A method of state-selective transfer of atoms between microtraps based on the Franck-Condon Principle.

A. B. Deb, G. Smirne, R. M. Godun, C. J. Foot
Clarendon Laboratory, University of Oxford, Parks Road, Oxford, OX1 3PU, UK
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We present a method of transferring a cold atom between spatially separated microtraps by means of a Raman transition between the ground motional states of the two traps. The intermediate states for the Raman transition are the vibrational levels of a third microtrap, and we determine the experimental conditions for which the overlap of the wave functions leads to an efficient transfer. There is a close analogy with the Franck-Condon principle in the spectroscopy of molecules. Spin-dependent manipulation of neutral atoms in microtraps has important applications in quantum information processing. We also show that starting with several atoms, precisely one atom can be transferred to the final potential well hence giving deterministic preparation of single atoms.

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Ultracold atoms in arrays of microtraps have been proposed as systems for storing quantum information in the internal states of the atoms [1]. To carry out quantum information processing of the information in such a register, the atoms must interact in a way that depends on their internal state, but because the interactions between neutral atoms are short range, this requires bringing the atomic wavepackets into ‘contact’, i.e. putting atoms into the same well. A method of achieving this has been demonstrated experimentally [2] in which the microtraps belonged to a spin-dependent optical lattice that was physically moved to transport the atomic wavepackets though space—in order to give a spin-dependent potential in that scheme the trapping light has a frequency closer to the atomic resonance frequency than would otherwise be the case and this introduced some undesirable inelastic light scattering leading to decoherence. Also, the movement of the potentials must be carried out sufficiently slowly to avoid motional heating. In this paper we analyse a scheme that differs from [2] in the following ways: a) it does not require the potentials to change position but only to be turned on and off adiabatically (by controlling the intensity of the light, which is necessary to loading the trap in any case), and b) although spin-dependence is introduced in the same way as in [2] the atoms are only exposed to this radiation transiently; atoms in the initial and final states are stored in traps where the scattering rate is very low and wavepackets are transferred between microtraps by a Raman process. Similar schemes are implicitly assumed in proposals for creating artificial magnetic fields [3] and fractional occupation of fermions in an optical lattice [4] but here we give explicit values for realistic experimental conditions. Instead of using dipole traps created by laser light, these ideas could be implemented using the strong spin-dependent potentials close to current-carrying wires on magnetic atom chips; suitable potentials can be either magnetostatic, associated with RF/microwave radiation, or some combination of these. To date, however, the distance scale over which the potentials are modulated by atom chips is considerably greater than the sub-micron length scales in optical lattices. In addition to realizing a collisional gate for quantum computation, the scheme described here can perform the operations of beam-splitting, spatial separation and recombination of atomic wavepackets that form the basis of atomic interferometry [5].

FIG. 1: (a) Franck-Condon Transfer: The spatial transfer of neutral atoms between two wells, L and R using the overlap of vibrational wavefunctions. Each of the vertical double-headed arrows denotes a microwave transition between hyperfine levels of the atomic ground configuration (or a Raman transition between these states). Note that the Franck-Condon scheme shown in (a) does not work for electronic transitions, as explained in this paper. (b) The Franck-Condon principle explains the relative strengths of the spectral lines between vibrational levels that arise in the electronic transitions in diatomic molecules. The strongest line in the vibrational spectra is indicated by the vertical arrow.

In this paper we analyse a scheme based on a Raman transition of a trapped neutral atom from the ground vibrational state of one well to that of a neighboring well as shown in Fig. 1(a). The left and right wells repre-
sent the (one-dimensional) potential experienced by the atom in internal states $|1\rangle$ and $|2\rangle$ respectively. In the deep central well the atom is in internal state $|3\rangle$ We assume that the atom is initially in the lowest vibrational level of the left well. A Raman transition brings the atom from $|1\rangle$ to $|2\rangle$ where the initial and final vibrational wave functions have a significant overlap with the vibrational wave functions of the intermediate state. The scheme has an analogy with the well-known Franck-Condon principle in molecular physics. Underlying this principle is the Born-Oppenheimer approximation which allows the electronic and the nuclear motions to be separated and the molecular wave function to be written as a product of the electronic and the vibrational wave function:

$$\Psi(r, R) = \psi_e(r, R) \psi_v(R),$$  \hspace{1cm} (1)$$

where $r$ and $R$ are the electronic and the center-of-mass coordinates, respectively. Thus when the molecule undergoes an electric dipole transition from a state $A$ to an excited state $B$ (Fig 1(b)), the electric dipole matrix element is proportional to

$$\langle \psi_v, A | \psi_v, B \rangle$$

where the initial and final vibrational wave functions have a significant overlap with the vibrational eigenstates corresponding to different potential functions do not need to be orthogonal. The modulus-squared of the Franck-Condon factor $\langle \psi_v, A | \psi_v, B \rangle$ determines the relative strength of transitions. Our scheme employs as the internal states hyperfine states of the atomic ground configuration. The hyperfine levels have typical energy splitting of order 1 GHz whereas the vibrational states of dipole traps have energies of tens of kHz, so we can write the wavefunction as a product of the internal and vibrational wavefunctions.

Usually, the potential corresponding to the intermediate atomic state will have a number of vibrational states with non-zero overlap with the initial and final states. The alternating parity of eigenfunctions of a given Hamiltonian leads to the fact that the overlaps between two nearest vibrational levels tend to cancel each other (the implications of this fact will be discussed later). We derive below under what conditions the problem reduces to a three-level problem. Fig. 2 shows the situation schematically. The ground states of the left and the right well, denoted by 1 and 2, are coupled to the vibrational manifold (denoted by $n$) of the potential associated with the intermediate atomic state 3 (these states are denoted by 3, $n$) by two lasers or microwaves of frequencies $\omega_{L1}$ and $\omega_{L2}$ respectively. The Hamiltonian

$$H = H_0 + H_I$$  \hspace{1cm} (3)$$

can be written in the basis $|1\rangle$, $|2\rangle$, $|3, n\rangle$, $|3, n+1\rangle$, ..., as

$$H_I = \hbar \sum_{i,j} M_{i,j} \omega_i \omega_j$$

where $H_0$ is the atomic Hamiltonian, and the interaction Hamiltonian $H_I$ is given by

$$H_{1,j} = -d \cdot E_{0, L_j},$$

for optical (electric dipole) transitions and

$$H_{1,j} = -\mu \cdot B_{0, L_j},$$

for microwave (magnetic dipole) transitions.

$$M_{3n,j} = \Omega_{3n,j} \cos(\omega_{L_j} t)$$

Here, $\Omega_{3n,j}$ is the Rabi frequency of the transition between levels $|3, n\rangle$ and $|j\rangle = 1, 2 \rangle$ which gives the coupling strength between these levels induced by the lasers/microwaves $\omega_{L_j}$ and is given by

$$\Omega_{3n,j} = \frac{\langle 3| H_{1,j} | n \rangle}{\hbar}$$  \hspace{1cm} (4)$$

and

$$\frac{3| H_{1,j} | n \rangle}{\hbar} = \frac{\langle 3| H_{1,j} | 2 \rangle}{\hbar} + \frac{\langle 3| H_{1,j} | 1 \rangle}{\hbar}$$  \hspace{1cm} (5)$$

where

$$\Omega_{3n,j} \sqrt{\Omega_{3n,j}}.$$  \hspace{1cm} (6)$$
where \( n_j = n_1 \) or \( n_2 \) are the vibrational quantum number of the initial/final well and \( n \) is the vibrational quantum number of the intermediate well. \( \Omega_{3n,j} \) is the Rabi frequency if the overlap is perfect and \( f_{n,j} \) is a dimensionless quantity representing the overlap of wave function squared. The zero of energy is taken to be the energy of \([1, n_1 = 1]\). Non-resonant transition between internal states \([1]\) and \([2]\) is ignored.

We make the usual transformation to the interaction picture using the unitary operator \( U = e^{-\frac{i}{\hbar}H_0 t} \), we obtain the transformed Hamiltonian,

\[
\bar{H} = \hbar \begin{pmatrix}
0 & 0 & N_{31,1} & N_{32,1} & N_{33,1} & . & . \\
0 & 0 & K_{31,2} & K_{32,2} & K_{33,2} & . & . \\
N_{31,1}^* & K_{31,2}^* & 0 & 0 & 0 & . & . \\
N_{32,1}^* & K_{32,2}^* & 0 & 0 & 0 & . & . \\
N_{33,1}^* & K_{33,2}^* & 0 & 0 & 0 & . & . \\
. & . & . & . & . & . & .
\end{pmatrix},
\]

In the RWA, the matrix elements are

\[
N_{3n,j} = \frac{1}{2} \Omega_{3n,j} e^{i\Delta_n t}
\]

\[
K_{3n,j} = \frac{1}{2} \Omega_{3n,j} e^{i(\Delta_n - \delta) t}
\]

The frequency detunings are (see Fig.2),

\[
\Delta_n = \omega_{L1} - \omega_{3n}
\]

and

\[
\delta = (\omega_{L1} - \omega_{L2}) - (\omega_2 - \omega_1).
\]

The time-evolution of the wavefunction

\[
\tilde{\Psi}(t) = c_1(t)|1, n_1 = 1\rangle + c_2(t)|2, n_2 = 1\rangle + \sum_n c_{3n}(t)|3, n\rangle
\]

is given by

\[
\hbar i \frac{d}{dt} \tilde{\Psi}(t) = \bar{H}(t)\tilde{\Psi}(t).
\]

Thereby we obtain a set of coupled first-order differential equations:

\[
\frac{dc_1}{dt} = i \sum_n N_{3n,1} c_{3n},
\]

\[
\frac{dc_2}{dt} = i \sum_n K_{3n,1} c_{3n},
\]

\[
\frac{dc_{3n}}{dt} = i(N_{3n,1}^* c_1 + K_{3n,2}^* c_2),
\]

for all \( n \). We can see from Eq. (7), (8) and (9) that under the condition:

\[
\Delta_n \gg \Omega_{3n,1}, \Omega_{3n,2},
\]

the variables \( c_{3n} \) (for all \( n \)) oscillate very fast compared to the slow variables \( c_1 \) and \( c_2 \) so that “adiabatic elimination” is possible where we integrate (9) considering \( c_1 \) and \( c_2 \) as constants to obtain:

\[
c_{3n} = \frac{\Omega_{3n,1} e^{-i\Delta_n t}}{2\Delta_n} c_1 + \frac{\Omega_{3n,2} e^{-i(\Delta_n - \delta) t}}{2(\Delta_n - \delta)} c_2,
\]

for all \( n \). Substituting in equations (7) and (8), we obtain

\[
\frac{dc_1}{dt} = i c_1 \sum_n \frac{\Omega_{3n,1}^2}{2\Delta_n} + i c_2 \sum_n \frac{\Omega_{3n,1} \Omega_{3n,2} e^{i\delta t}}{2(\Delta_n - \delta)}
\]

\[
\frac{dc_2}{dt} = i c_1 \sum_n \frac{\Omega_{3n,1} \Omega_{3n,2} e^{-i\delta t}}{2(\Delta_n - \delta)} + i c_2 \sum_n \frac{\Omega_{3n,2}^2}{2\Delta_n}
\]

Thus under condition (10) the system reduces to an effective two-level system. The additional condition

\[
\Delta_n \gg \delta,
\]

for all \( n \) allows us to make another unitary transformation using the operator

\[
U' = \begin{pmatrix}

\end{pmatrix}
\]

which reduces everything to an effective two-level problem with an effective Rabi frequency:

\[
\Omega_{eff} = \sum_n \frac{\Omega_{3n,1} \Omega_{3n,2}}{2\Delta_n}
\]

\[
= \tilde{\Omega}_{3,1} \tilde{\Omega}_{3,2} \sum_n \frac{\langle n_1 = 1|n\rangle \langle n|n_2 = 1\rangle}{2\Delta_n},
\]

The effective detuning of the two-level system is given by

\[
\delta_{eff} = \delta - \sum_n \left( \frac{\Omega_{3n,1}^2}{4\Delta_n} - \frac{\Omega_{3n,2}^2}{4\Delta_n} \right).
\]
transfers an atom initially in the lowest vibrational level of the left well completely to that of the right well when the conditions leading to Eq.(16) are satisfied.

In what follows we discuss the transfer scheme only in the situations where the initial, the intermediate and the final internal states are ground hyperfine states of the atom. In the appendix, we show that the Franck-Condon transfer scheme cannot be carried out using electronic transitions.

To create potential landscapes that depend on the internal state for ground hyperfine states of alkali atoms, there are different viable options - among them are i) using spin-dependent dipole potentials created by off-resonant laser light [2], ii) magnetic potentials on atoms chips, including magnetostatic trapping modified by RF fields or near-field microwave potentials [6], or combinations of these or a combination of any of these with conservative optical dipole potentials. As shown below, the Franck-Condon transfer scheme requires the intermediate state potential to be very deep and the initial and final state potentials only moderately deep, therefore with a pure spin-dependent optical dipole potential, there would be a high light scattering rate since the dipole trap laser needs to be tuned between D1 and D2 lines. As we shall see below, the transfer time can be made of order of milliseconds; thus if one uses spin-dependent dipole potentials only for initial and final states and keeps them on only during the transfer process, light scattering will not be a serious problem. Furthermore, it is possible to create blue-detuned spin-dependent optical potentials [7] which could further reduce the light scattering in the initial and final states.

FIG. 3: Creating microwave potential for \(^{87}\text{Rb}\). For a near-field microwave positively detuned from both \(|F = 1, M_F = -1\rangle \leftrightarrow |2, 0\rangle\) and \(|1, 1\rangle \leftrightarrow |2, 0\rangle\) transitions, one has a trapping potential for \(|2, 0\rangle\) and and anti-trapping potentials for both \(|1, -1\rangle\) and \(|1, 1\rangle\) (see Ref. [3]).

To give an estimate of the parameter regime for which the spatial transfer scheme works, we consider the situation of two harmonic wells separated by a distance \(1 \mu\text{m}\). The left well predominantly traps atoms in \(|F = 1, m_F = -1\rangle\) state whereas the right well traps predominantly \(|F = 1, m_F = 1\rangle\) in the ground state of \(^{87}\text{Rb}\); states \(|1\rangle\) and \(|2\rangle\) respectively in the earlier notation. This means that the left well is deep for atoms in state \(|1\rangle\) and shallow for atoms in \(|2\rangle\), so that the lowest vibrational wavefunction for atoms in \(|1\rangle\) is much more localized than that for atoms in \(|2\rangle\), so that Franck-Condon overlap for state \(|2\rangle\) is negligible. Similarly for right well, only overlaps for atoms in state \(|2\rangle\) is relevant. In between them is a tighter harmonic well with trap frequency \(\omega_{\text{vib}} = 2\pi \times 50 \text{kHz}\) which only traps a \(m_F\)-state of the upper hyperfine level \(F = 2\), e.g., \(|F = 2, m_F = 0\rangle\).

The ground state of \(^{87}\text{Rb}\) has a hyperfine splitting of \(6.8 \text{GHz}\). The Zeeman energy is given by \(g_F m_F \mu_B B\) where \(g_F = -1/4\) for \(F = 1\), so a bias magnetic field of a few Gauss will create a situation similar to Fig. 2. Spin-dependent potentials in the above-mentioned length scale and trap frequencies are technically achievable using microwave potentials as shown in Fig. 4. For example, the intermediate potential can be created by using near-field microwave with a positive frequency detuning from both of \(|F = 1, m_F = 1\rangle \leftrightarrow |F = 2, m_F = 0\rangle\) and \(|F = 1, m_F = -1\rangle \leftrightarrow |F = 2, m_F = 0\rangle\) transitions.
(Fig.3) so that one has a trapping potential for an $F = 2$ atom and anti-trapping potential for an $F = 1$ atom. Unlike in [ ] where the state $|F = 2, m_F = 1\rangle$ is used as a qubit state, in our case the atom stays in the intermediate potential only for a very short time (as we will see below) and therefore the choice of a $F = 2$ spin-state not crucial. The left and the right wells can be created, for example, using a combination of conservative dipole trap and a spin-dependent dipole trap with suitable choice of beam polarization and detuning, so that the left trap provides good Franck-Condon overlap only for atoms in $|F = 1, m_F = -1\rangle$ state and the right well, for $|F = 1, m_F = 1\rangle$. This can be further ensured by adjusting the relative position and depth of the conservative and spin-dependent dipole traps (Fig.4). The spin-dependent part of the dipole trap can be switched off adiabatically after the transfer to reduce spontaneous light scattering.

In the following, the overall trap frequencies of the left and right wells for the appropriate spin-state is assumed to be $2\pi \times 10$ kHz. The spin-dependent dipole beam will also modify the potential for the intermediate state equally on both sides and this in fact enhances the overall Franck-Condon overlap. If we tune the two microwaves connecting $|F = 1, m_F = -1\rangle \rightarrow |F = 2, m_F = 0\rangle$ and $|F = 2, m_F = 0\rangle \rightarrow |F = 1, m_F = 1\rangle$ midway between the 13th and 14th vibrational levels of the intermediate potential, the resultant of the summation in Eq.(16) is calculated to be $(0.053)/(2\pi \times 50)$ kHz$^{-1}$. If the powers of the microwaves are adjusted so that the Rabi frequencies $\tilde{\Omega}_{3,1}$ and $\tilde{\Omega}_{3,2}$ in Eq.(16) are $2\pi \times 16$ kHz each (the maximum of the Franck-Condon factors is $\sim 0.2$, so the individual two-level Rabi frequencies are $2\pi \times 3.2$ kHz $\ll \Delta$, since we assume $\Delta \sim 2\pi \times 25$ kHz, condition (10) is satisfied. Impurity of transfer arising from this approximation will be estimated below), the effective Rabi frequency is about $2\pi \times 273$ Hz leading to a pi-pulse time $\sim 1.8$ ms. The coherence time in microwave potentials is estimated [ ] to be of order of seconds, and up to few tens of seconds in far-off resonant dipole traps, so the transfer time is well-suited for coherent manipulations of cold atoms for realizing phase-gates for quantum computation, inter alia.

It turns out that fairly large values of the summation is possible even with small individual Franck-Condon factors. This arises from the symmetry of the intermediate potential - the wavefunctions of the alternate vibrational levels have opposite parities. Thus if we tune the microwaves midway between the $n$ and $(n + 1)$-th vibrational levels, the matrix elements in the numerator of the term inside the summation of Eq.(16) have opposite signs for $n$ and $(n + 1)$, but since the detunings for $n$ and $(n + 1)$ have opposite signs too, the contributions from $n$ and $(n + 1)$ add up. However, for the same reason, the contribution from the pair $(n - 1, n + 2)$ will tend to add destructively, but these levels are further detuned (e.g. $\Delta_{n-1} = (1/3)\Delta_n$, for pure harmonic potential) and overlap factors are also smaller. A great part of it is further compensated by the contribution from the next pair $(n - 2, n + 3)$ Those levels which do not have a counterpart have negligibly small Franck-Condon factors and their contributions are not important. This shows that it is helpful to choose the potential profiles such that the Franck-Condon overlap falls off sharply above and below a desired pair of vibrational levels. The parity of the wavefunctions leading to alternate sign of the quantities in the summation also is exactly the reason why the transfer is not possible in the optical regime since when the vibrational levels cannot be resolved, the contributions all cancel out (see Appendix).

It is also interesting note that in Eq.(17), the net detuning is the Raman detuning as shown in Fig.2 minus the net AC Stark shift generated by the Raman microwave beams summed over the vibrational ladder of the intermediate potential. The AC Stark shift coming from the individual beams $((-1)^{p-1} \sum_j \Omega_{3j,p}/4\Delta_j$ with $p = 1, 2$) is very small due to the alternating signs of $\Delta_j$ for levels $n$ and $n + 1$ and similarly for all such pairs (as discussed in the above paragraph) and given that the numerator was always positive and in the numerical example given above, this is less than 0.1 percent of $\Omega_{eff}$. Of course, for symmetric choice of Franck-Condon factors and Raman microwave beam powers (i.e. $\Omega_{3j,1} = \Omega_{3j,2}$ for all $j$), the net AC Stark shift (the term under summation in Eq.(17)) is essentially zero. Negligible AC Stark shifts for this Raman process is suitable for the phase coherence of qubits required for quantum information processing.

To estimate the inaccuracy involved in the adiabatic elimination of the intermediate levels, it is useful to consider the system as an effective three-level system with an effective Franck-Condon factor by re-writing Eq.(16) in the following form:

$$\Omega_{eff} = \frac{\tilde{\Omega}_{3,1}\tilde{\Omega}_{3,2}}{2\Delta} f_{eff}. \tag{19}$$

Here $\Delta$ is half the mode-spacing of the levels $n$ and $(n + 1)$, midway between which the microwaves have been tuned and $f_{eff}$ is defined by comparing Eq.(19) with Eq.(16). For the simplified case where $\sqrt{f_{eff}} = \tilde{\Omega}_{3,1}\sqrt{f_{eff}} = \tilde{\Omega}_{3,2}\sqrt{f_{eff}} = \Omega$, the set of equations (7), (8) and (9) become,

$$\frac{dc_1}{dt} = \frac{i\Omega}{2} e^{i\Delta t} c_3 \tag{20}$$

$$\frac{dc_2}{dt} = \frac{i\Omega}{2} e^{i(\Delta - \delta) t} c_3 \tag{21}$$

$$\frac{dc_3}{dt} = \frac{i\Omega}{2} e^{-i\Delta t} c_1 + \frac{i\Omega}{2} e^{-i(\Delta - \delta) t} c_2 \tag{22}$$

These coupled equations are numerically solved for the same parameters as above and Fig.[] shows the result.
We can see that the peak population of the intermediate level is below 1 percent. This impurity decreases rapidly with increased pi-pulse time (less power on the microwaves). It is interesting to note at this point that with microwaves, the sideways push on the atom comes from the different potential gradient experienced by the atom when transferred to a different internal state, so momentum is conserved. Such physical movements of a particle during internal state transition occurs also in the proposed scheme for microwave Raman sideband cooling of ions where a differential magnetic field gradient is necessary for creating state-dependent potential profile.

In the case where both atoms in left well and right well go to the central well, separating them afterwards at the end of the phase accumulation can be a problem, which can, at least in principle, be surmounted by using the adiabatic transfer technique described in the next paragraph. Using other atomic species with a wider choice of spin-states, one can have states \( |c \rangle \) and \( |d \rangle \) different to each other (and to \( |0 \rangle \) and \( |1 \rangle \)), e.g., for \(^{133}\text{Cs}\) the lowest ground hyperfine state \( (F = 3) \) has seven different spin-states.

One of the preliminary requirements for using neutral atoms in lattice structures as scalable quantum computers is to deterministically prepare one atom per lattice site in the motional ground state. Several proposals to this end have been made \([10], [11], [12]\). In the following we show how the spatial separation scheme can be useful for realizing the purification scheme suggested in \([10]\) which consists of an adiabatic transfer of an atom from one internal state with low inter-atom interaction (Hubbard-U) to another with a high interaction energy (e.g., by choosing the second internal state to be one with a Feshbach resonance and applying a magnetic field close to the resonance to get the required high \(U\)). Initially, a small number of atoms \( (N = 3, 4, \text{on an average}) \) is loaded into the first internal state from a BEC with a Poissonian number distribution, so the number uncertainty is \( \sim \sqrt{N} \) leading to an uncertainty in the interaction energy of the atoms in the first internal state \( \sim \sqrt{NU} \), and a very low probability of there being zero atoms. Adiabatically scanning the Raman detuning over a suitable range can ensure that only one atom is transferred to the second internal state in the same well. State-selectively removing the remaining atoms in the first internal state leaves one with a pure atomic crystal with one atom in the motional ground state of each site. A scheme in which atoms are transferred between internal

![Figure 5: Population of the initial (top), final (middle) and the intermediate (bottom) levels for the parameters mentioned in the text.](image)

![Figure 6: The scheme for implementing a collisional phase gate with Franck-Condon transfer. The states are labelled \( |1 \rangle \) and \( |0 \rangle \) in the left and right wells respectively according to the usual QIP conventions. Atoms starting in state \( |1 \rangle \) are connected to the state \( |c \rangle \) in the central well, and similarly \( |0 \rangle \leftrightarrow |d \rangle \).](image)
states within the same well means that there must be a separation of these states at the end of the process. Removing the atoms state-dependently while maintaining high purity of the desired single-atom state is not straightforward: an obvious option is to use a pulse of resonant light to kick the unwanted atoms out of the trap. However if these atoms are in the same potential well, inelastic light scattering can leave some of the atoms in the second state which limits the purity of the final state. Using a spin-dependent lattice to separate the two spin-species spatially is another option but for states which can be connected by magnetic dipole transitions, it is not possible to make the force on one spin-species more than 3 times bigger than that on the other at low magnetic fields, so one needs to effect the separation process very slowly. Another possibility is to transfer the atoms into the first excited Bloch band of the lattice and then lower the depth of the lattice such that the atoms in the first internal state are released while the only atom in the second internal state is still trapped \[13\], but for a number of closely spaced wells this may lead to tunneling, and thus affect the purity. Also in all these schemes, atoms in their initial and final internal states are in the same region of space and thus collisional loss such as three-body recombination will limit the purity. With the Franck-Condon spatial transfer scheme, since the atom transferred to the second state is in a different well, removing the atoms in the first internal state is straightforward and there is no collisional loss. Suppose we want to transfer only one atom to the right well in Fig. 2, starting with a few atoms \( N \sim 4 \) in the left well with a number uncertainty of \( \sim \sqrt{N} \). For this scheme, it is advantageous to have less tight confinement in the starting well and strong confinement in the final well to make the ratio of on-site interaction energy in the final and initial wells as large as possible. Such adjustments are possible whilst keeping good overlap of wavefunctions. This means the region of desirable avoided crossings between number states (i.e. ones between \( |N, 0⟩ \rightarrow |N+1, 1⟩ \) with a \( \sqrt{N} \) uncertainty in N) is small enough to be scanned adiabatically, and this region is small enough so that condition (14) is fulfilled and the region of unwanted avoided crossings (\( |N−1, 1⟩ \rightarrow |N−2, 2⟩ \)) are driven far from the former region. For \( N_{\text{ave}} = 4 \), trap frequencies for left and right well = \( 2\pi \times 3\) kHz and = \( 2\pi \times 15\) kHz, same bare Rabi frequencies and \( \Delta \) as above and Raman detuning and Rabi frequency ramps chosen as suggested in \[14\], a transfer time of 35 ms gives 99.5% purity of transfer. As suggested in \[10\], the transfer time can be minimized by optimizing pulse shapes for Raman detuning and effective Rabi frequency. Switching off the traps holding the atoms in the initial state will leave an array of wells, each of which contains only a single atom.

In summary, we have discussed a scheme of spatially transferring atomic wavepackets between different micro-wells and derived the conditions for such a transfer scheme to work effectively. We have shown that such a transfer can work in an experimentally achievable parameter regime and can be useful for realizing two-qubit phase gates and realizing a deterministic single atom occupation scheme on a realistic time scale. Such a scheme can also be useful for atomic interferometry with localized atomic wavepackets.

**APPENDIX**

In this appendix we show why the Franck-Condon transfer cannot easily be implemented using transitions between electronic states (which would be the most direct analogy with molecular transitions such as that shown in Fig.1b). Using \(^{87}\text{Rb}\), for example, a state-dependent potential profile can be created by using two focussed Gaussian beams red-detuned from the \( ^{5}\text{S}_{1/2} - ^{5}\text{P}_{3/2} \) transition to form the initial and the final wells and inserting in between the beams a central well formed by another focussed Gaussian beam red-detuned from, say, \( ^{5}\text{P}_{3/2} - ^{6}\text{P}_{3/2} \). The problem with this kind of potential for the current scheme is that the natural linewidths of such transitions are several MHz or more. To make the spacing of the vibrational states of the intermediate states many MHz so that they could be resolved, one needs the intermediate potential very deep which is practically impossible for any available laser power and without enormous loss due to spontaneous emission. When the vibrational states cannot be resolved, \( \Delta_n \) in the denominator of Eq.(16) is same for all \( n \):

\[
\Omega_{\text{eff}} = \frac{\bar{\Omega}_{3,1}\bar{\Omega}_{3,2}}{2\Delta} \sum_n \langle n_1 = 1|n⟩⟨n|n_2 = 1 \rangle
\]

\[
= \frac{\bar{\Omega}_{3,1}\bar{\Omega}_{3,2}}{2\Delta} \langle n_1 = 1|n_2 = 1 \rangle,
\]

since by completeness,

\[
\sum_n |n⟩⟨n| = 1.
\]

The direct overlap of the two lowest vibrational levels of the two spatially separated traps is essentially very small. Thus the Franck-Condon (FC) transfer scheme cannot be carried out using optical transitions.

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