Fast Quantum Gate via Feshbach-Pauli Blocking in Quantum Nano-Trap

Krzysztof Jachymski\textsuperscript{1,2}, Zbigniew Idziaszek\textsuperscript{1} and Tommaso Calarco\textsuperscript{2}

\textsuperscript{1}Faculty of Physics, University of Warsaw, Hoża 69, 00-681 Warsaw, Poland,
\textsuperscript{2}Institut für Quanteninformationsverarbeitung, Universität Ulm, D-89069 Ulm, Germany

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We propose a simple idea for realizing a quantum gate with two identical fermions in a double well trap via external optical pulses without addressing the atoms individually. The key components of the scheme are Feshbach resonance and Pauli blocking, which decouple unwanted states from the dynamics. As a physical example we study atoms in the presence of a magnetic Feshbach resonance in a nanoplasmonic trap and discuss the constraints on the operation times for realistic parameters, reaching a fidelity above 99.9\% within 42\,\mu s.

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Identifying physical systems in which quantum algorithms \cite{1} can be implemented is a crucial element for the development of quantum information. A number of different systems, including trapped ions, photons and superconducting circuits, can be considered suitable for building a quantum gate. Among the most promising candidates are ultracold atoms and molecules \cite{2,3,4,5,6,7,8,9,10,11,12,13}. Neutral particles in optical lattices \cite{16,17,18} are amenable to operations with single site resolution \cite{19,20,21}. However, achievable gate speeds with such systems are comparatively low due to weak atomic interactions and limited trapping frequencies.

A powerful tool used to control the interactions of trapped neutral atoms is a Feshbach resonance, which allows for manipulation of the scattering length \cite{22,23} and production of ultracold molecules \cite{24}. The resonance mechanism comes from the coupling of a free pair of atoms with a molecular bound state. The energy of the bound state can be controlled by an external field and the resonance occurs when it crosses the energy of the open channel.

Recently a new kind of traps for ultracold atoms has been proposed \cite{25,26,27,28,29}, allowing to reach significantly higher trapping frequencies than before. In these novel systems, the atoms are trapped by the potential formed from the near-field scattering of laser light on plasmonic nanostructures. The resulting trapping frequencies can be of the order of several MHz and the separation between the potential wells is much smaller than the laser wavelength. The combination of strong resonant interactions with tight subwavelength traps would allow in principle for much faster quantum gates. However, there is no way to achieve single site addressability in those systems with existing techniques, so standard gate schemes would not work.

In this letter we propose a way to make use of strong confinement and resonant interactions to achieve a fast quantum gate with high fidelity but without the need for individual particle addressing, schematically presented on Figure 1. We consider a pair of identical fermions in a tight double well trap. Using the exchange blockade mechanism and manipulating the trap shape in time, it would be possible to realize a quantum gate with this setup \cite{30}, but the operation time can be expected to be long as the trap shapes need to be changed adiabatically with respect to the small tunneling energy splitting. Instead, we suggest to use external fields to induce transitions between different trap levels. The time evolution of the pair will then depend on the spin state due to symmetry requirements. The Feshbach resonance plays a crucial role here as a mechanism for suppressing unwanted states in the evolution. It shifts the energy of the states having both atoms in antisymmetric spin state occupy the same potential well, decoupling it from the dynamics, whereas the Pauli exclusion principle blocks transitions to states with both atoms in the symmetric internal state and in the same trap level. Non-adiabatic effects, such as leakage to highly excited trap states, can be suppressed by means of optimal control \cite{31}.

We calculate the energy levels of a model double well

\begin{figure}[h]
\centering
\includegraphics[width=0.8\textwidth]{fig1.png}
\caption{(color online) Schematic view of the gate operation. Two particles (purple balls) are initially localized in separated wells of the trap, then an external pulse with Rabi frequency $\Omega$ (blue arrows) is applied to induce coupling to an excited, delocalized trap state. The state with doubly occupied site is detuned by $\delta_F$ due to the Feshbach resonance when the atoms are in antisymmetric internal state or forbidden by Pauli blocking when they are in symmetric internal state (crossed orange arrows and balls).}
\end{figure}
trap in the vicinity of a magnetic field, assuming that an s-wave Feshbach resonance is present. The trapping potential does not allow for separation of center of mass and relative motion, which has to be included in the calculations \[32, 35\]. Then we consider the dynamics of the pair when an external laser pulses are applied. We optimize the pulse shape using optimal control \[31\] to achieve high gate fidelity. Our scheme does not need single site resolution and can thus be implemented even in very tight traps.

**Double well trap and its eigenstates.** Let us consider a pair of neutral atoms trapped by the light scattered on a set of nanospheres or nanotips \[25, 26\]. We assume that the trap is designed to produce a double well potential. For simplicity we describe the trap as a one-dimensional harmonic potential with frequency $\omega$ with a Gaussian barrier in the middle, parametrized by width $w$ and height $b$. We assume that the trap in the remaining two dimensions is so tight that the particles stay in its lowest state and the dynamics in those directions is frozen. Submicrometer precision of arranging the nanostructures and tunability of polarization of light sources \[21\] allows for realization of a trapping potential of this kind. Setting $\sqrt{\hbar/m\omega}$ as the length unit, where $m$ is the atomic mass, the single particle Hamiltonian is

$$\frac{H}{\hbar\omega} = -\frac{1}{2} \frac{\partial^2}{\partial x^2} + \frac{1}{2} x^2 + \frac{b}{\sqrt{2\pi w}} e^{-x^2/2w^2}.$$  

We diagonalise the Hamiltonian \[1\] in the basis of harmonic oscillator wavefunctions. The matrix elements in this basis can be calculated analytically. For high enough barriers, the two lowest lying states become degenerate in energy and separated from the others. One of them corresponds to the even and the other to the odd parity solution. Combining them yields two states localized in one of the potential wells. A two-mode approximation can then be used, which allows for separation of center-of-mass and relative motion, also in the multwell case (an optical lattice) \[36\]. On the other hand, highly excited states of this potential are just harmonic oscillator states. The only important difference between our model potential and a realistic nanoplasmonic trap is the finite depth of the latter one. We thus have to make sure that the states above the realistic trap depth will not be populated during the gate process.

**Feshbach resonance in a double well.** The crucial component of our proposal is a magnetic Feshbach resonance that couples the pair of atoms with the molecular bound state \[22\]. We will describe the resonance using an effective two-channel configuration interaction model \[37, 38\]. The open channel can then be characterized by the hyperfine state of the atomic pair, which we will label by $|\chi\rangle$, while the closed molecular channel is denoted as $|m\rangle$. We neglect the background interaction between the atoms, describing the interactions far from the resonance, as it gives little contribution close to the resonance. We also treat the molecule as a pointlike particle of mass $M = 2m$. Under these assumptions the Hamiltonian can be written as (see \[35\] for a more detailed derivation in the general case)

$$H = |\chi\rangle \langle \chi| \left( -\frac{1}{2} \frac{\partial^2}{\partial x^2} - \frac{1}{2} \frac{\partial^2}{\partial y^2} + V_{DW}(x) + V_{DW}(y) \right) + (|\chi\rangle \langle m| + |m\rangle \langle \chi|) W(x - y) + |m\rangle \langle m| \left( -\frac{1}{4} \frac{\partial^2}{\partial R^2} + 2V_{DW}(R) \right).$$  

(2)

Here $x$ ($y$) is the position of the first (second) particle, $V_{DW}$ is the double well trapping potential and $W$ is the interchannel coupling. The general wave function can be conveniently written in the form

$$|\Psi\rangle = |\chi\rangle \sum_{ij} C_{ij} \psi_i(x) \psi_j(y) + |m\rangle \sum_k A_k \Phi_k(R),$$  

(3)

where $C_{ij}$ and $A_k$ are the amplitudes and $\psi_i$ are single-particle eigenstates. The molecular wave functions $\Phi_k$ obey the equation

$$\left( -\frac{1}{4} \frac{\partial^2}{\partial R^2} + 2V_{DW}(R) \right) \Phi_k(R) = (\epsilon_k + \nu(B)) \Phi_k(R),$$  

(4)

where $\nu(B)$ is the energy shift resulting from coupling with the open channel and it depends on the external magnetic field. Close to the resonance it may be expanded to first order, giving $\nu = s(B - B_0)$, where $s$ is the difference of magnetic moments between the open and closed channel states \[22\].

Substituting \[3\] into the Schrödinger equation $H |\Psi\rangle = E |\Psi\rangle$ leads to a set of equations for the amplitudes

$$(\epsilon_i + \epsilon_j) C_{ij} + \sum_k V_{ij}^k A_k = EC_{ij}$$  

(5)

$$(\epsilon_k + \nu) A_k + \sum_{ij} C_{ij} (V_{ij}^k)^* = E A_k$$  

(6)

where $V_{ij}^k = \alpha \int dR \phi_i^*(R) \phi_j^*(R) \Phi_k(R)$ and $\alpha$ is the coupling constant. By extracting $C_{ij}$ from the first equation, we obtain

$$(E - \epsilon_k - \nu) A_k = \sum_{ijl} A_l \frac{V_{ij}^k (V_{ij}^l)^*}{E - \epsilon_i - \epsilon_j}.$$  

(7)

In our treatment the eigenstates of the double well in which we expanded the solution \[3\] are superpositions of harmonic oscillator states, so $V_{ij}^k$ can be computed using the matrix elements between harmonic oscillator states. This quantity can be computed analytically and written in terms of hypergeometric functions, which allows for obtaining the energy levels from Eq. \[7\].

Figure 2 shows the level structure of trapped $^{40}$K atoms near a 202G s-wave Feshbach resonance for three
exemplary cases: (i) a pure harmonic potential, (ii) a moderate barrier where \( b = 15 \) and \( w = 1 \) and (iii) a higher barrier with \( b = 100 \) with the same \( w \). When the barrier is absent, the center of mass motion can be decoupled from the relative degrees of freedom and the energy spectrum has a simple structure as all the bound states behave in the same way. As the barrier grows, the spectrum becomes more complicated. The two lowest bound levels become close in energy and separate from the rest, as can be seen in the middle panel of Figure 2. For even higher barriers (right panel), also the other bound states form degenerate pairs. In the limit of infinite barrier all the levels are doubly degenerate, which is intuitively clear as the system can be thought of as two completely separated wells. The horizontal lines represent states with odd symmetry, which are not affected by the s-wave resonance.

In general, eq. (7) may contain divergent terms and requires renormalization \[35\]. However, in one dimension all the sums in (7) converge, in contrast to the three-dimensional case. For the one-dimensional description to be valid, the energy of the particles has to be much smaller than \( \hbar \omega_\perp \), where \( \omega_\perp \) is the transverse trapping frequency, so that particles occupy the ground state in the transverse direction at each stage of the gate process. This in our case requires \( \omega_\perp \gtrsim 5\omega \).

**Gate idea.** To introduce the idea of a quantum gate, it is essential to include the quantum statistics and the spin state of the atomic pair in our considerations. In the case of identical fermions, the wave function consists of the spatial and spinor part and it has to be globally antisymmetric. We identify qubit spin states with \(|\uparrow\rangle\) and \(|\downarrow\rangle\). The basis of spin states is \(|\uparrow\uparrow\rangle, |\uparrow\downarrow\rangle, (|\uparrow\rangle + |\downarrow\rangle)/\sqrt{2} = |\uparrow_T\rangle\) (symmetric) and \(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)/\sqrt{2} = |\downarrow_S\rangle\) (antisymmetric).

For the spatial part in the lowest energy sector \([30, 39]\) one may consider only the two lowest eigenstates of the trap, an odd and an even state \(|\psi_o\rangle\) and \(|\psi_e\rangle\). If the barrier height is sufficiently large, those states will have approximately the same energies. One may then construct two localized solutions \(|E\rangle = (|\psi_e\rangle - |\psi_o\rangle)/\sqrt{2}\) and \(|R\rangle = (|\psi_e\rangle + |\psi_o\rangle)/\sqrt{2}\), which will be approximate eigenstates of the Hamiltonian \([1]\). Within this assumption, there are six antisymmetric low energy states:

\[
\frac{1}{\sqrt{2}}(|LR\rangle - |RL\rangle)|\uparrow\rangle, \frac{1}{\sqrt{2}}(|LR\rangle - |RL\rangle)|\downarrow\rangle, \frac{1}{\sqrt{2}}(|LR\rangle - |RL\rangle)|\chi_T\rangle, \frac{1}{\sqrt{2}}(|LR\rangle + |RL\rangle)|\chi_S\rangle,
\]

\[
\frac{1}{\sqrt{2}}(|LL\rangle - |RR\rangle)|\chi_S\rangle.
\]

Now let us add the Feshbach resonance to our considerations. We will work with an s-wave resonance, where only the singlet spin state is coupled to the molecular channel and others do not have the right symmetry. The dynamics of the pair will be spin-dependent due to both the quantum statistics and the presence of the resonance. The idea of how the gate will work is as follows (see Figure 1): initially we will consider two fermions in separate wells. An external field will then be applied, inducing transition between the ground states and an excited trap state \(|E\rangle\) with Rabi frequency \(\Omega\). Due to the Pauli blocking, which will forbid occupation of the same trap state by symmetric spin states, the symmetric and anti-symmetric states will evolve differently and accumulate different phases \(\phi_s\) and \(\phi_a\) during the process. The phase depends only on the state symmetry as the pulse is assumed to couple only to the spatial part of the wavefunction. A phase gate will then be realized when the pair will return to its initial trap state with relative phase \(\phi_s - \phi_a = (2n + 1)\pi, n \in \mathbb{N}\). One potential source of errors is that if we consider the singlet spin state, the particles can in principle end up in the same potential well. This problem is avoided by the resonance, which shifts the energy of such state and thus decouples it from the transitions.

Coupling the trap states can be achieved using various methods, such as Raman transitions or radio-frequency pulses. Ideally it could be desirable to couple only to a single target state \(|E\rangle\), chosen in such a way that it is energetically separated from other trap states and that the Franck-Condon factors \(\langle E| e^{ikz} |R\rangle, \langle E| e^{ikz} |L\rangle\) (denoted by \(\eta_{RE}\) and \(\eta_{LE}\) respectively) are large. However, other trap states will also unavoidably get populated during the gate process, unless the ratio \(\Omega/\omega \ll 1\) (equivalent to
the Lamb-Dicke regime in ion trapping experiments \cite{40}). On the other hand, keeping \(\Omega\) low will result in long operation times, so one can expect that a shaped pulse will be needed to operate at high Rabi frequencies while maintaining high fidelity. To minimize the transitions to levels other than the first excited one, we will work at barrier height \(b = 36\) and width \(w = 1.5\) in oscillator units. This choice of trap parameters gives two almost degenerate lowest states, while the first excited state is already separated from the next one. In the high barrier regime the Franck-Condon factors are equal for the states localized in left and right potential wells, \(\eta_{LE} = \eta_{RE} = \eta\).

It is also important to choose the value of the magnetic field. By analysing Figure 2, one may conclude that the optimal choice is to work at fields slightly lower than the position of the resonance, where the energy shift of the bound levels is large. In this case particles in the same well form a deeply bound state, far detuned from the transitions driven by the external field.

**Implementation and optimization of the gate.** We will now consider more specifically a gate implementation with \(^{40}\)K atoms, for which an s-wave Feshbach resonance occurs at about 202G \cite{22}. When trying to find optimal and realistic experimental parameters which will give shortest operation times, one finds two interesting trade-offs. Firstly, higher Rabi frequencies (more laser power) lead to faster dynamics but also introduce losses via leakage to highly excited states. Secondly, large trapping frequencies reduce the characteristic timescales, but at the same time lower the Franck-Condon factors as the trap becomes smaller and the laser wavelength cannot. Thus the time needed for the operation does not scale linearly with the trapping frequency. For the Raman transition the achievable wavenumbers are of the order of 0.03nm\(^{-1}\). Using UV transitions would allow to improve it by around 50\%, but we will assume optical transitions which are far more convenient experimentally.

The target state after the operation is to have particles again in the lowest trap states \((|LR| \pm |RL|)\) depending on the spin state), but with relative phase \(\pi\) between the symmetric and antisymmetric spin states. The fidelity of the gate can be defined as \(f = |\langle \psi_{\text{out}} | \psi_{\text{target}} \rangle|^2\), where \(|\psi\rangle\) contains both internal and trap states. We choose the initial pulse to have the form \(\Omega(t) = \Omega_0 t / \tau (1 - t / \tau)\), where \(\tau\) is the operation time. We set the trapping frequency \(\omega = 2\pi \times 5\) MHz for which the well minima are \(~250\)nm apart and \(\tau = 1300 / \omega \approx 42\) \(\mu s\). To optimize the pulse and achieve high fidelity we applied the CRAB optimization method \cite{31}. After optimization the fidelity of the solution reached over 99.9\%. The gate operation corresponding to it is depicted on Figure 3. The Rabi frequency of the pulse \(\Omega\) does not exceed 1.8 \(\omega \approx 2\pi \times 9\) MHz, which is a reasonable value for \(^{40}\)K \cite{11} and needs much less laser power than the plasmonic trap itself \cite{28}. The gate time obtained here is limited by the value of \(\Omega\) and does not reach the quantum speed limit \cite{42}. However, using stronger pulses makes the leakage effects stronger and would require adding more driving fields.

**Conclusions.** We proposed a new scheme for realizing a quantum gate with ultracold atoms, which uses two identical fermions in a double well potential and an external optical field. The scheme does not need access to individual particles, but rather relies on using a Feshbach resonance and Pauli exclusion principle. We discussed the implementation of our method in a tight nanoplasmonic trap for realistic experimental conditions and showed that it is possible to obtain a high fidelity phase gate with short operation times using optimal control. Our scheme does not crucially depend on the details of the trapping potential or internal structure of the atoms. It also does not require unrealistic precision in controlling the pulse shapes and can be implemented in various trap types, including standard optical lattices as well as nanoplasmonic traps.

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[1] M. A. Nielsen and I. L. Chuang, *Quantum computation and quantum information* (Cambridge university press, 2010).
[2] J. I. Cirac and P. Zoller, Phys. Rev. Lett. **74**, 4091 (1995).
[3] J. I. Cirac and P. Zoller, Nature **404**, 579 (2000).
[4] J. Benhelm, G. Kirchmair, C. F. Roos, and R. Blatt, Nature Physics **4**, 463 (2008).
[5] P. Kok, W. J. Munro, K. Nemoto, T. C. Ralph, J. P. Dowling, and G. J. Milburn, Rev. Mod. Phys. **79**, 135 (2007).
[6] G. Burlard, D. Loss, and D. P. DiVincenzo, Phys. Rev. B **59**, 2070 (1999).
[7] D. Jaksch, H.-J. Briegel, J. I. Cirac, C. W. Gardiner, and P. Zoller, Phys. Rev. Lett. **82**, 1975 (1999).
[8] G. K. Brennen, C. M. Caves, P. S. Jessen, and I. H. Deutsch, Phys. Rev. Lett. **82**, 1060 (1999).
[9] D. Jaksch, J. I. Cirac, P. Zoller, S. L. Rolston, R. Côté, and M. D. Lukin, Phys. Rev. Lett. **85**, 2208 (2000).
[10] D. DeMille, Phys. Rev. Lett. **88**, 067901 (2002).
[11] T. Calarco, U. Dorner, P. S. Julienne, C. J. Williams, and P. Zoller, Phys. Rev. A **70**, 012306 (2004).
[12] M. Murphy, S. Montangero, T. Calarco, P. Grangier, and A. Browaeys, arXiv:1111.6083 (2011).
[13] A. Negretti, P. Treutlein, and T. Calarco, Quantum Information Processing **10**, 721 (2011).
[14] I. Bloch, J. Dalibard, and W. Zwerger, Rev. Mod. Phys. **80**, 885 (2008).
[15] M. Anderlini, P. J. Lee, B. L. Brown, J. Sebby-Strabley, W. D. Phillips, and J. Porto, Nature **448**, 452 (2007).
[16] D. Jaksch, C. Bruder, J. I. Cirac, C. W. Gardiner, and P. Zoller, Phys. Rev. Lett. **81**, 3108 (1998).
[17] M. Greiner, O. Mandel, T. Esslinger, T. W. Hänsch, and I. Bloch, Nature **415**, 39 (2002).
[18] I. Bloch, Nature Physics **1**, 23 (2005).
[19] P. Würtz, T. Langen, T. Gericke, A. Koglbauer, and H. Ott, Phys. Rev. Lett. **103**, 080404 (2009).
[20] W. S. Bakr, J. I. Gillen, A. Peng, S. Fölling, and M. Greiner, Nature **462**, 74 (2009).
[21] C. Weitenberg, M. Endres, J. F. Sherson, M. Cheneau, P. Schauß, T. Fukuhara, I. Bloch, and S. Kuhr, Nature **471**, 319 (2011).
[22] C. Chin, R. Grimm, P. Julienne, and E. Tiesinga, Rev. Mod. Phys. **82**, 1225 (2010).
[23] S. Inouye, M. R. Andrews, J. Stenger, H. J. Miesner, D. M. Stamper-Kurn, and W. Ketterle, Nature **392**, 151 (1998).
[24] M. Bartenstein, A. Altmeyer, S. Riedl, S. Jochim, C. Chin, J. H. Denschlag, and R. Grimm, Physical review letters **92**, 120401 (2004).
[25] D. E. Chang, J. D. Thompson, H. Park, V. Vuletić, A. S. Zibrov, P. Zoller, and M. D. Lukin, Phys. Rev. Lett. **103**, 123004 (2009).
[26] B. Murphy and L. V. Hau, Phys. Rev. Lett. **102**, 033003 (2009).
[27] C. Stehle, H. Bender, C. Zimmermann, D. Kern, M. Fleischer, and S. Slama, Nature Photonics **5**, 494 (2011).
[28] M. Gullans, T. Tiecke, D. Chang, J. Feist, J. Thompson, J. Cirac, P. Zoller, and M. Lukin, Phys. Rev. Lett. **109**, 235309 (2012).
[29] B. Juliá-Díaz, T. Graß, O. Dutta, D. Chang, and M. Lewenstein, Nature Communications **4** (2013).
[30] D. Hayes, P. S. Julienne, and I. H. Deutsch, Phys. Rev. Lett. **98**, 070501 (2007).
[31] T. Caneva, T. Calarco, and S. Montangero, Phys. Rev. A **84**, 022326 (2011).
[32] J. P. Kestner and L.-M. Duan, New Journal of Physics **12**, 053016 (2010).
[33] H. P. Büchler, Phys. Rev. Lett. **104**, 090402 (2010).
[34] S. Sala, P.-I. Schneider, and A. Saenz, Phys. Rev. Lett. **109**, 073201 (2012).
[35] K. Jachymski, Z. Idziaszek, and T. Calarco, Phys. Rev. A **87**, 042701 (2013).
[36] N. Nygaard, P. Fil, and K. Mølmer, Phys. Rev. A **78**, 023617 (2008).
[37] P. S. Julienne, E. Tiesinga, and T. Köhler, Journal of Modern Optics **51**, 1787 (2004).
[38] S. J. J. M. F. Kokkelmans, J. N. Milstein, M. L. Chiofalo, R. Walser, and M. J. Holland, Phys. Rev. A **65**, 053617 (2002).
[39] C. Foot and M. Shotter, Am. Journ. Phys. **79**, 762 (2011).
[40] D. Leibfried, R. Blatt, C. Monroe, and D. Wineland, Reviews of Modern Physics **75**, 281 (2003).
[41] K.-K. Ni, S. Ospelkaus, M. H. G. de Miranda, A. Pe’er, B. Neyenhuis, J. J. Zirbel, S. Kotochigova, P. S. Julienne, D. S. Jin, and J. Ye, Science **322**, 231 (2008).
[42] T. Caneva, M. Murphy, T. Calarco, R. Fazio, S. Montangero, V. Giovannetti, and G. E. Santoro, Phys. Rev. Lett. **103**, 240501 (2009).