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Citation for published version (APA):

Document status and date:
Published: 01/08/2020

Please check the document version of this publication:
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Phonon-mediated spin-spin interactions between trapped Rydberg atoms

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(Dated: September 1, 2020)

We theoretically investigate the possibility of creating phonon-mediated spin-spin interactions between neutral atoms trapped in optical tweezers. By laser coupling the atoms to Rydberg states, collective modes of motion appear. We show that these can be used to mediate effective spin-spin interactions or quantum logic gates between the atoms in analogy to schemes employed in trapped ions. In particular, we employ Rydberg dressing in a novel scheme to induce the needed interaction, and we show that it is possible to replicate the working of the Mølmer-Sørensen entanglement scheme. The Mølmer-Sørensen gate is widely used in emerging quantum computers using trapped ion qubits and currently features some of the highest fidelities of any quantum gate under consideration. We find arbitrarily high fidelity for the coherent time evolution of the two-atom state even at non-zero temperature.

The quest for scalable, high fidelity quantum logic gates is on [1]. State-of-the-art quantum gates based on trapped ions show the best fidelities in the field of quantum logic. A notable quantum gate protocol, inspiring this work, is the so-called Mølmer-Sørensen (MS) gate [2–4], which uses trapped ions to create a quantum gate. It is based on phonon-mediated interactions, and in combination with the Hadamard- and π/2-gates the MS gate can be used to implement a C-NOT gate. This gate has been experimentally realized and has shown very high fidelities [5–10], but trapped ion gates lack in terms of scalability, as it is difficult to control many trapped ions. On the other hand, quantum gates using neutral, highly excited Rydberg atoms [11–18], constitute a much more scalable platform [19, 20], but show significantly lower experimental fidelities. Rydberg atom quantum gates rely on strong dipole-dipole interactions between electrically neutral Rydberg atoms to facilitate entanglement.

These considerations raise the question: “Can phonon-mediated interactions be used to implement quantum gates between neutral atoms in a similar way as between ions?” In this paper we will justify that the answer is "yes" and we present both a model and a recipe for the formation of maximally entangled Bell states of neutral atoms.

Phonon-mediated interactions between Rydberg atoms have been treated in a recently published paper by Gambetta et al. [21]. This work, however, focuses on multi-body interactions in optical lattices, while our paper focuses on phonon-mediated two-body interactions, and we demonstrate that these interactions can be made independent of the temperature of the atoms in direct analogy to the trapped ion case [22, 23].

Although the external degrees of freedom play a central role in the trapped ion quantum system, their use has not been fully explored in ultracold Rydberg platforms. The recent [21] work proposes the occurrence of non-binary interactions by electron-phonon coupling, while there has also been a number of works studying mediated interactions in self-assembled dipolar crystals e.g. [23–31]. Here we aim for a scalable high fidelity platform for the creation of Bell states using trapped, neutral, Rydberg-dressed rubidium atoms for our qubits, and rely on the strong dipole-dipole interactions to induce motion, like in the Mølmer-Sørensen trapped ion gate, where entanglement is achieved via phonon mediated interactions [23–31]. This is realized by transient mapping of the qubit states of the atoms onto a mode of collective motion. At the end of the sequence, the qubit state is disentangled from the motion again [24]. This phonon-mediated interaction, treated in the original MS paper [2], does not depend on the initial state of the phonon modes to lowest order. This makes for a reliable entanglement mechanism, even if the qubits are strongly coupled to a thermal reservoir [2], and can possibly be used as the basis for a two-qubit quantum gate.

Our approach starts with two (Rb) atoms with four distinct states each, two long lived states |g0⟩ and |g1⟩ and two Rydberg states |r0⟩ and |r1⟩, trapped in two well separated harmonic traps

\[ V = \frac{1}{2} m \nu^2 [(x_1 - l/2)^2 + (x_2 + l/2)^2] + V_{Ryd}(x_1 - x_2), \]

with \( x_j \) the position of atom \( j \), \( l \) the distance between the oscillator minima, \( m \) the mass of each atom and \( V_{Ryd}(x) = C_6/x^6 \) the state dependent, repulsive (in the case of rubidium \( nS \)-states) Rydberg-Rydberg van der Waals interaction. This can be rewritten in relative and center-of-mass (CM) coordinates

\[ V = \frac{1}{2} \nu^2 [m_r (r-l)^2 + m_R R^2] + V_{Ryd}(r), \]

where \( m_r = m/2 \) and \( r \) are the reduced mass \( m_1 m_2/(m_1 + m_2) \) and relative coordinates and \( m_R = 2m \) and \( R \) are the CM mass and coordinate.

In order to lift the degeneracy of the CM and relative modes, we will use Rydberg dressed qubit states. We
The interaction between the atoms and the laser light not only changes the internal state of the atom, but also their external state, i.e., the atoms gain momentum. Therefore we have to consider the full laser interaction Hamiltonian Eq. (3), including the exponential factors. Using the shorthand notation \( \theta_j = \eta_j (\hat{a}^\dagger + \hat{a}) - \omega_j t \), and projecting \( \hat{H}^{(1)} \) onto the basis

\[
S = (D_0, D_1, O, I) = \frac{1}{\sqrt{1 + \beta^2}} \begin{pmatrix}
0 & -\beta & 1 & 0 \\
-\beta & 0 & 0 & 1 \\
1 & 0 & 0 & \beta \\
0 & 1 & \beta & 0
\end{pmatrix},
\]

constructed from the dark and qubit states of \( \hat{H}^{(1)} \), we get

\[
S^{-1} \hat{H}^{(1)} S = \hbar \Omega \left( \beta (e^{-i\theta_0} - e^{-i\theta_1}) |D_0\rangle \langle O| + \beta (e^{-i\theta_1} - e^{i\theta_1}) |D_1\rangle \langle I| + e^{i\theta_1} |O\rangle \langle I| \right) + H.C.,
\]

ignoring terms higher than second order in \( \beta \), since a realistic setup would be \( n \approx 100 \), \( l \approx 3 \mu m \) and \( \nu \approx 2\pi \times 100 \text{kHz} \), we can expect \( \beta < 0.1 \), as we will explain below. Therefore neglecting these terms lead to errors on the order of 1%.

Additionally, assuming \( \eta \) to be small and taking the Lamb-Dicke approximation, we get

\[
\Phi = \exp \left[ -i \eta_k (\hat{a}^\dagger + \hat{a}) \right] - \exp \left[ -i \eta_l (\hat{a}^\dagger + \hat{a}) \right] \\
\approx i (\eta_k - \eta_l) (\hat{a}^\dagger + \hat{a}) - \frac{1}{2} (\eta_k^2 - \eta_l^2) (\hat{a}^\dagger + \hat{a})^2.
\]

We will here assume that \( \eta_0 \) and \( \eta_1 \) are not only small and comparable to \( \eta_0 \approx 0.05 \), but in fact of equal absolute value. This is not only desirable, but also easily realizable as the Lamb-Dicke parameter can be tuned.
for two-photon transitions. With counter propagating dressing lasers and with Lamb-Dicke parameters close to that of the ground state to ground state coupling, \( \eta_0 = \eta_g + \xi = -\eta_l \) (with dimensionless \( \xi << \eta_g \)), we can ensure that the exponential factors of the \( |D_0 \rangle \langle O | \) and \( |D_1 \rangle \langle I | \) terms in Eq. (7) are limited in absolute value, to leading order, by

\[
\Phi \approx \beta \xi |i(\hat{a} + \hat{a}^\dagger)^2| - \eta_g (\hat{a} + \hat{a}^\dagger)^2|  
\leq 0.001 |i(\hat{a} + \hat{a}^\dagger)^2|,  
\tag{9}
\]

which we can neglect, for reasonably low vibrational states i.e. the CM mode quantum number \( n_R < 10 \), as they contribute on the order of 1% to the Hamiltonian, leaving

\[
S^{-1} H^{(1)} S = \hbar \Omega e^{i(\eta_g (\hat{a} + \hat{a}^\dagger) - \omega_r^R)} |O \rangle \langle I | + H.C.  
\tag{10}
\]

With these approximations, \( H^{(1)} \) only cycles between the two-qubit states. Allowing for a detuning of the ground state to ground state coupling and one of the dressing lasers, we add \( D = -\hbar \Delta (|g_1 \rangle \langle g_1 | + |r_0 \rangle \langle r_0 |) \) to \( H^{(1)} \), resulting in the qubit detuning

\[
S^{-1} DS = -\hbar \Delta (|D_0 \rangle \langle D_0 | + |I \rangle \langle I |).  
\tag{11}
\]

This dressing makes the Van der Waals interaction between the two atoms independent of state, while having long life time compared to bare Rydberg atom qubits. The Van der Waals interactions will lift the degeneracy of the CM and relative modes of motion, as the oscillator frequency of the CM mode remains unchanged and the relative mode frequency increases. This results in a simplified Hamiltonian, in the absence of laser light,

\[
H_0 = \hbar \left[ \nu_r \left( \hat{a}_r^\dagger \hat{a}_r + \frac{1}{2} \right) + \nu \left( \hat{a}_R^\dagger \hat{a}_R + \frac{1}{2} \right) + \sum_{\sigma \in S} \omega_\sigma |\sigma \rangle \langle \sigma | \right],  
\tag{12}
\]

with \( \nu_r \) the relative mode oscillator frequency, \( \hat{a}_R \) (\( \hat{a}_r \)) and Hermitian conjugate are the CM (relative) mode ladder operators, the sum runs over the internal states and \( \hbar \omega_\sigma \) is the energy of state \( \sigma \).

The inter-particle Rydberg-Rydberg interaction will only affect the relative mode. The relative frequency and the shift in the relative minimum position are also a function of the trapping frequency \( \nu \) and the distance between the traps \( l \), and to fully characterize the mode splitting we have to take all four parameters \( \nu, l, C_0 \), and \( \beta \) into account. We introduce the dressed interaction strength

\[
W = \beta^4 C_0,  
\tag{13}
\]

since the strength of the interaction between Rydberg dressed atoms is scaled by \( \beta^4 \) [22].

Ideally we would like to achieve a splitting ratio \( \nu_r / \nu = \sqrt{3} \), as this would mimic to the ion-ion case. However, at the same time we have to minimize the shift in minimum position, realize sufficiently large life time (scaling with \( \beta^{-2} \)) and keep gate operation times low, therefore we have to consider splitting ratios smaller than \( \sqrt{3} \). We find that the splitting needs to be larger than 1.15, in order to make a reliable transfer with good fidelity.

For a given dressed interaction strength \( W \) only one local minimum exists in the potential Eq. (2) for (real) positive relative coordinate, see Fig. 2. This minimum is located at \( r_{\text{min}} \), which is the solution to

\[
r_{\text{min}}^8 - lr_{\text{min}}^7 - \frac{6 \hbar W}{\nu^2 m_r} = 0.  
\tag{14}
\]

Expanding the potential around this minimum, we find the splitting ratio \( f_{\nu} = \nu / \nu_r \) as

\[
f_{\nu} = \sqrt{8 - \frac{l}{r_{\text{min}}}}, \quad l > 0,  
\tag{15}
\]

which is shown in Fig. 2. Since \( r_{\text{min}} \) grows monotonically for increasing \( W \), the upper limit of the splitting fraction is \( \sqrt{3} \) and lower limit is 1. This gives us a large range of controllable splitting fraction, limited the distance between the single atom traps. Inversely, it is more convenient to determine what strength is needed to result in a sufficient splitting fraction and the shift in minimum position can then be determined as

\[
r_{\text{min}} = \frac{7l}{8 - f_{\nu}^2} , \quad l > 0,  
\tag{16}
\]

from which \( W \) can be derived, using Eq. (14). This treatment is limited by the validity of the harmonic approximation of the effective potential around the local minimum \( r_{\text{min}} \). However, for reasonable values of \( l \) and \( W \) the
approximation holds for a large range around the minimum and a large number of bound states are consistent with this approximation.

We induce spin-spin interactions by letting both qubits interact with bichromatic laser light, slightly detuned both above and below resonance. Including the photon recoil in the dressed frame, the effect of the laser light acting on both qubits, each with internal states $|O\rangle$ and $|I\rangle$ and trap states $|n_R, n_I\rangle$, where $n_R$ ($n_I$) is the CM (relative) mode vibrational quantum number, can be expressed in the two-qubit Hamiltonian

$$H^{(2)} = \sum_{k} \frac{\hbar \Omega_{kj}}{2} \sigma_{+,j} e^{-i\omega_{k} t} \times \exp \left[ i \eta_{kj} \left( \hat{a}_{R} \hat{a}_{R} + \frac{(-1)^{j} \sqrt{\nu}}{2} \left( \hat{a}_{I}^{\dagger} + \hat{a}_{I} \right) \right) \right] + H.C.,$$

(17)

where $k_j$ is used to label the laser beams interacting with the $j$ atom and $\sigma_{+,j}$ are the internal state step operator for atom $j$. We will use a sufficiently large mode splitting such that the relative mode is effectively frozen out. Changing to the interaction picture, we define the rotated creation operator

$$\hat{b}_{j} = e^{-i\omega_{j} t} \hat{a}_{R} - \frac{(-1)^{j} \sqrt{\nu}}{2} e^{-i\omega_{I} t} \hat{a}_{I},$$

(18)

where $j = 1, 2$ is the atom site number, and get the two-qubit interaction picture Hamiltonian

$$H_{I} = \frac{\hbar}{2} \sum_{j} \sum_{k_j} \Omega_{kj} e^{i\delta_{kj} t} \sigma_{+,j} e^{i\eta_{kj} \left( \hat{b}_{I}^{\dagger} + \hat{b}_{I} \right)} + \Omega_{kj} e^{-i\delta_{kj} t} \sigma_{-,j} e^{-i\eta_{kj} \left( \hat{b}_{I}^{\dagger} + \hat{b}_{I} \right)},$$

(19)

where $\delta_{kj} = \omega_{kj} - \omega_{O} + t$ is the detuning from the $|O\rangle \rightarrow |I\rangle$ transition. This Hamiltonian Eq. (19) reduces to a spin-spin interaction Hamiltonian. Assuming $\eta_{kj} = \eta, \Omega_{kj} = \Omega$ and $|\delta_{kj}| = \delta \approx \nu$, we can, in the Lamb-Dicke limit, simplify the interaction picture Hamiltonian

$$H_{I} \approx \frac{\hbar \Omega}{2} \sum_{k_j} e^{i\delta_{kj} t} \sigma_{+,j} \left[ 1 + i \eta \left( \hat{b}_{I}^{\dagger} + \hat{b}_{I} \right) \right] + H.C.,$$

which we further simplify by using

$$e^{i\delta_{kj} t} \hat{b}_{j} = e^{i\left( \nu - \nu \right) t} \hat{a}_{R} - \frac{(-1)^{j} \sqrt{\nu}}{2} e^{i\left( \nu - \nu \right) t} \hat{a}_{I},$$

(20)

and by neglecting fast rotating terms. This results in

$$H_{I} \approx \left[ 2 \hbar \cos(\delta t) J_{x} - \sqrt{2 \hbar \nu} \eta_{I} J_{y} \left( \cos(\nu t - \delta t) R + \sin(\nu t - \delta t)p_{R} \right) \right] - H_{r},$$

(21)

where $J_{x}$ and $J_{y}$ are collective spin operators, $p_{R}$ is the CM mode momentum operator and

$$H_{r} = \frac{\hbar m_{r} \nu}{2} \Omega_{r} \tilde{J}_{y} \left( \cos(\nu t - \delta t) R + \sin(\nu t - \delta t) \nu \right),$$

(22)

with $p_{r}$ the relative mode momentum operator, $\tilde{J}_{y} = \sigma_{y,2} - \sigma_{y,1}$ and $\eta_{r} = \sqrt{\nu} \eta_{r}$ the relative mode Lamb-Dicke parameter. If we ignore the fast rotating $J_{x}$ term, we can write the propagator by virtue of the Zassenhaus formula

$$U(t) = \exp \left[ -i \frac{\eta^{2} \Omega^{2}}{\nu - \delta} \tilde{J}_{y}^{2} A(t) \right] \exp \left[ -i \frac{\eta^{2} \Omega^{2}}{\nu - \delta} \tilde{J}_{y}^{2} B(t) \right] \times \exp \left[ -i \alpha_{R} \frac{\nu - \delta}{\nu} \tilde{J}_{y} \right] \times \exp \left[ -i \alpha_{R} \tilde{J}_{y} \right] \times \exp \left[ i \alpha_{R} \tilde{J}_{y} \right] \times \exp \left[ i \alpha_{R} \tilde{J}_{y} \right] \times \exp \left[ i \alpha_{R} \tilde{J}_{y} \right],$$

(23)

with $\alpha_{R} = \sqrt{\frac{2 m_{r} \nu}{\hbar}} \eta \Omega$ and $\alpha_{r} = \sqrt{\frac{2 m_{r} \nu}{\hbar}} \eta_{r} \Omega$. $A(t)$ and $B(t)$ can be determined from the Schrödinger equation similar to $A(t)$ in Eq. (9) of ref. [4].

At times $\tau_{k} = 2k\pi / (\nu - \delta)$ (with $k$ an integer), the propagator Eq. (23) reduces to that of a spin-spin Hamiltonian

$$U(\tau_{k}) \approx \exp \left[ -i \frac{\eta^{2} \Omega^{2}}{\nu - \delta} \tilde{J}_{y}^{2} A(\tau_{k}) - \frac{\eta^{2} \Omega^{2}}{\nu - \delta} \tilde{J}_{y}^{2} B(\tau_{k}) \right],$$

(24)

with exact equality if $\nu(\nu - 1) / (\nu - \delta)$ is an integer, however, the approximation always has merit if $\frac{\nu - \delta}{\nu - \delta} >> 1$.

We apply the Hamiltonian Eq. (19) in the time-dependent Schrödinger equation in the interaction picture with interaction picture state $\psi_{t}$ [34] [35]. We set the Rabi frequency such that

$$\Omega = \frac{\nu - \delta}{2\eta} \cdot (1 + \alpha) \cdot T(t),$$

(25)

with alpha being a small dimensionless number and

$$T(t) = \begin{cases} \sin^{2} \left( \frac{\tau_{t}}{2\tau_{c}} \right) & t < t_{s} \\ 1 & t_{s} < t < t_{p} - t_{s} \\ \cos^{2} \left( \frac{\tau_{t} + t_{p} - t_{s}}{2\tau_{c}} \right) & t_{p} - t_{s} < t < t_{p} \\ 0 & \text{otherwise} \end{cases}$$

(26)

is a ramping function with $t_{s}$ being the ramping time and $t_{p}$ is the length of the pulse. In the original MS
Our simulation shows reliable creation of Bell states, at all temperatures starting from all four of the internal two-qubit states. Tracing out the vibrational states, we find fidelities of Bell state creation to be higher than 0.999 for all input states even at non-zero temperature, under the approximations given above. We expect both the anharmonicity of the trap and non-magic trapping of the Rydberg part \cite{36} to influence the fidelity of the entanglement mechanism negatively: We estimate the trap quality issues to reduce the fidelity of Bell state creation by ~2%. Further we expect the finite life-time of the Rydberg-dressed qubits, which we estimate to influence the overall fidelity by ~1% for the 100S Rydberg level in rubidium-85. Additional losses and reductions in fidelity, due to neglected terms in the Hamiltonian are all below 1%, as they are all higher order in $\beta \sim 0.1$ or $\eta \sim 0.01$. By increasing the principal quantum number of the Rydberg level $n$ of the dressed qubits, we expect these approximations to have a smaller effect on the overall fidelities, as $\beta \propto n^{-11/4}$. The lifetime of the Rydberg-dressed state will also increase \cite{32,37,39} as $\beta^{-2n^3} \propto n^8 \sqrt{n}$ by neglecting black body radiation, which of course limits the lifetime, but is not detrimental to this analysis, and can be reduced by means of a cryostat. This leaves only the quality of the traps as a significant source of errors, which can not simply be reduced by a change of the dressing parameter, and we expect this will be the limiting factor.
Recent years have seen many implementations of single-atom traps, like optical tweezers [10-12], holographic trapping [13-14], photonic crystals trapping [15], cavity trapping [16-17], magneto optical traps [18] or magnetic microtraps [19-20]. Both magnetic microtraps and optical tweezer arrays [10-11] can be very tight with frequencies in the 10–100kHz and the separation of two trap sites is on the μm scale. This development of tight single-atom traps with high filling factors forms the main motivation of this paper to investigate the MS gate for dressed Rydberg atoms. An interesting future development would be to employ a trapped ion crystal to mediate interactions between atomic qubits. This would combine long-range Coulomb interactions with the favorable scaling properties of neutral quantum devices [50].

In this paper, we have shown that it should be possible to implement a Mølmer-Sørensen gate between two atoms trapped in tweezers. Combined with single qubit gates, the MS gate forms a universal set of quantum gates that has been implemented in trapped ions with very high fidelity [2-4]. Our work shows, that it should be possible to extend its use to neutral atomic systems, that have much better scalability prospects. We have shown that, by appropriate choices of Rydberg level and dressing parameters, it is possible to create maximally entangled states with qubits consisting of Rydberg-dressed atoms in a Boltzmann-distributed statistical mixture of oscillator states, with experimentally realistic laser parameters, and we have quantified the order of magnitude of the errors. Besides the quantum gate described in this work, the scheme may be beneficial for the creation of atomic quantum simulators of quantum spin models [51]. Here the tweezer setup offers in particular the benefit of creating nearly arbitrary trapping geometries [21].

During the preparation of this paper, we became aware of a related work by Gambetta et al. [21], which focuses on many-body interactions in tweezer arrays. Our work has been conducted independently of Gambetta et al. and focuses instead on two-body interactions.

**ACKNOWLEDGMENTS**

This research was financially supported by the Foundation for Fundamental Research on Matter (FOM), and by the Netherlands Organization for Scientific Research (NWO). We also acknowledge the European Union H2020 FET Proactive project RySQ (grant N. 640378). RG and SK acknowledge support by Netherlands Organization for Scientific Research (Vrije Programma 680.92.18.05). RG acknowledges support by the Netherlands Organization for Scientific Research (Vidi Grant 680-47-538 and Start-up grant 740.018.008).

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