Intensity landscape and the possibility of magic trapping of alkali Rydberg atoms in infrared optical lattices

Turker Topcu and Andrei Derevianko

Department of Physics, University of Nevada, Reno, NV 89557, USA

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Motivated by compelling advances in manipulating cold Rydberg (Ry) atoms in optical traps, we consider the effect of large extent of Ry electron wave function on trapping potentials. We find that when the Ry orbit lies outside inflection points in laser intensity landscape, the atom can stably reside in laser intensity maxima. Effectively, the free-electron AC polarizability of Ry electron is modulated by intensity landscape and can accept both positive and negative values. We apply these insights to determining magic wavelengths for Ry-ground-state transitions for alkali atoms trapped in infrared optical lattices. We find magic wavelengths to be around 10 μm, with exact values that depend on Ry state quantum numbers.

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Magic trapping [1] of cold atoms and molecules is a powerful technique that has recently enabled ultrastable optical lattice clocks [2,4], long-lived quantum memory [5], and precision manipulation of ultracold molecules [6]. When neutral atoms are trapped, their internal energy levels are necessarily perturbed by spatially inhomogeneous trapping fields. For a cold atomic cloud, typical mK temperatures translates into the 10 MHz trap depths. In other words, as the atom travels about the trap, its energies are modulated at the 10 MHz level with associated coherence times of just 100 ns. If it were not for magic trapping techniques, such decoherences would be prohibitive for the enumerated cold-atom applications. The key idea of magic trapping is the realization that one is interested in differential properties of two levels, such as the clock frequency or a differential phase accumulated by two qubit states. Then if the trapping field affects both levels in the very same way, the differential perturbations vanish. Such engineered traps are commonly referred to as “magic”. These ideas enabled precision clock spectroscopy at the sub-100 mHz level [7] and second-long coherence times [8], orders of magnitude better than the quoted “non-magic” values.

Application of magic trapping techniques to Rydberg (Ry) states of alkali atoms has turned out to be challenging. Generic quantum-information protocols involve qubits encoded in hyperfine manifolds of the ground state (GS) and conditional multiqubit dynamics mediated by interactions of Ry states [9–11]. Therefore, the trapping field must be magic both for the GS hyperfine manifolds and also for the GS-Ry transition [11]. The first part by itself is a non-trivial problem and has been a subject of several studies [9,12–14]. The GS-Ry transition presents another challenge [11,15,16].

To appreciate the problem, let us first review commonly invoked arguments. In optical fields, the trapping potential is proportional to the AC polarizability \( \alpha(\omega) \), leading to trapping potential \( U(R) = -\alpha(\omega) F^2(R)/4 \), where \( F \) is the local value of the electric field [32]. The GS polarizability \( \alpha_g(\omega) > 0 \) when red-detuned from atomic resonances, and the atoms are attracted to intensity maxima. On the other hand, loosely-bound Ry electron is nearly “free”; therefore its polarizability \( \alpha_r(\omega) \approx -1/\omega^2 \) is negative and the atoms are pushed towards intensity minima. Then as the GS population is driven to a Ry state during gate operations, an atom experiences time-varying trapping potential. This causes undesirable motional heating. The resulting decoherence is so severe that experimentalists simply turn off trapping fields during GS-Ry excitations [10,17,18]. This process is also detrimental because this again leads to heating. Such “pulsed” operation of the trap is the leading heating mechanism in gate experiments, with heating rate of \( \sim 1\% \) per gate cycle [17]. In addition, there is a problem of scalability: it is impossible to turn off the trapping field at individual trapping sites, therefore the entire ensemble becomes heated during pulsed trap operations [18].

One way to evade the AC Stark shifts is to use blue detuned bottle beam traps [19]. Here, the atoms are trapped in intensity minima. Experimentally, such a multi-trap setup is arguably more challenging than using optical lattices as discussed below.

Because of the GS-Ry polarizability sign difference, it is usually accepted that magic trapping in red-detuned fields is unattainable (see however Ref. [20] for evidence to the contrary). Here we present clear arguments that Ry atoms can in fact be attracted to intensity maxima, and demonstrate trapping of GS and Ry state in red detuned magic infrared lattices.

We start by presenting a qualitative argument (see Fig. 1) that makes the underlying physics transparent. First of all one realizes that Ry wave function is spread over large distances that can be comparable to spatial scale of the laser intensity variations. For example, for a lattice formed by CW lasers of wavelength \( \lambda \), the laser intensity is spatially modulated with a lattice constant \( \lambda/2 \): \( F^2(z) = F_0^2 \sin^2(k z) \), \( k = 2\pi/\lambda \). Ry orbit is larger than the lattice constant if its principal quantum number \( n > \sqrt{3}a_0 \), e.g., \( n \gtrsim 100 \) for \( \lambda = 10\mu m \). As a result, the ponderomotive potential experienced by the nearly free electron must be averaged over local field in-
Here the frame, size and the lattice constant can be made for a 1D optical core, and (a), the slope, intensity minimum and is proportional to the local intensity dipole force exerted on each lump is directed towards nearby (unstable equilibrium). When 2\(z_e > \lambda/4\) (panel (b)), they act as restoring forces, with Ry atom stably resting at the intensity maximum.

There are two distinct contributions, \(U_i(Z) = U_0^0 + U_0^2 \sin^2(kZ)\): the \(U_0^0\) term is a uniform shift across the lattice and the second contribution is proportional to the standing wave intensity. The uniform offset does not affect atomic motion as it does not contribute to the force. The lattice depth prefactor, \(U_0^2 = F_0^2/4\omega^2\) shows that the atoms are attracted to lattice nodes if \(\cos(2kz_e) > 0\), i.e. when \(p - 1/4 < 2z_e/\lambda < p + 1/4\), \(p = 0, 1, 2, \ldots\). Otherwise, atoms reside at antinodes. At critical values \(2z_e/\lambda = (p+1/2)/2\), the trapping potential vanishes altogether and the atom travels through the lattice uninhibited. These observations are consistent with our dipole force analysis in Fig. We as increase the principal quantum number and the orbit grows larger, the atoms initially stably reside at nodes. Then as \(2z_e\) reaches \(\lambda/4\), the atoms move freely, and then are pushed towards the anti-nodes. This pattern repeats itself with further increase in the Ry orbit size.

Having qualitatively understood the nature of various trapping regimes, we now proceed with a rigorous evaluation of trapping potentials for realistic Ry atoms [23]. One starts with the Hamiltonian \((p_e - A/c)^2/2\), where \(p_e\) is the electron momentum and \(A\) is the vector potential. Upon expanding the square, we encounter the kinetic energy term, \(p_e \cdot A\) cross terms and an \(A^2\) contribution. It is the \(A^2\) term in the Coulomb gauge that leads to the ponderomotive potential, and in the lowest order perturbation theory we recover Eq. [21]. Further discussion of the validity of this approximation can be found in [23].

Explicitly evaluating the integral [21], we find that the Ry atom potential in a 1D lattice is identical to that of our toy problem in Eq. [3], but with potential shift and depth redefined in terms of expectation values

\[
U^r(x) = \frac{F_0^2}{4\omega^2} \langle nlm | \cos(2kz_e) | nlm \rangle \equiv -\alpha^{lsc}_r(\omega) \frac{F_0^2}{4},
\]

\[
U^0_r(x) = -\alpha^{lsc}_r(\omega) - \alpha_r(\omega) \frac{F_0^2}{4},
\]

Fig. 1: (Color online) Influence of Ry orbit size on stability of atomic motion at the 1D lattice anti-node for a toy model of Ry atom. The vertical axis is the laser intensity \(I(z)\). Electron cloud is localized in two “lumps”. The optical dipole force exerted on each lump is directed towards nearby intensity minimum and is proportional to the local intensity slope, \(dI(z)/dz\). When the Ry orbit size \(2z_e < \lambda/4\) (panel (a)), the \(f_L\) and \(f_R\) acting on the localized “lumps” of electron density pull the atom away from the intensity maximum (unstable equilibrium). When \(2z_e > \lambda/4\) (panel (b)), they act as restoring forces, with Ry atom stably resting at the intensity maximum.

\[
U(R) = \frac{1}{4\omega^2} \int d^3r_e \left| \Psi(r_e) \right|^2 F^2(R + r_e).
\]
for a Ry state \(|nlm\rangle\). Here we introduced the effective intensity landscape-averaged polarizability \(\alpha^\text{loc}(\omega) = -\langle \cos(2kz_r) \rangle / \omega^2\), which unlike the free electron polarizability, \(\alpha_e = -1/\omega^2\), can accept both positive and negative values. One can view \(\alpha^\text{loc}(\omega)\) as landscape-modulated free-electron polarizability as \(\alpha^\text{loc}(\omega) = \langle \cos(2kz_r) \rangle \alpha_e(\omega)\) and \(|\alpha^\text{loc}(\omega)| \leq |\alpha_e(\omega)|\).

The optical potential is \(U_r(Z) = U_r^0 + U_r^Z \sin^2(kZ)\). As in our toy model, the potential consists of a term that depends on the position of the atom in the lattice and a uniform offset \(U_r^0\). Note that without properly accounting for the finite size of Rydberg cloud, one would conventionally write \(U_r^\text{conv}(Z) = P_0^2/(4\omega^2) \sin^2(kZ)\). The two potentials, conventional and ours, are equal only in the limit \(\langle r_e \rangle \ll \lambda\) as \(U_r^0 \to 0\), and \(U_r^Z \to P_0^2/(4\omega^2)\) in this limit. Our potential can support stable equilibrium in lattice anti-nodes, while the conventional potential does not.

The expectation value of \(\cos(2kz_r)\) can be evaluated by expanding \(\cos(2kz_r)\) over spherical Bessel functions. For example, for \(l = 0\) states,

\[
\langle n| \cos(2kz_r)|n\rangle = \int_0^{\infty} dr_e P_{ns}(r_e) j_0(2kr_e).
\]

Here \(P_{ns}(r_e)\) is the radial wave function of Ry electron; we computed \(P_{ns}(r_e)\) using well-known model potentials \cite{26}.

\[\text{FIG. 2: The “landscape-modulated” polarizability } \alpha^\text{loc} \text{ for } n \text{-states of Rb with } n = 100 \text{ (dashed orange), } 160 \text{ (dashed black) and } 180 \text{ (dashed blue). The scalar ground state polarizability } \alpha_s \text{ (solid red) and the free electron polarizability } \alpha_e \text{ (dashed gray) are also shown. The magic wavelengths can be found for all } n \geq 154 \text{ in the infrared wavelength range spanning the CO}_2\text{ and the frequency-doubled CO}_2\text{ laser bands.}
\]

Our computed landscape-averaged polarizabilities for several Ry states are shown in Fig. 2. For all the Ry states, \(\alpha^\text{loc}\) is essentially zero at wavelengths below \(\sim 1000\) nm and starts oscillating with increasing amplitude before dropping off like \(\alpha_e(\omega)\).

By recasting \(\alpha^\text{loc}(\omega) = -(1 - 2\langle \sin^2(kz_e) \rangle) / \omega^2\), one could conclude \(\alpha^\text{loc}(\omega) \approx 0\) for \(\lambda \ll \langle r_e \rangle\), so that \(\alpha^\text{loc} \approx 0\). As \(\lambda\) is increased, \(kz_e\) gets smaller and \(\langle \sin^2(kz_e) \rangle\) becomes smaller than \(1\). This explains the short- and long-wavelength behavior of \(\alpha^\text{loc}(\omega)\) in Fig. 2. As to the \(n\)-dependence of \(\alpha^\text{loc}\), one could show on general grounds that \(\langle \cos(2kz_r) \rangle = f((n*)^2 \alpha_0 / \lambda)\), where \(f\) has some universal function of the effective quantum number \(n^*\). Thus our discussion is applicable to all Ry atoms.

A possible detrimental effect on the gate fidelity can arise if the wavefunctions of the Ry atoms trapped at adjacent lattice sites start to overlap. In order to avoid such overlaps, one can fill in the optical lattice by leaving empty lattice site(s) between trapped atoms. Such experimental capabilities have been demonstrated \cite{25}.

Furthermore, the Rydberg blockade mechanism, central for the gate operations relies on the repulsive long-range interaction \cite{27}. Penning ionization requires close approach of two atoms, so the rate is suppressed. As experimentally shown in Ref. \cite{28}, since the collisional ionization requires attractive potentials, the Ry states first need to be redistributed (mainly by black body radiation \cite{26}) to populate Ry states that would correlate to attractive molecular potentials at long range. Therefore decoherence rates due to ionization is limited from above by the BBR-induced decoherences. BBR-induced decoherence were studied in \cite{17}: at room temperature Ry-state lifetime is greater than 0.1 ms for \(n > 65\). Thereby, collisional ionization being the secondary step, is not an issue for Ry gates.

Now since \(\alpha^\text{loc}(\omega)\) can become positive, we show that the GS and Ry potentials can be matched at red-detuned “magic” wavelengths. For the GS atoms, the trapping potential reads

\[
U_g(Z) = -\frac{P_0^2}{4} \alpha_g(\omega) \sin^2(kZ),
\]

with the dynamic polarizability \((D\text{ is the dipole operator and } E_i \text{ are atomic energy levels})

\[
\alpha_g(\omega) = \sum_i \frac{(E_g - E_i)(\langle \psi_g | D | \psi_i \rangle)^2}{(E_g - E_i)^2 - \omega^2}.
\]

We evaluated \(\alpha_g(\omega)\) with a high-accuracy procedure \cite{29}.

The two spatial parts of Ry and GS potentials match when \(U_r^Z = U_g^Z\), which is attained at “magic” values of laser frequencies \(\omega^*\) when \(\alpha_g(\omega^*) = \alpha^\text{loc}(\omega^*)\). In Fig. 2, we plot both polarizabilities to search for such magic wavelengths \(\lambda^*\). We find that for Rb \(ns\) states the two curves cross for all \(n \geq 154\) with \(\lambda^* \approx 5600\) nm for \(n = 154\). Above this critical value of \(n\), there are at least two values of \(\lambda^*\) (e.g., \(\alpha^\text{loc}\) for the 160s and 180s states cross twice with the GS polarizability). The number of \(\lambda^*\)‘s increases further with increasing \(n\). Table I lists \(\lambda^*\) for Rb and Na atoms. In addition to the \(l = 0\) states, Table II lists \(\lambda^*\) for the \(l = 1\) and \(l = 2\) states (all \(m = 0\)).

All these \(\lambda^*\) are in the \(\text{CO}_2\) and the frequency-doubled \(\text{CO}_2\) laser bands. This provides an advantage of individual lattice-site addressing \cite{30}. These wavelengths are
far from any resonances which reduces photon scattering rate.

In a trap red-detuned from the Rb 5s – 6p resonance but blue-detuned from the 5s – 5p resonance, the ground state polarizability is negative and can be matched to the free-electron polarizability. This allows for a λ* ≈ 432 nm [13][16]. However, this magic wavelength being very close to the 5s – 6p resonance can lead to enhanced photon scattering and heating. Even then, as the “landscape averaging” reduces the free-electron polarizability employed in [16], the feasibility of working at that lattice wavelength needs to be revised. Our calculations show (see Fig. 2) that for n = 100 at λ* ≈ 432 nm, α^Re(λ*)/α^Re(ω*) ≈ 3 × 10^-3, a substantial suppression factor. This reduces the trapping depth and to make up for the suppression the laser intensity would need to be increased by a factor of 360.

In quantum gate protocols such as the CNOT gate, the conditional logic requires driving a π-pulse transition between one of the qubit (ground) states and a Ry state. Although both the qubit and the Ry states see the same trapping potentials in magnetic lattices, the differential energy shift between these states does not vanish because of the uniform offset term (Eq. [3]). Drifts in the lattice laser intensity introduce an error Δω in the Rabi frequency Ω. This error in the actual Rabi frequency Ω leads to the fractional error in GS-Ry rotation angle: Δφ/π ≈ (Δω/Ω)^2/2. For Rb, we estimate this error to be Δφ/π = 25 (λ/1000 nm)^4 (1 MHz/Ωo)^2 (λ/1000 nm)^4 (150 a.u./α_s)^2, where δI/I is the fractional intensity fluctuation and U is the trap depth. For example, when δI/I = 10^-4 for a 0.16 mK deep trap, Ωo/2π = 1 MHz, and 1000 nm lasers, Δφ/π = 6.5 × 10^-9. For CO2 wavelengths the errors are below 10^-4, which is considered to be tolerable [31].

Finally, although we focused on the magic trapping on the Ry-GS transition, simultaneous magic trapping on the qubit transition can be also carried out. For example, techniques employing additional compensating CW traveling laser wave [3] are fully compatible with our proposal. Indeed, since the intensity profile of a traveling wave is uniform in space, it does not affect the spatially-varying part of optical potentials.

We have demonstrated that although nominally the Ry state AC polarizability is essentially that of a free electron and always negative, laser intensity landscape can profoundly affect the effective “landscape-averaged” polarizability and can lead to positive values of polarizability. “Landscape-averaging” depends on the relative size of Ry orbit and the lattice constant in a non-monotonic way. A Ry atom can be attracted to intensity maxima. This opens up the possibility of magic trapping of Ry atoms in infrared lattices. The separation between adjacent atoms at these IR wavelengths is comparable to Ry blockade radius of a few microns, which provides an additional convenience for Ry gate experiments utilizing dipole blockade mechanism.

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TABLE I: Magic wavelengths (nm) for Rydberg states of Na and Rb atoms. l = 0, 1, 2 and m = 0.

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[32] Unless specified otherwise, atomic units, $|e| = \hbar = m_e \equiv 1$ are used throughout the paper