Engineering non-binary Rydberg interactions via electron-phonon coupling

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Coupling electronic and vibrational degrees of freedom of Rydberg atoms held in optical tweezers arrays offers a flexible mechanism for creating and controlling atom-atom interactions. We find that the state-dependent coupling between Rydberg atoms and local oscillator modes gives rise to two- and three-body interactions which are controllable through the strength of the local confinement. This approach even permits the cancellation of two-body terms such that three-body interactions become dominant. We analyze the structure of these interactions on two-dimensional bipartite lattice geometries and explore the impact of three-body interactions on system ground state on a square lattice. Our work shows a highly versatile handle for engineering multi-body interactions of quantum many-body systems in most recent manifestations on Rydberg lattice quantum simulators.

Introduction.— In the past years Rydberg atoms [1–3] held in optical tweezer arrays have emerged as a new platform for the implementation of quantum simulators and, potentially, also quantum computers [4–10]. One- [6], two- [11] and three-dimensional [12] arrays containing hundreds of qubits are in principle achievable and the wide tunability of Rydberg atoms grants high flexibility for the implementation of a whole host of quantum many-body spin models. The physical dynamics of these quantum simulators takes place in the electronic degrees of freedom which mimic a (fictitious) spin particle. Effective magnetic fields and interactions are achieved via light-shifts effectuated by external laser fields and the electronic degrees of freedom and consisting of both two- and three-body contributions; see text for details. This also results in a state-dependent clustered phases occur as well as signatures of frustration phenomena. Our work is directly relevant for recent developments on the domain of quantum simulation with Rydberg tweezer arrays where it highlights a so far unanticipated mechanism for realizing exotic interactions.

2D model.— We consider a 2D lattice of N Rydberg atoms in the x – y plane, whose sites are labeled by \( k = (k_x, k_y) \). The electronic degree of freedom is modeled as effective two-level system (with \( |\downarrow\rangle \) and \( |\uparrow\rangle \) denoting the ground state and the Rydberg excited state, respectively) [3, 40]. The two levels are coupled by a laser with Rabi frequency \( \Omega \) and detuning \( \Delta \). The atom is trapped inside a tight harmonic optical tweezer (grey line) and, at low temperature, it occupies the ground state of the associated phonon degree of freedom (red curve). For simplicity, we assume that Rydberg and ground state experience the same trapping potential. (b) Energy diagram of a two atom system arranged along the x-axis. When both atoms are excited to the Rydberg state, \( |rr\rangle \), they experience, in addition to the standard interaction \( V \), the potential change \( \delta V \) arising as a consequence of the coupling between spin and phonon degrees of freedom and consisting of both two- and three-body contributions; see text for details. This also results in a state-dependent displacement \( \delta x_{1,2} \) of the atoms from their equilibrium position \( x_{1,2}^0 \), separated by the lattice spacing \( a \).

FIG. 1. Setup. (a) Each atom is modeled as a two-level system with ground state \( |g\rangle \) and excited Rydberg state \( |r\rangle \). The two levels are coupled by a laser with Rabi frequency \( \Omega \) and detuning \( \Delta \). The atom is trapped inside a tight harmonic optical tweezer (grey line) and, at low temperature, it occupies the ground state of the associated phonon degree of freedom (red curve). For simplicity, we assume that Rydberg and ground state experience the same trapping potential. (b) Energy diagram of a two atom system arranged along the x-axis. When both atoms are excited to the Rydberg state, \( |rr\rangle \), they experience, in addition to the standard interaction \( V \), the potential change \( \delta V \) arising as a consequence of the coupling between spin and phonon degrees of freedom and consisting of both two- and three-body contributions; see text for details. This also results in a state-dependent displacement \( \delta x_{1,2} \) of the atoms from their equilibrium position \( x_{1,2}^0 \), separated by the lattice spacing \( a \).
of its local potential, with situations with harmonic trapping potentials in the three spatial directions the inter-particle distance \(r\). Here, we have introduced the coefficients \(\tilde{W}_{k,m} = \sum_{\mu} \tilde{W}_{k,m,\mu}\), with \(\tilde{W}_{k,m,\mu} = W_{k,m,\mu}/\sqrt{\hbar \omega_{\mu}}\). Equations (8b) and (8c) show that, as consequence of the spin-phonon coupling, an effective atom-atom interaction emerges. The latter consists of an extra two-body [Eq. (8b)] and a novel three-body term [Eq. (8c)], whose strengths are both \(\propto \tilde{W}_{k,m,\mu}\). Importantly, \(\tilde{W}_{k,m,\mu}\) depends on the trapping frequencies \(\omega_{\mu}\) and, therefore, the strength of the effective interactions can be tuned by varying the harmonic confinement.

We note that the new phonon operators \(B_{k,\mu}\) appearing in Eq. (8a) mix the original phonon and spin degrees of freedom. However, in the limit of small \(\tilde{W}_{k,m,\mu}\) this mixing is negligible \([43,44]\). In this regime the phonon dynamics decouples from the spins. Details on the validity of this approximation are provided in the next section and in the Supplemental Material (SM) \([45]\).

**Tailoring the three-body interaction.**—The strength of the phonon-mediated effective interactions in Eqs. (8b) and (8c) is directly connected to the strength of the dipolar ones: This is because the coefficients \(\tilde{W}_{k,p}\) are proportional to the gradient of \(V(r_k, r_m)\). Typical dipolar interactions exhibit a power-law behavior \(\propto |r_k - r_m|^{-\alpha}\) (e.g., \(\alpha = 6\) for a van der Waals potential). In which case, one generally finds that \(V(r_k, r_m) \gg \tilde{W}_{k,p}\). This means that, in common situations, phonon-mediated interactions only represent a small correction. However, the interaction potential between excited atoms can be tailored via microwave (MW) dressing of two different
Rydberg states [45–47], allowing to make the effective interactions dominant. Such dressed potential can be parameterized, to a good degree of approximation, as

$$V(r_k, r_m) \approx \begin{cases} \frac{C_1}{2|r_k - r_m|^\beta} + \frac{C_2}{2|r_k - r_m|^\beta} & \text{for } |r_k - r_m| \approx a, \\ \frac{C_1}{2|r_k - r_m|^\beta} + \frac{C_2}{2|a_{\text{NNN}}|^\beta} & \text{for } |r_k - r_m| \approx a_{\text{NNN}}. \end{cases}$$ (9)

Here, $a$ and $a_{\text{NNN}}$ are the distances at equilibrium between next nearest (NN) and next-to-next nearest (NNN) neighbors, respectively. For a typical dressed potential, $V(r_k, r_m) \approx 0$ for $|r_k - r_m| > a_{\text{NNN}}$ [45]. MW dressing allows to control the values of the constants $C_{1,2}$ and $c_{1,2}$ in Eq. (9) independently and, in turn, to tune the strength of the dipolar potential (as well as its gradient) at NN and NNN neighbors distances, denoted by $V_1$ and $V_2$, respectively. In this way we can achieve regimes dominated by the phonon-mediated interactions, whose strength along the $\mu$ direction is

$$V_{3,\mu} = \frac{36\ell^2_{\mu}}{\hbar \omega_\mu a^2} \left( \frac{C_1}{a^6} \right)^2.$$ (10)

In this case, Eqs. (8b) and (8c) become

$$H_{3B} = \sum_{\langle k,m \rangle} V_1 \sum_\mu V_{3,\mu} \left( \hat{R}^0_{k,m,\mu} \right)^2 n_k n_m + \sum_\mu \sum_{\langle k,m \rangle} V_2 n_k n_m, \quad (11a)$$

$$H_{3B} = -\sum_\mu \sum_{\langle k,p,q \rangle} V_{3,\mu} \hat{R}^0_{k,p,\mu} \hat{R}^0_{k,q,\mu} n_k n_p n_q, \quad (11b)$$

where we have used that $\hat{W}_{k,m,\mu} = \sqrt{V_{3,\mu}} \hat{R}^0_{k,m,\mu}$, with $\hat{R}^0_{k,m,\mu} = a^{-1} \hat{R}^0_{k,m} - \hat{R}^0_{m}$. The symbols $\langle k, m \rangle$ and $\langle k, m \rangle$ denote the sum over NN and NNN neighbors, respectively, while $\langle k, p, q \rangle$ implies that the sum is restricted to sites satisfying $|k| \leq a$. Note that, due to the presence of the factors $\hat{R}^0_{k,m,\mu}$, the terms $\propto V_{3,\mu}$ strongly depend on the lattice geometry and, as we will show for the case of bipartite lattice, they give rise to anisotropic contributions in atom-atom interactions even if original dipolar forces are isotropic.

The strength of the phonon-mediated interactions can be tailored by tuning the trapping frequencies $\omega_\mu$, which are typically of the order of hundreds of kHz [6, 9, 38, 40]. In particular, Eq. (11a) implies that it is possible to make the overall two-body term vanish and maximize the effects of three-body interactions. Recalling Eq. (8), in order to decouple the electronic and vibration degrees of freedom and to focus only on the spin dynamics we have to require $W_{k,m,\mu} \ll \hbar \omega_\mu$. On the other hand, to access regimes governed by the effective two- and three-body interactions one should also consider $V_{3,\mu} \gtrsim V_{1,2}$. From Eqs. (6) and (10), the above conditions translate into the following bounds on $\omega_\mu$.

$$\sqrt{\frac{18\hbar}{ma^2} \left( \frac{C_1}{a^6} \right)^2} \ll \omega_\mu \leq \sqrt{\frac{72}{ma^2 V_{1,2}} \left( \frac{C_1}{2a^6} \right)^2}. \quad (12)$$

As can be seen from the blue area in Fig. 2(b), there exists a finite region of system parameter space in which Eq. (12) holds.

**Phase diagram for a bipartite lattice.** We now focus on system of atoms arranged on a bipartite lattice and investigate the effects of the interplay between (two-body) dipolar and effective (two- and three-body) interactions on its phase diagram. The simplest case of a square lattice is shown in
two-body interactions and four-excitation clustered phase, dominated by attractive $\propto$ are melted due to the three-body repulsive contribution phase with one missing line (here, the trimers occurring in (2) of density of trimers dominated by the repulsive contribution $\propto f_{\text{trim}}$, respectively. Dashed red lines represent guide for the eye to distinguish between the different system phases. In panel (d) we show typical configurations in the different regions of the phase diagram. Dark (red) spots correspond to excited atoms. See text for details. In all panels, $L = 10$, $V_a/\hbar = 2\pi \times 0.2$ MHz and $\Delta/\hbar = 2\pi \times 1$ MHz.

Fig. 3(a). The different contributions to atom-atom interaction are listed in Fig. 3(a,c). Importantly, the lattice-dependent structure of $H_{3\Omega}$ in Eq. (8c) implies that effective two-body interactions are attractive while, on the contrary, three-body terms have a repulsive character. This feature is quite general and, e.g., in Ising spin models on non-bipartite lattices (triangular, kagome) it could be employed to implement frustrated interactions [15, 19–21]. The study of such phenomena will constitute the focus of future investigations. Due to the competition between two- and three-body interactions, we expect that different phases emerge. To map out the phase diagram we consider the classical limit (i.e., with vanishing Rabi frequency $\Omega$) and determine its ground state through a classical Metropolis algorithm [48, 49] by employing an annealing scheme [50].

Results are displayed in Fig. 4(a,b,c). Here, we show the behavior in the $V_2 - V_3$ plane (with $V_1 > 0$) of the average value of the Rydberg excitation density $\langle n \rangle$, of the density of dimers $\langle n_{\text{dim}} \rangle$ [defined as in the left column of Fig. 3(c,d)], and of density of trimers $\langle n_{\text{trim}} \rangle$ [defined as in the right column of Fig. 3(c,d)]. Beyond the trivial states with all excited and all de-excited atoms (dark blue and white regions, respectively), four further phases emerge [see Fig. 4(d)]: (1) checkerboard phase, dominated by the repulsive contribution $\propto V_1$, (2) striped phase with a single three-atom stripe, dominated by NNN neighbor two-body (attractive) interaction $\propto V_2$, (3) frustrated striped phase with one missing line (here, the trimers occurring in (2) are melted due to the three-body repulsive contribution $\propto V_3$, and (4) four-excitation clustered phase, dominated by attractive two-body interactions $\propto V_{3,\mu}$. Concerning this latter, we note that the transition is not as sharp as the other ones. Indeed, as can be seen from the last panel of Fig. 4(d), the lattice is not entirely covered by four-particle clusters. This may suggest either that (4) is a liquid phase or that it represents a critical region. A full covering can be obtained for $V_2 > 0$, where attractive NNN neighbor interactions contribute to enhance the energy gain in forming cluster.

Interestingly, effective interactions due to spin-phonon coupling give rise to finite-size frustration phenomena even in a square lattice in the presence of isotropic dipolar interactions. This is manifest in the emergence of the different striped phases (2) and (3): see Fig. 4, which displays the case of a lattice with an even number of sites. On the contrary, if an odd number of sites is considered only a single regular striped phase emerges in this region of the phase diagram. However, a frustrated phase forms inside region (1) (see SM [45]).

In non-square lattices, the geometrical factors characterizing phonon-mediated interactions [see Eq. (11)] give rise to anisotropic two- and three-body contributions even if the original dipolar interactions between atoms are isotropic. This can be seen in Fig. 3(d), where the various interaction contributions arising in a honeycomb lattice are displayed. Here, though the phase diagram is similar to the one shown in Fig. 4, non-trivial and anisotropic system configurations emerge (see SM [45] for details).

The various phases shown in Fig. 4 can be probed in state-of-the-art Rydberg simulators consisting of 2D defect-free arrays of optical tweezers [37]. Here, desired many-body states can be accessed via a generalization of the adiabatic protocol proposed in Refs. [22–24].

**Conclusions.** — We have shown that electron-phonon interactions in Rydberg lattice quantum simulators permit the engineering of tunable multi-body interactions. We have illustrated the underlying mechanism in bipartite lattices, discussing in particular the case of an isotropic square lattice, where we studied the phase diagram in the classical limit. Going beyond this limit and considering the impact of quantum fluctuations ($\Omega > 0$) will be possible in Rydberg quantum simulator experiments.

Many future directions of this work can be envisioned: In particular, we expect that, as a consequence of the lattice-dependent structure of the induced interactions, peculiar two- and three-body terms would arise in non-bipartite lattices (e.g., triangular, kagome), allowing for the investigation of frustrated magnetism in spin models with non-trivial multi-body interactions. Moreover, so far we have focused on the conceptually simple case in which each atom experiences a state-independent trapping potential. In practice, this may not be always possible to achieve and modifications to the effective interactions may arise. Finally, the mechanism leading from the spin-phonon coupling to effective many-body interactions can be generalized to different kinds of bare atom-atom potentials (e.g., exchange interactions, oscillating potentials) and may allow for engineering effective interactions with different structure and/or even $n$-body (with $n > 3$) contributions.
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