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

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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 ultra-stable optical lattice clocks [2,3], long-lived quantum memory [6], and precision manipulation of ultracold molecules [6]. When neutral atoms are trapped, their internal energy levels are necessarily perturbed by spatially inhomogeneous trapping fields as the gradients of position-dependent energy-shifts determine mechanical forces on the atoms. 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, in practice, one is interested in differential properties of two atomic levels, such as the clock transition frequency or a differential phase accumulated by two qubit states. Then if the trapping field affects both levels of interests in the very same way, the differential perturbations vanish. The parameters of such engineered traps are commonly referred to as “magic”. These ideas enabled precision clock spectroscopy at the sub-100 mHz level [2] and second-long coherence times [3], orders of magnitude better than the quoted “non-magic” values.

Application of magic trapping techniques to Rydberg (Ry) states of widely-used 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 long-range interactions of Ry states [7–10]. 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 [5,12,13]. The GS-Ry transition presents another challenge [11,14,18].

To appreciate the problem, let us first review commonly invoked arguments. In off-resonant optical fields, the AC Stark shift and thereby the trapping potential is proportional to the dynamic polarizability α(ω), leading to trapping potential $U(R) = -\alpha(\omega)F^2(R)/4$, where $F$ is the local value of the electric field [20]. For conventionally-used lasers, 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 it’s polarizability $\alpha_r(\omega) \approx -1/\omega^2$ is negative and now the atoms are pushed by optical dipole forces 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 the atom becomes untrapped during this operation.

Because of the GS-Ry polarizability sign difference, it is usually accepted that magic trapping in red-detuned fields is unattainable. The prevailing view is that Ry atoms are always expelled from maxima of laser intensity. Here we demonstrate that the above arguments are overly simplified and these conclusions must be substantially revised, and for sufficiently large Ry wave function extents, can be reversed.

Before proceeding with rigorous formalism, we present 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 an optical lattice formed by counter-propagating CW lasers of wavelength λ, the laser intensity of the standing wave is spatially modulated with a lattice constant $\lambda/2$: $F^2(z) = F_0^2 \sin^2(\kappa z)$, $\kappa = 2\pi/\lambda$. Ry orbit is larger than the lattice constant if its principal quantum number $n > \sqrt{3\alpha_0}/(2\kappa)$, e.g., $n \geq 100$ for $\lambda = 10\mu m$. As a result, the ponderomotive potential experienced by the nearly free electron must be averaged over local field intensities $18,20$,

$$U(R) = \frac{1}{4\omega^2} \int d^3r_e |\Psi(r_e)|^2 F^2(R + r_e).$$

(1)

Here $R$ is the position of atomic core (Rb+ ion for Rb...
atom) in the laboratory frame, \( r_e \) is the Ry electron coordinate relative to the core, and \( |\Psi(r_e)|^2 \) is the Ry electron probability density.

An illustration of the important interplay between the Ry orbit size and the laser intensity variations length scale can be made for a 1D optical lattice and a toy model of a Ry atom, (see Fig. 1). Here \( |\Psi(z_e)|^2 \) is localized in two “lumps” positioned symmetrically (at relative distances \( \pm z_e \)) about the core. This toy model resembles a cross-section of a Ry atom in a circular state \([21]\). The optical-dipole force acting on each lump is transferred to the core by the Coulomb interaction, so that the net force the atom experiences no net force regardless of displacement. However, as the size of the Ry orbit is increased, \( 2z_e > \lambda/4 \) the atom stably resides in intensity maxima. This is a crucial point. As the atom is displaced in some direction the wave function lump on the side opposite to the displacement experiences larger dipole-force tug towards nearby node, resulting in a restoring force.

From this model, we can generalize to an arbitrary 3D laser intensity landscape: a Ry atom is drawn to intensity maxima if in an equilibrium position \( \nabla I(\mathbf{r}) = 0 \) the bulk of the Ry wave function straddles outside of the nearby surface of inflection points in intensity landscape, parametrically given by \( \Delta I(\mathbf{r}) = 0 \). For example, for a 2D Gaussian intensity cone, \( I(x, y) = I_0 \exp(-\rho/\rho_0)^2 \), the radius of Ry orbit must be greater than \( \rho_0(\sqrt{3} - 1)/2\rho_0 \). Then a Ry atom can be attracted to the intensity maximum and its motion can be guided by the beam.

Further insight can be gained by explicitly computing trapping potential in our toy problem. Integrating over “lumps” in Eq. (1), we obtain

\[
U_t(Z) = \frac{F^2}{4\omega^2} (\sin^2(kz_e) + \cos(2kz_e)\sin^2(kZ)) \quad .
\]

There are two distinct contributions, \( U_t(Z) = U_t^0 + U_t^2 \sin^2(kZ) \): the \( U_t^0 \) term is a uniform Stark shift across the lattice and the second spatially-modulated contribution is proportional to the standing wave intensity. The uniform offset does not affect atomic motion as it does not contribute to the force \([22]\). The lattice depth prefactor, \( U_t^2 = F^2/4\omega^2 \cos(2kz_e) \) shows that the atoms are attracted to lattice nodes if \( \cos(2kz_e) > 0 \), i.e. when \( p - 1/4 < 2z_e/\lambda < p + 1/4 \). 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. 1. As we 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 of Ry atoms in inhomogeneous intensity distributions, we now proceed with a rigorous evaluation of trapping potentials for realistic Ry atoms in optical lattices \([22]\). 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. While usually neglected, 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. (1). Eq. (1) remains valid for field strengths where we could neglect the laser-field admixtures of other states. Such constraints can be easily satisfied \([18]\). The second-order contribution in the cross term \( p_e \cdot A \) leads to the traditional AC polarizability \( \alpha(\omega) \). For Ry states, the \( \alpha(\omega) \) contribution can be neglected compared to the ponderomotive potential when

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**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 dipole force exerted on each lump is directed towards nearby unstable equilibrium. When 2 \( z_e < \lambda/4 \) (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.

This is a crucial point. As the atom is displaced in some direction the wave function lump on the side opposite to the displacement experiences larger dipole-force tug towards nearby node, resulting in a restoring force.
away from resonances. For the GS, by contrast, the $\alpha(\omega)$ contribution dominates over the ponderomotive potential.

Explicitly evaluating the integral $\int$, 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

$$U_r^Z = \frac{F_0^2}{4\omega^2} |nlm| \cos(2kz_r)|nlm| \equiv -\alpha^{bc}_{lsc}(\omega) \frac{F_0^2}{4},$$

$$U_r^0 = -\frac{\alpha^{bc}_{lsc}(\omega) - \alpha(\omega)}{2} \frac{F_0^2}{4},$$

for a Ry state $|nlm\rangle$. Here we introduced the effective intensity landscape-averaged polarizability $\alpha^{lsc}_{bc}(\omega) = -\langle \cos(2kz_r) \rangle/\omega^2$, which unlike the free electron polarizability, $\alpha_e = -1/\omega^2$, can accept both positive and negative values. One can view $\alpha^{bc}_{lsc}$ as landscape-modulated free-electron polarizability as $\alpha^{bc}_{lsc} = \langle \cos(2kz_r) \rangle \alpha_e(\omega)$ and $|\alpha^{bc}_{lsc}(\omega)| \leq |\alpha_e(\omega)|$.

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 term $U_r^0$. It is worth emphasizing that without properly accounting for the finite size of Rydberg cloud, one would conventionally write $U_{conv}^r(Z) = F_0^2/(4\omega^2) \sin^2(kZ)$. The two potentials, conventional and ours, are equal only in the limit $r_e \ll \lambda$ as $U_r^0 \to 0$, and $U_r^Z \to F_0^2/(4\omega^2)$ in this limit. Spatial averaging of both potentials yields the same interaction energy of $F_0^2/(8\omega^2)$. The essential effect distinguishing the two cases is that 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,

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

Here $P_{ns}(r_e)$ is the radial wave function of Ry electron; we computed $P_{ns}(r_e)$ by directly integrating the one-electron Schrödinger equation using well-known quantum defect potentials [28].

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

The oscillating behavior of $\alpha^{bc}_{lsc}(\omega)$ seen in Fig. 2 was qualitatively captured by our toy model. That model breaks down for Ry wave functions with local wavelengths longer than the lattice wavelengths. Then by recasting $\alpha^{bc}_{lsc}(\omega) = -(1 - 2\langle \sin^2(kz_r) \rangle)/\omega^2$, one could conclude [29] that, $\langle \sin^2(kz_r) \rangle \approx 1/2$ for $\lambda \ll \langle r_e \rangle$, so that $\alpha^{bc}_{lsc} \approx 0$. As $\lambda$ is increased, $kz_r$ gets smaller and $\langle \sin^2(kz_r) \rangle \ll 1$ resulting in $\alpha^{bc}_{lsc} \to \alpha_e$. This explains the short- and long-wavelength behavior of $\alpha^{bc}_{lsc}(\omega)$ in Fig. 2.

We also explore the $n$-dependence of the modulation factor $\langle \cos(2kz_e) \rangle$ in Fig. 3.

Now since $\alpha^{bc}_{lsc}(\omega)$ 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

$$U_g(Z) = -\frac{F_0^2}{4} \alpha_g(\omega) \sin^2(kZ),$$

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

FIG. 3: Landscape modulation factor $\langle \cos(2kz_e) \rangle$ as a function of $n$ for $l = 0$ states of Rb at various lattice wavelengths. For small $n$, $\langle \cos(2kz_e) \rangle \to 1$ at a given wavelength, resulting in the limit $\alpha^{lsc}_{bc}(\omega) \to \alpha_e$. As $n$ is increased, $\alpha^{lsc}_{bc}$ undulates around zero, and the trapping potential minima switch back and forth between the nodes and the anti-nodes of the lattice. The longer the wavelength the higher $n$ it takes to modulate $\alpha_e$. The inset shows that all these curves follow a nearly universal dependence on $k(r_e) \propto n^2 \alpha_0/\lambda$. 

FIG. 4: The “landscape-modulated” polarizability $\alpha^{lsc}_{bc}$ for $ns$-states of Rb with $n = 100$ (dashed orange), 160 (dashed black) and 180 (dashed blue). The scalar ground state polarizability $\alpha_g$ (solid red) and the free electron polarizability $\alpha_e$ (dashed gray) are also shown. The magic wavelengths can be found for all $n \geq 154$ in the infrared wavelength range spanning the CO$_2$ and the frequency-doubled CO$_2$ laser bands.

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

$$\alpha_g(\omega) = \sum_i \frac{(E_g - E_i)(\langle \psi_g | \mathbf{D} | \psi_i \rangle)^2}{(E_g - E_i)^2 - \omega^2}. \quad (8)$$

We evaluated $\alpha_g(\omega)$ with a high-accuracy procedure [24].

The two spatial parts of Ry and GS potentials match when $U_r^Z = U_g^Z$, therefore the motionally-equivalent trapping is attained at some “magic” values of laser frequencies $\omega^*$ (or wavelengths $\lambda^*$) when $\alpha_g(\omega^*) = \alpha_r^{bc}(\omega^*)$.

In Fig. [2] we plot both $\alpha_g(\omega)$ and $\alpha_r^{bc}(\omega)$ to search for wavelengths at which the two AC polarizabilities match. 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., $\lambda_r^{bc}$ for the 160s and 180s states cross twice with the GS polarizability). The number of $\lambda^*$’s increases further with increasing $n$. Table I compiles the magic wavelengths for Rb and Na atoms. In addition to the $l = 0$ states, Table I lists $\lambda^*$ for the $l = 1$ and $l = 2$ states (all $m = 0$).

| $n$ | $s$ | $p$ | $d$ | $s$ | $p$ | $d$ |
|-----|-----|-----|-----|-----|-----|-----|
| 100 | 1961 | 2798 | 2734 | 3894 |       |     |
| 120 | 4655 | 3762 | 6766 | 5532 |       |     |
| Na  | 2022 | 3016 | 2750 | 3942 |       |     |
| 160 | 4421 | 3401 | 6525 | 5301 |       |     |
| Rb  | 5550 | 3356 | 6923 | 4305 | 4231 |     |
| 6791 | 4762 | 6792 | 8695 | 6606 | 8567 |     |
|     | 12134 | 9961 | 15386 | 12631 |     |     |
| Na  | 5755 | 3132 | 6098 | 4124 | 4095 |     |
|     | 4714 | 6743 | 8358 | 5934 | 8490 |     |
|     | 11836 | 9740 | 15059 | 12402 |     |     |

All these magic wavelengths are in the CO$_2$ and the frequency-doubled CO$_2$ laser bands. This provides an additional advantage that the lattice-constant is large enough to allow for individual lattice-site addressing [24]. These wavelengths are far from any resonances which reduces the photon scattering rate and thereby reduces the motional heating. Again, working at the magic conditions fully eliminates the necessity to turn off [10] or to invert [26] the trapping fields while performing gate operations.

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 $\lambda^* \approx 432$ nm [10]. 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 [10], the feasibility of working at that lattice wavelength needs to be amended. Our calculations show (see Fig. [2]) that for $n = 100$ at $\lambda^* \approx 432$ nm, $\alpha_{\text{free}}(\omega^*)/\alpha_r(\omega^*) \approx 3 \times 10^{-3}$, 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.

So far we focused on one dimension. If the 1D lattice is formed by Gaussian beams, the Ry atom can escape in the radial direction. As discussed above, for a sufficiently highly-excited atom, the bulk of its wave function can be outside the beam intensity inflection points, providing radial confinement. Alternatively one could work with 3D lattices. Since s-electron wave functions are spherically symmetric, the $x$, $y$, and $z$ axes are equivalent and the 1D arguments can be directly transferred to 3D lattices: s-state Ry atoms can be trapped at the anti-nodes of red-detuned 3D optical lattices. As to the $l \neq 0$ states, the 3D trapping in intensity maxima requires further consideration as the quantization axis and three optical beam axes are no longer aligned [27].

In quantum gate protocols such as the CNOT gate, the conditional logic requires driving a $\pi$-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 magic lattices, the different energy shift between these states does not vanish because of the uniform offset term (Eq. [5]). Drifts in the lattice laser intensity introduce an error $\Delta \omega$ in the Rabi frequency $\Omega_0$ of the GS-Ry transition: $\Omega = \sqrt{\Omega_0^2 + \Delta \omega^2}$. This error in the actual Rabi frequency $\Omega$ leads to the fractional error in GS-Ry rotation angle: $\frac{\Delta \phi}{\pi} = \frac{\Delta \omega}{\Omega} \approx \frac{1}{2} \left( \frac{\Omega_0}{\Omega} \right)^2$. For Rb, we estimate this error to be $\frac{\Delta \phi}{\pi} = 25 \left( \frac{\delta I}{I_0} \right)^2 \left( \frac{1 \text{ MHz}}{10^6 \text{ Hz}} \right)^2 \left( \frac{U}{1 \text{ mK}} \right)^2 \left( \frac{\lambda}{1000 \text{ nm}} \right)^4 \frac{350 \text{ a.u.} \sqrt{\alpha_g}}{\alpha_g} \frac{2}{3}$, where $\delta I/I$ is the fractional intensity fluctuation and $U$ is the trap depth. For example, when $\delta I/I = 10^{-4}$ for a 0.16 mK deep trap, $\Omega_0/2\pi = 1 \text{ MHz}$, and 1000 nm lasers, $\Delta \phi/\pi = 6.5 \times 10^{-9}$. For CO$_2$ wavelengths the errors are below $10^{-4}$, which is considered to be tolerable [28].

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 [8] 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.
ity. “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 ponderomotive lattices.

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