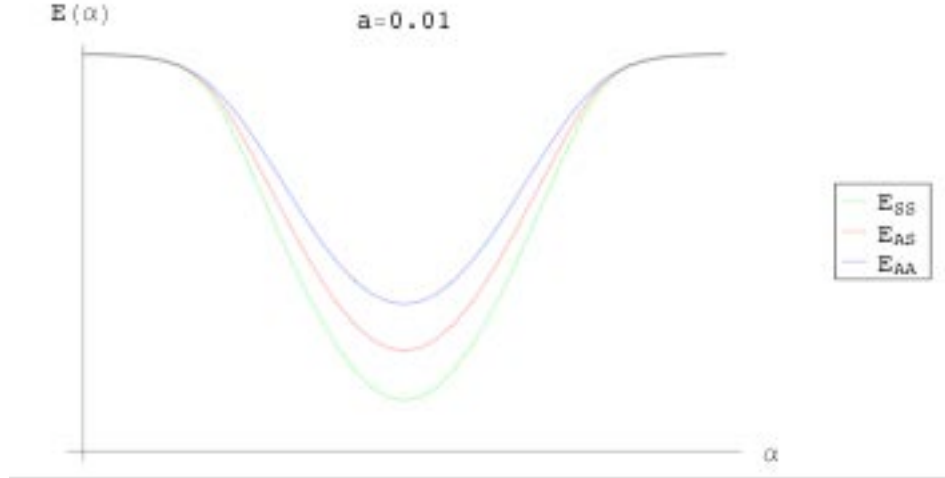


Figure 6: Trap separation ($-2\sigma \leq \alpha \leq 2\sigma$)

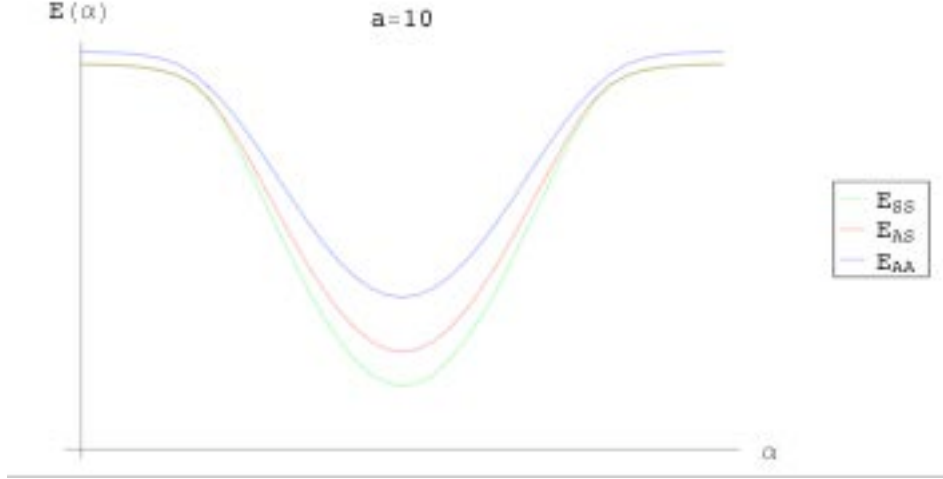


Figure 7: Trap separation ($-2\sigma \leq \alpha \leq 2\sigma$)

Results:

I used a grid method procedure to calculate the single particle atom-laser interaction energy eigenvalues and eigenfunctions first derived in [9]. To find acceptable velocities and interaction times predicted by the adiabatic evolution (see Appendix 1) we must find the $E_{\tilde{S}\tilde{S}}$, E_{AS} and $E_{\tilde{A}\tilde{A}}$ energy curves as a function of trap separation. Because the state corresponding to the E_{AS} is a triplet state the energy curve is not a function of the interaction strength and can therefore be defined as $E_{AS}(\alpha) = E_S(\alpha) + E_A(\alpha)$. The two single particle curves can be found by interpolating a list of energy values that are calculated by evaluating the code at different trap separations and tabulating the ground and first excited state values. The code by itself is not capable of solving the interaction problem and therefore will find the $E_{\tilde{S}\tilde{S}}$ and $E_{\tilde{A}\tilde{A}}$ curves by diagonalizing the full problem, using the non-interacting states as a basis. We define a non-interacting Hamiltonian as \hat{H}_0 as diagonal matrix with elements given by $\langle \Phi_i | \hat{H}_0 | \Phi_j \rangle = \delta_{ij} E_i$ then the full Hamiltonian is given by $\hat{H} = \hat{H}_0 + \hat{H}_I$ where the interaction-Hamiltonian matrix

elements are given by $H_{1,ij} = \langle \Phi_i | \hat{H}_1 | \Phi_j \rangle$ and the first order energy corrections due to the interaction can be by calculating the eigenvalues of \hat{H} . If we introduce new indices where q and r refer to the single particle orbitals that make of the two-particle states indexed by i , likewise s and t refer to the single particle orbitals that make the two-particle states indexed by j .

$$\begin{aligned}
H_{1,ij} &= \langle \Phi_i | \hat{H}_1 | \Phi_j \rangle = f(\alpha) \\
&= \iint dx_1 dx_2 \left(\frac{\phi_q(x_1)\phi_r(x_2) + \phi_r(x_1)\phi_q(x_2)}{\sqrt{2}} \right) a \delta(x_1 - x_2) \left(\frac{\phi_s(x_1)\phi_t(x_2) + \phi_t(x_1)\phi_s(x_2)}{\sqrt{2}} \right) \quad (35) \\
&= \int_{-\infty}^{\infty} (\phi_q(x)\phi_r(x)\phi_s(x)\phi_t(x)) dx
\end{aligned}$$

These single particle orbitals can be calculated using the code, and the routine to find these functions of trap separation is shown in the Appendix 2. In order to calculate the fidelity we define $F = |\langle \psi' | \psi \rangle|^2$ where the primed wave function is what results from the physical gate operation and the unprimed wave function is what an ideal square root of swap gate would produce. If we take the input state of $|01\rangle$ then

$$|\psi\rangle = \left(\frac{|AS\rangle - |SA\rangle}{2} \right) \chi_0^T + i \left(\frac{|SS\rangle - |AA\rangle}{2} \right) \chi_0^S \quad (36)$$

$$\begin{aligned}
|\psi'\rangle &= \left(C_{AS} \frac{|AS\rangle - |SA\rangle}{\sqrt{2}} + \sum_{k \neq AS} C_k^T |\Phi_k^T\rangle \right) \chi_0^T + \left(C_{SS} |SS\rangle + C_{AA} |AA\rangle + \sum_{\substack{k' \neq AA \\ k' \neq SS}} C_{k'}^S |\Phi_{k'}^S\rangle \right) \chi_0^S \\
&\quad (37)
\end{aligned}$$

Now we can see that $F = \left| \frac{C_{AS}}{\sqrt{2}} - \frac{i}{2} C_{SS} + \frac{i}{2} C_{AA} \right|^2$.

We will solve the time-dependent Schrödinger equation to find $|\psi'\rangle$ by expanding

the solution in terms energy eigenfunctions of the unperturbed Hamiltonian.

$$\text{Expansion: } |\psi'\rangle = \sum_n C_n(t) |\Phi_n(t)\rangle \quad (38)$$

For the triplet states we arrive at a set of coupled differential equations similar to Eq. (23)

$$\dot{C}_m^T(t) + \frac{\partial\alpha}{\partial t} \sum_n^{N(N-1)} C_n^T \langle \Phi_m | \frac{\partial}{\partial\alpha} | \Phi_n \rangle = \frac{-i}{\hbar} E_m^T(t) C_m^T(t) \quad (39)$$

Where N is the number of single particle bound states the double well configuration can support. In order to get a solution for the singlet states we decompose the full Hamiltonian into the non-interacting and perturbation matrices that have already been defined,

$$i\hbar|\dot{\psi}'\rangle = \hat{H}|\psi'\rangle = (\hat{H}_o + \hat{H}_1)|\psi'\rangle \quad (40)$$

$$\dot{C}_m^S(t) + \frac{\partial\alpha}{\partial t} \sum_n^{N(N+1)} C_n^S \langle \Phi_m | \frac{\partial}{\partial\alpha} | \Phi_n \rangle = \frac{-i}{\hbar} \left(E_m^S(t) C_m^S(t) + \sum_n^{N(N+1)} C_n^S \langle \Phi_m | \hat{H}_1 | \Phi_n \rangle \right) \quad (41)$$

If we use the q, r, s, t notation introduced earlier and look at singlet state, the triplet matrix elements have a similar form, we arrive at the following form,

$$\begin{aligned} \langle \Phi_i | \frac{\partial}{\partial\alpha} | \Phi_j \rangle &= g_{ij}(\alpha) \\ &= \iint dx_1 dx_2 \left(\frac{\phi_q(x_1, \alpha) \phi_r(x_2, \alpha) + \phi_r(x_1, \alpha) \phi_q(x_2, \alpha)}{\sqrt{2}} \right) \frac{\partial}{\partial\alpha} \left(\frac{\phi_s(x_1, \alpha) \phi_t(x_2, \alpha) + \phi_t(x_1, \alpha) \phi_s(x_2, \alpha)}{\sqrt{2}} \right) \\ &= \delta_{qs} \int \phi_r(x, \alpha) \frac{\partial}{\partial\alpha} \phi_t(x, \alpha) dx + \delta_{qt} \int \phi_r(x, \alpha) \frac{\partial}{\partial\alpha} \phi_s(x, \alpha) dx + \\ &\delta_{rs} \int \phi_q(x, \alpha) \frac{\partial}{\partial\alpha} \phi_t(x, \alpha) dx + \delta_{rt} \int \phi_q(x, \alpha) \frac{\partial}{\partial\alpha} \phi_s(x, \alpha) dx \end{aligned} \quad (42)$$

These matrix elements have additional factors $\sqrt{2}$ when $q = r$ and $s = t$. A function like

$g_{rs}(\alpha) = \int \phi_r(x, \alpha) \frac{\partial}{\partial \alpha} \phi_s(x, \alpha) dx$ can be evaluated for a specific trap separation numerically by recalling the definition of the partial derivative of $f(x, y)$ with respect to x at the point (x_0, y_0) , [10]:

$$\left. \frac{\partial f}{\partial x} \right|_{(x_0, y_0)} = \lim_{h \rightarrow 0} \frac{f(x_0 + h, y_0) - f(x_0, y_0)}{h} \quad (43)$$

Giving the following form for $g_{rs}(\alpha)$ evaluated at a specific trap separation:

$$g_{rs}(\alpha_0) = \int \phi_r(x, \alpha_0) \frac{\phi_s(x, \alpha_0 + \varepsilon) - \phi_s(x, \alpha_0)}{\varepsilon} dx \quad \text{Where } \varepsilon \ll \sigma \quad (44)$$

Once Eq. (44) is evaluated at several different separations, an interpolation function can be used to approximate $g_{rs}(\alpha)$. The numerical routine used to evaluate these matrix elements is shown in appendix section [3]. Once all the necessary functions have been calculated, the coupled differential equations, Eq. (39), (41), can be solved numerically using Mathematica's numerical routine, shown in appendix section [4,5].

If we take the case where the traps are overlapped and expand the Gaussian potential in a power series, taking the quadratic coefficient as the spring constant, we arrive at $\omega = \sqrt{\frac{2V_o}{m\sigma^2}}$ where V_o is the depth of an individual well and we can then define a characteristic energy as $E_c = \hbar\omega$. The characteristic energy should be a good approximation of the non-interacting energy of two atoms in the ground state of overlapped wells. For this study, the chosen parameters yield $E_c = \sqrt{3} \approx 1.73205$, whereas the actual value of two atoms in the ground state of overlapping wells is calculated to be $E_{SS}(0) = 1.696$. Calculating ω allows us to define a characteristic time

as $t_c = \frac{2\pi}{\omega} \approx 3.6276$ and a characteristic velocity as $v_c = \frac{\sigma}{t_c} = 0.551329$.

Interaction strength	v/v_c	t/t_c	Fidelity
a = 0.001	0.02861975	28.6040357	0.994453
	0.03273145	26.0957107	0.993156
	0.03822291	23.5873029	0.989876
a = 0.01	0.02912308	28.1114235	0.969835
a = 0.1	0.01257937	67.8443048	0.912787
	0.01373973	64.5145551	0.929059
	0.01513592	61.1961076	0.943393
	0.01684796	57.8553313	0.956499
	0.01785792	56.1903187	0.963157
	0.03413461	24.0022053	0.989627
	0.03855212	22.3373305	0.991279
	0.04428281	20.6724556	0.986309
	0.05201468	19.0075808	0.972878
	0.06301791	17.3427335	0.97231
0.07992524	15.6778586	0.960569	
0.10923151	14.0129838	0.791559	
a = 0.25	0.04237071	19.364318	0.947109
	0.0469705	18.5542507	0.964924
	0.0526905	17.744211	0.955282
a = 0.4	0.05050179	16.271171	0.939334
a = 0.5	0.05220222	14.6697817	0.911449
a = 0.6	0.06120991	13.4527787	0.916877
a = 1	0.02733123	29.7135847	0.370697
	0.08220881	10.0599294	0.806297

Discussion and Outlook:

The fidelity is a function of at least three variables, the strength of the interaction,

the velocity at which the traps are brought together, and the time for which the traps are overlapped. These results seem fairly good as long as two conditions are met: (i) the chosen velocity must be about two orders of magnitude smaller than the characteristic velocity defined earlier, (ii) the strength of the delta interaction must be about an order of magnitude smaller than a characteristic energy which can be defined as the ground state energy of a single particle when the traps are overlapped. These requirements are to be expected since the predicted acceptable velocities and interaction times were derived using the adiabatic theorem and first order perturbation theory. If the strength of the delta interaction gets too large, it can no longer be correctly thought of as a perturbation and more importantly the approximation $\langle \tilde{S}\tilde{S} | SS \rangle \approx \langle \tilde{A}\tilde{A} | AA \rangle \approx 1$ quickly becomes invalid. In fact the actual value of the overlap integrals might be a good measure of the fidelity not including diabatic effects, something that I will be investigating soon. It is also thought that the initial separation of the traps might play an important role in the fidelity, a notion that can be illustrated by noting that,

$$|SS\rangle = \frac{|LL\rangle + |RR\rangle + |LR\rangle + |RL\rangle}{2} \quad (45)$$

$$|AA\rangle = \frac{|LL\rangle + |RR\rangle - (|LR\rangle + |RL\rangle)}{2} \quad (46)$$

and therefore the corresponding perturbed states can be written as,

$$|\tilde{S}\tilde{S}\rangle = \frac{|\tilde{L}\tilde{L}\rangle + |\tilde{R}\tilde{R}\rangle + |\tilde{L}\tilde{R}\rangle + |\tilde{R}\tilde{L}\rangle}{2} \quad (47)$$

$$|\tilde{A}\tilde{A}\rangle = \frac{|\tilde{L}\tilde{L}\rangle + |\tilde{R}\tilde{R}\rangle - (|\tilde{L}\tilde{R}\rangle + |\tilde{R}\tilde{L}\rangle)}{2}. \quad (48)$$

However, in the case that the traps are very far apart, atoms in different wells will not feel

a weak interaction giving $|\tilde{L}\tilde{R}\rangle \approx |LR\rangle$ and $|\tilde{R}\tilde{L}\rangle \approx |RL\rangle$, and therefore,

$$|\tilde{S}\tilde{S}\rangle - |\tilde{A}\tilde{A}\rangle \approx |LR\rangle + |RL\rangle = |SS\rangle - |AA\rangle, \quad (49)$$

which is the approximation we made in order to get (27).

An unexpected result is that longer interaction times also lead to lower fidelities. This simply might be a result of not having sufficient initial separation, but further analysis is needed. I believe a Landau-Zener analysis could yield an optimization scheme that might maximize the fidelity. A Landau-Zener analysis aims to quantify the probability of a particle making a transition from one energy eigenstate to another based on the gap between the relevant energy curves and the speed at which the curves are being traversed. One basic test that must be carried out is the addition of other possible states that the atoms can be excited into that were excluded from this solution for the reason of greatly reducing the length of code that is necessary. I believe that including these states will result in relatively small corrections, perhaps reductions, in the calculated fidelities, that will need to be verified. I also want to gather more data in order to quantify how the fidelity falls off with increasing velocity and the strength of the delta interaction and compared this to the predictions made by the Landau-Zener theorem. Other velocity profiles should also be experimented with to investigate the possibility of an increase in fidelity when the magnitude of acceleration is decreased. In this study we have assumed we have access to neutral spin 1/2 atoms, an assumption that can never be realized since any real atom will have a nucleus that also has spin. The hyperfine interaction will have to taken into account in any simulation claiming to be realistic.

Appendix

1. Adiabatic prediction routine
2. Interaction exchange functions routine
3. Diabatic coupling functions routine
4. Coupled ODE triplet solution routine
5. Coupled ODE singlet solution routine