Possibility of magic trapping of a three-level system for Rydberg blockade implementation

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The Rydberg blockade mechanism has shown noteworthy promise for scalable quantum computation with neutral atoms. Both qubit states and gate-mediating Rydberg state belong to the same optically trapped atom. The trapping fields, while being essential, induce detrimental decoherence. Here we theoretically demonstrate that this Stark-induced decoherence may be completely removed using powerful concepts of magic optical traps. We analyze magic trapping of a prototype three-level system: a Rydberg state along with two qubit states: hyperfine states attached to a J = 1/2 ground state. Our numerical results show that, while such a magic trap for alkali metals would require prohibitively large magnetic fields, the group IIIB metals such as Al are suitable candidates.

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I. INTRODUCTION

Multiparticle quantum gates have been successfully implemented in neutral atoms using the Rydberg blockade mechanism [1–4]. In this method, qubits are encoded in hyperfine sublevels of the electronic ground state in each atom. Gate operations utilize interactions between pairs of neutral atoms with a separation on the order of 10 μ m. At this range, ground-state atoms have negligible interactions, while Rydberg states interact strongly with each other. Blockade refers to the inhibition of excitation of a target atom by the prior excitation of another (control) atom. This can be used to entangle the qubits and execute CNOT gates, which in principle forms a universal set of two-qubit gates for arbitrary quantum computation.

Unfortunately, such a qubit implementation suffers from decoherence due to the trapping lasers. All three (two qubit and Rydberg) atomic levels are shifted via the Stark effect, leading to undesired differential phase accumulation. Even worse, the shift accumulation is uncontrollable as it depends on the local laser intensity, which varies as the atom moves in the trap.

This problem is similar to that encountered in optical lattice clock experiments. So-called magic traps were proposed as a powerful solution and have seen widespread use in clock experiments (see, e.g., reviews [5,6] and also [7,8]). Just as for neutral atom implementation of qubits, clocks depend on the transition frequency between two particular atomic energy levels. With a particular choice of trapping laser wavelength (and, in some cases, magnetic fields and polarization; see [5,9]), both levels experience the same shift regardless of laser intensity, so the perturbation from the trap effectively vanishes. Figure 1 depicts the level structure.

In the case of the alkalis, qubit transitions can be made Stark and Zeeman insensitive at a range of trapping wavelengths using a bias magnetic field tuned to a magic value, as described in Ref. [10]. The hyperfine structure of Al is also favorable for magic trapping, discussed in Refs. [9,11], and the formalism from Ref. [10] for alkalis is also applicable to Al. Thus the problem of removing decoherence for the qubit levels has already been solved.

However, excitation to a Rydberg level also causes decoherence of the qubit since in general the Rydberg trapping potential differs from the ground-state potential. This third level and additional source of decoherence must be addressed. Previous proposals have considered magic trapping for a two-level system, including a Rydberg state in alkalis [12] and in alkaline earths [13,14]. However, such treatments are not sufficient for the present problem, as the remaining Stark shifts of the qubit states would cause decoherence. We must therefore treat all three levels simultaneously. This problem is more akin to the situation in Ref. [9], which considered two-level systems in two species sharing the same trap.

Our goal in this paper is to find magic trapping conditions such that all three levels experience the same optical trapping potential. We begin by reviewing the Stark effect theory underlying such magic traps. We then present results of numerical calculations for Rb, Cs, and Al.

II. THEORY

A. Nonmagnetic states

We begin by summarizing the Stark effect formalism necessary for Rydberg states. This treatment is similar to that in Refs. [9,15] and references therein. The ac Stark shift of an atomic state $|nF, M_F\rangle$ with total angular momentum $\vec{F} = \vec{J} + \vec{I}$ and projection M_F can be written as¹

$$\delta E_{nFM_F}(\omega) = -\alpha_{nFM_F}^{\text{tot}}(\omega) \left(\frac{\mathcal{E}_L}{2}\right)^2, \qquad (1)$$

where \mathcal{E}_L and ω are the amplitude and frequency of the trapping laser field. The prefactor $\alpha_{nFM_F}^{\text{tot}}(\omega)$ is the total polarizability of the state; note that it depends on ω but not on \mathcal{E}_L . $\alpha_{nFM_F}^{\text{tot}}(\omega)$ may be decomposed using irreducible tensor operators as

$$\alpha_{nFM_F}^{\text{tot}}(\omega) = \alpha_{nF}^S(\omega) + (\hat{k} \cdot \hat{B}) \mathcal{A} \frac{M_F}{2F} \alpha_{nF}^a(\omega) + \frac{1}{2} (3|\hat{\epsilon} \cdot \hat{B}|^2 - 1) \frac{3M_F^2 - F(F+1)}{F(2F-1)} \alpha_{nF}^T(\omega).$$
(2)

Here \mathcal{A} is the degree of circular polarization ($|\mathcal{A}| \leq 1$), while α_{nF}^{S} , α_{nF}^{a} , and α_{nF}^{T} are the irreducible scalar, vector, and tensor

¹We use atomic units throughout unless noted otherwise.



FIG. 1. (Color online) Stark shifts affecting the Rydberg blockade three-level system (not to scale). Qubit levels $|0\rangle$ and $|1\rangle$ are hyperfine levels attached to the electronic ground state, while $|R\rangle$ is a Rydberg state. The unperturbed levels (solid) acquire a shift from the trapping laser. (a) For an arbitrary trapping laser, each state is shifted (dashed) by a different amount according to the local laser intensity. (b) With magic trapping conditions, all levels experience the same shift (dotted), and differential phase accumulation due to the trap vanishes.

polarizabilities, respectively. The unit vectors are the laser wave vector (\hat{k}), laser polarization ($\hat{\varepsilon}$), and bias magnetic field (\hat{B}). Their relative geometry is shown in Fig. 2. The bias magnetic field is a static, externally applied field which defines the quantization axis. This "quantizing magnetic field" guarantees that M_F remains a "good" quantum number for the ac Stark effect perturbation formalism, from which Eq. (2) follows.² For linearly polarized light, $\hat{\varepsilon} \cdot \hat{B} = \cos \theta_p$, where θ_p is the angle between the polarization and quantization unit vectors. If we consider circularly polarized light, defining $\hat{\varepsilon}$ using Jones calculus conventions, then $|\hat{\varepsilon} \cdot \hat{c}_z|^2 = \frac{1}{2} \sin^2 \theta_k$, where θ_k is the angle between the wave vector and quantization unit vectors.

Equations (1) and (2) determine our task: we must find ω and either θ_k or θ_p such that the Rydberg polarizability $\alpha_{Ryd}(\omega)$ and the qubit state polarizabilities $\alpha_{nFM_F}(\omega)$ and $\alpha_{nF'M_{F'}}(\omega)$ are all equal. Note that the polarizabilities in Eqs. (1) and (2) may be the conventional second-order quantities, as in Ref. [15], or they may be replaced with third-order hyperfine mediated polarizabilities, denoted β and described in detail in Ref. [8]. The second-order definition considers only the interaction with the external electric field, neglecting the hyperfine interaction. This is sufficient for matching Rydberg and ground-state polarizabilities, but it cannot be used to find magic conditions for the qubit levels. As shown in Ref. [8], if the hyperfine interaction is neglected, the qubit levels are degenerate and always experience the same shift, so any choice of ω and θ is trivially magic. Therefore a third-order treatment including hyperfine and external electric-field interactions is necessary for the qubit states.

For Rydberg states, the tensor polarizability is highly suppressed at optical frequencies [12,15], so the total polarizability is dominated by the scalar part, which is essentially equal to that of a free electron, $\alpha_{Ryd}^S(\omega) = -1/\omega^2$. Our *ab initio* numerical calculations confirmed this conclusion; see Sec. III below for details. Since α_{Ryd}^S has negligible dependence on geometry (either θ_k or θ_p), the magic trap frequency will be





FIG. 2. (Color online) Relation of angles to unit vectors in Eq. (2). (a) For linear polarization, \hat{k} , $\hat{\varepsilon}$, and \hat{B} are the laser wave vector, laser polarization, and quantization axis, respectively. θ_p is the angle between the polarization and the quantization axis, defined by the magnetic field. (b) For circular polarization, the relevant angle is θ_k , the angle between the wave vector and the magnetic field. (θ_p is no longer well defined as $\hat{\varepsilon}$ is time dependent.)

determined by $\alpha_{\text{Ryd}}^{S}(\omega) = \alpha_{nl_{1/2}}^{\text{tot}}(\omega)$, i.e., when the ground- and Rydberg state polarizabilities are equal.

Equations (1) and (2) also apply for qubit states in Al, with β in place of α as detailed above. Using Al in a linearly polarized trap, magic conditions for qubit transitions between nonmagnetic states will be set entirely by geometry. For the alkalis, magic trapping is not possible using nonmagnetic states, so we consider magnetic states below.

B. Magnetic states

Here we review the formalism to find magic conditions for qubit states with nonzero M_F projection. The methods developed above in Sec. II A are not sufficient to find magic conditions for the qubit transition in alkalis. As was shown in Ref. [8], magic conditions do not exist for the nonmagnetic hyperfine states. This is due to the smallness of α^T in comparison with α^S , along with the strict proportionality of $\alpha_{nF'M_{F'}}^S$ and $\alpha_{nFM_F}^S$. However, if we move to magnetic substates (with $M_F \neq 0$) we acquire unacceptable Zeeman sensitivity.

A solution to this problem was developed in Ref. [10]. Atoms with a J = 1/2 ground state are held in a circularly polarized trap to take advantage of vector polarizabilities. By utilizing multiphoton transitions between magnetic states with opposite projections (i.e., $|nF', M_F\rangle$ and $|nF, -M_F\rangle$) most of the first-order Zeeman shift goes away as these states have opposite electronic g factors.³ The remaining first-order shift is due only to the much smaller nuclear magnetic moment, which can be made to cancel the second-order shift with the application of a static magnetic field. The magic value of the

³Since J = 1/2, there are only two hyperfine states, and F' = F + 1.

B field is given by

$$B_m \approx \frac{g_I \mu_N M_{F'}}{2 |\langle nF, M_{F'} | \mu_z^e | nF', M_{F'} \rangle|^2} \,\omega_{\text{qubit}},\tag{3}$$

where ω_{qubit} is the energy splitting between the hyperfine levels. Although this expression for B_m is only accurate to second order, it agrees well with the exact answer [10].

Having dealt with Zeeman sensitivity, we turn to the Stark shift due to the trapping lasers. We need the differential shift between the qubit states to vanish, i.e., both states must experience the same shift. This condition is satisfied when [10]

$$\left(\beta_{nF'}^{s} - \beta_{nF}^{s}\right) + \delta\beta^{T} + \mathcal{A}\cos\theta_{k}M_{F'} \left[\left(\frac{1}{2F'}\beta_{nF'}^{a} + \frac{1}{2F}\beta_{nF}^{a}\right) + g_{I}\frac{\mu_{N}}{\mu_{B}}\left(\frac{B}{B_{m}}\right)\overline{\alpha}_{nl_{1/2}}^{a} \right] = 0.$$

$$(4)$$

Here β^S , β^a , and β^T are the third-order hyperfine mediated polarizabilities referred to above, while $\overline{\alpha}^a_{nl_{1/2}}$ is the conventional second-order polarizability. Note the distinction between coupling schemes used in $\overline{\alpha}^a_{nl_{1/2}}$ and α^a_{nF} . $\delta\beta^T$ absorbs lengthy prefactors. The full form is

$$\delta\beta^{T} = -\beta_{nF'}^{T} \frac{3M_{F}^{2} - F'(F'+1)}{2F'(2F'-1)} + \beta_{nF}^{T} \frac{3M_{F}^{2} - F(F+1)}{2F(2F-1)}.$$
(5)

 B_m is set by Eq. (3), while *B* is the actual applied field. Ideally $B = B_m$, but as suggested in Ref. [10] this is not always possible.

Clearly we need the third-order polarizabilities for the two states to cancel, but the appearance of the last term involving $\overline{\alpha}_{nl_{1/2}}^a$ may be surprising. It arises due to interference between the Zeeman shift and the vector part of the Stark shift, as these are both (axial) vector operators; see [10] for a full discussion. Although $\mu_N \ll \mu_B, \overline{\alpha}_{nl_{1/2}}^a \gg \beta_{nF}^T$, so this term is of a comparable order of magnitude and must be included in Eq. (4).

Evaluating Eq. (3) with representative values, we find that B_m is on the order of a few G. This relatively large magnetic field may adversely impact the blockade interactions. A detailed treatment of these effects is beyond the scope of this paper. However, the case of Zeeman degenerate states is treated in Ref. [16], and a qualitatively similar approach should suffice to calculate the effect of B_m on the blockade.

III. NUMERICAL EVALUATION

We used the same codes as in Ref. [9] for the ground states in all atoms considered. To summarize, we use the B-spline technique to generate a quasicomplete set of orbitals that are solutions to the Dirac-Hartree-Fock equations. To refine these solutions, we find the second-order self-energy operator to build the so-called Brueckner orbitals. Matrix elements are then calculated using the relativistic random-phase approximation.

For the Rydberg state calculations, we extended and modified our *B*-spline codes; the original codes are described in detail in Ref. [17]. To generate a complete basis set including physically accurate Rydberg states, we dramatically increased the size of the cavity and the number of basis functions. As an illustration, a typical run to calculate low-lying states uses \sim 40 splines in a \sim 50*a_B* cavity. For calculations aimed at the

50s state, we obtained accurate results using \sim 200 splines in a \sim 8000 a_B cavity. We also used a logarithmic rather than an exponential distribution of spline knots. This increased the accuracy of matrix elements by improving the representation of wave functions at large *R* near the cavity wall.

Correlations were included by building the self-energy operator using a small basis set (~40 splines in a ~50 a_B cavity) and using this potential to build Brueckner orbitals for a large set. This is justified since the self-energy operator diminishes rapidly outside the core, so highly excited states have a negligible contribution. Neglecting these states decreases calculation time dramatically. Inclusion of correlations introduced small but detectable corrections to Rydberg state energies and matrix elements. Corrections were around the fourth significant figure for n = 50 states and diminished with increasing n.

IV. RESULTS

We first present results for ⁸⁷Rb. This isotope has nuclear spin I = 3/2, and we are interested in transitions between the $|F' = 2, M_{F'} = 1\rangle$ and $|F = 1, M_F = -1\rangle$ qubit states attached to the $5s_{1/2}$ electronic ground state. The hyperfine splitting is 6.83 GHz, and from Eq. (3), $B_m \approx 3.25$ G [10]. In Fig. 3 we plot α_{Ryd} , $\alpha_{5s_{1/2}}^S$, and the ratio B/B_m . To achieve magic trapping using the scheme above, we require $|B/B_m| \leq 1$ in Eq. (4). If $|B/B_m|$ is slightly greater than 1, "nearly magic" trapping is possible as considered in Ref. [10]. But in this case, B/B_m diverges near ω_m , and the necessary B to achieve Stark-insensitive trapping is prohibitively large. The reason for this divergence can be seen from Eq. (4) by solving for B/B_m :

$$\frac{B}{B_m} = -\frac{\mu_B}{g_I \mu_N \overline{\alpha}^a_{nl_{1/2}}} \left[\frac{\left(\beta^s_{nF'} - \beta^s_{nF}\right) + \delta \beta^T}{\mathcal{A} \cos \theta_k M_{F'}} + \left(\frac{1}{2F'} \beta^a_{nF'} + \frac{1}{2F} \beta^a_{nF}\right) \right].$$
(6)

As B/B_m is inversely proportional to $\alpha_{5s_{1/2}}^a$, this ratio diverges wherever $\alpha_{5s_{1/2}}^a$ is zero. The situation is qualitatively the same for ¹³³Cs; our numerical calculations show a similar divergence near ω_m . For the lighter alkalis, there are no doubly magic or nearly magic points for the qubit transition.

Since it is not possible to build a magic three-level trap with the alkalis, we need another candidate. Alkaline-earth atoms and similar divalents are a popular choice for many cold-atom trapping experiments, but they have J = 0 ground states (zero electronic angular momentum). They therefore lack hyperfine structure and are unsuitable for our trapping scheme. Instead, we turn to ²⁷Al. It has been successfully laser cooled [18], and as was shown in Ref. [11], magic trapping of its hyperfine states is aided by comparatively large tensor polarizabilities. This is because the ground state $3p_{1/2}$ is part of a fine-structure multiplet $(3p_{1/2} \text{ and } 3p_{3/2})$: the presence of this nearby state leads to terms with small energy denominators in the perturbation theory expressions for α , but due to angular selection rules these terms enhance only α^T and not α^S .

With nuclear spin I = 5/2, we consider the $|F' = 3, M_{F'} = 1$ and $|F = 2, M_F = -1$ qubit states attached to the $3p_{1/2}$ electronic ground state. The hyperfine splitting is 1.506 GHz,



FIG. 3. (Color online) Polarizabilities of the 5*s* state (dashed), the Rydberg state (solid), and the ratio B/B_m (lower frame) for the hyperfine transition $|F = 2, M_F = 1\rangle$ to $|F = 1, M_F = -1\rangle$ in ⁸⁷Rb. Since $\alpha_{5s}^a \ll \alpha_{5s}^s$, the magic ω simply occurs where $\alpha_{Ryd} = \alpha_{5s_{1/2}}^s$ at approximately $\omega = 0.1062$ a.u. ($\lambda = 429$ nm). B/B_m is obtained from Eq. (4). Near the circled magic ω , B/B_m diverges, so magic trapping is impossible.

and Eq. (3) gives $B_m \approx 4.32$ G. We may use either a linearly or circularly polarized trapping laser. In the case of a linearly polarized trap, the situation is closely analogous to that in Ref. [9]. The magic wavelength is set where $\alpha_{\text{Ryd}} = \alpha_{3p_{1/2}}^S$, near $\omega = 0.121$ a.u. ($\lambda = 377$ nm). The enhanced tensor polarizability all but guarantees that the qubit transition can be made magic. Numerical calculations show that this does occur with a magic angle $\theta_p \approx 65^\circ$.

For a circularly polarized trap, no divergence of B/B_m occurs near the magic frequency ω_m as for the alkalis. However, the magic condition is more complex, as the ground-state second order $\alpha^a_{3p_{1/2}}$ is not negligible compared with $\alpha^s_{3p_{1/2}}$. The total second-order polarizability of the ground state is given by Eq. (2).⁴ This must equal the Rydberg polarizability, leading to

$$\alpha_F^S(\omega) + \mathcal{A}\,\cos\theta_k \frac{M_F}{2F} \alpha_F^a(\omega) = \alpha_{FM_F}^{\text{Ryd}}(\omega). \tag{7}$$

Our choice of ω and θ_k must simultaneously satisfy Eqs. (4) and (7). We may solve for $M_F \mathcal{A} \cos \theta_k$ appearing in Eqs. (4)



FIG. 4. (Color online) Left-hand side (solid) and right-hand side (dashed) of Eq. (8). The range for magic trapping of the Rydberg transition is given by Eq. (7) and lies between the resonance at $\omega = 0.1155$ a.u. ($\lambda = 394$ nm) and the dotted line at $\omega = 0.121$ a.u. ($\lambda = 377$ nm). The magic frequency and magic angle for the qubit transition are set by the curves' intersection, just under $\omega = 0.121$ a.u. This combination of ω_{magic} and θ_{magic} will allow Stark and Zeeman insensitive trapping for the three-level system in Al.

and (7) and equate the results, giving

$$2F'\frac{\omega^{-2}+\alpha_F^S}{\alpha_F^a} = \frac{\beta_{F'}^s - \beta_F^s + \delta\beta^T}{\frac{1}{2F'}\beta_{F'}^a + \frac{1}{2F}\beta_F^a + g_I\frac{\mu_N}{\mu_B}\frac{B}{B_m}\overline{\alpha}_{np_{1/2}}^a}.$$
 (8)

We plot the left- and right-hand sides of Eq. (8) in Fig. 4. Since they intersect in the range allowed by Eq. (7), magic trapping for this three-level system in Al is possible. While circularly polarized trapping would be more complex than the linearly polarized trap presented above, it has the additional advantage of less Zeeman sensitivity. This is because the magic *B* field removes Zeeman effects to second order, while the linearly polarized trap only removes Zeeman decoherence to first order in the *B* field.

V. CONCLUSION

We have presented a method to remove differential Stark shifts for a three-level atomic system consisting of a Rydberg state and two hyperfine states attached to the ground electronic state. Such a system is an essential element of the CNOT gates utilizing the Rydberg blockade mechanism. Although such a trap is not possible for the alkalis, our numerical calculations show that Al may be trapped using this method. Such a trap could prove useful for removing decoherence from trapping lasers in implementing the Rydberg blockade mechanism. It is worth noting that this scheme is possible thanks to the presence of fine-structure levels near the ground state. Since the majority of atoms share this structure, as laser cooling techniques advance, this style of magic trapping could be adopted for many atomic species.

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 $^{{}^{4}\}alpha^{T}$ is identically zero as J = 1/2.

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