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Engineering spin-spin interactions with optical tweezers in trapped ions

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We propose a method for generating programmable interactions in one- and two-dimensional trapped-ion quantum simulators. Here we consider the use of optical tweezers to engineer the sound-wave spectrum of trapped ion crystals. We show that this approach allows us to tune the interactions and connectivity of the ion qubits beyond the power-law interactions accessible in current setups. We demonstrate the experimental feasibility of our proposal using realistic tweezer settings and experimentally relevant trap parameters to generate the optimal tweezer patterns to create target spin-spin interaction patterns in both one- and two-dimensional crystals. Our approach will advance quantum simulation in trapped-ion platforms as it allows them to realize a broader family of quantum spin Hamiltonians.

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I. INTRODUCTION

Trapped ions are one of the leading platforms for quantum computation and quantum simulation [1–4]. Numerous experiments have demonstrated the ability of the analog trapped-ion quantum simulator to emulate the dynamics of quantum magnetism models [3,5–8] and to study the dynamics of quantum information and quantum entanglement [9–11].

One of the main advantages of the trapped-ion quantum simulators is the tunability of the interaction range, as well as the ability to realize one- and two-dimensional (1D and 2D) systems. Hence, this platform provides an ideal setup in which one can explore the interplay of interaction range and dimensionality in the dynamics of quantum information, entanglement, and speed of thermalization [9,10,12,13], while simultaneously allowing one to simulate models relevant to condensed matter physics that are beyond the state-of-the-art numerical methods.

However, the current simulator setups do not offer enough versatility to explore the above questions. This is because, theoretically, the types of engineered interactions which can be realized in these systems is limited to those with power-law decay, $1/r^\xi$, where $r$ is the separation between two ions and $0 \leq \xi \leq 3$ [14]. In order to understand the source of this limitation, we note that the ion-ion interactions in the simulator are phonon mediated and depend on the spectrum and structure of the collective vibrational modes of the ion crystal [15]. Furthermore, considering experimental constraints such as laser power and decoherence rates, the range of interactions tends to be even more limited, and most experiments are operated with $0 \leq \xi \leq 1.5$ [12,14,16].

In the following, we illustrate an approach for realizing a highly tunable trapped-ion simulator in terms of connectivity, range, and sign of the interactions in both linear (or 1D) and triangular (2D) ion crystals in Paul traps [17–21]. We use optical tweezers to manipulate the frequencies and structures of the collective vibrational modes of the crystal. The triangular crystal structure in 2D makes it a natural platform for implementing quantum simulation of frustrated spin systems [22,23] and there has been rapid experimental progress in this area in recent years [24–26].

II. EFFECTIVE ISING INTERACTIONS

The spin-spin interactions in an ion crystal are generated when the electronic state of each ion is coupled to the phonon modes of the ion crystal by applying a state-dependent force generated by a pair of counterpropagating laser beams. The resulting Hamiltonian, in the Lamb-Dicke (LD) limit and in the interaction picture with respect to $\hat{H}_0 = \sum_{m=1}^N \hbar \omega_m \hat{a}_m$, is given by

$$\hat{H}_I = -i \sum_{j=1}^N g \cos(\mu t) \hat{\sigma}^z_j \times \sum_{m=1}^N \sqrt{\frac{\hbar}{2M\omega_m}} (\hat{a}_m e^{-i\omega_m t} - \hat{a}_m^\dagger e^{i\omega_m t}),$$

(1)

where $\mu$ is the beat-note frequency between the two counterpropagating bichromatic lasers used to generate the state-dependent force and $g$ is the interaction strength of the laser which is assumed to be homogeneous throughout the crystal. Here $\hat{a}_m$ ($\hat{a}_m^\dagger$) is the annihilation (creation) operator for a phonon in mode $m$, $\hat{a}_m = \hat{a}^\dagger_m \hat{a}_m$, and $b_{m}^{(m)}$ is the amplitude of the corresponding eigenvector at the position of ion $j$. The LD parameter is given by $\eta_j^{(m)} \equiv k_q b_{j}^{(m)} \sqrt{\frac{\hbar}{2M\omega_m}}$, where $k_q$ is the wave vector for the Raman beam pair and $M$ is the ion mass.
The form of the Hamiltonian in Eq. (1) allows us to find an explicit expression for the propagator governing the evolution of the system. The propagator can be written explicitly as its Magnus series expansion truncates at second order [15,27,28]:

\[ \hat{U}(t, 0) = \exp \left( -\frac{i}{\hbar} \int_0^t dt' \hat{H}_J(t') \right) \]

\[ \approx \exp \left( i \int_0^t dt' \left[ \int_0^t dt'' \left( \hat{H}_J(t'), \hat{H}_J(t'') \right) \right] \right) \]

where

\[ \gamma_j^{(m)}(t) = \frac{-i g \eta_j^{(m)}}{\mu^2 - \omega_m^2} \left[ \mu - e^{i \omega_m t} \left[ \mu \cos(\mu t) - i \omega_m \sin(\mu t) \right] \right] \]

and

\[ \beta_{j,k}(t) = g^2 \sum_m \frac{\eta_j^{(m)} \eta_k^{(m)}}{\mu^2 - \omega_m^2} \left( \frac{\mu \sin(\mu t) - \omega_m t}{\mu - \omega_m} \right) \]

\[ - \frac{\mu \sin(\mu t) - \omega_m t}{2\mu - \omega_m} \left( \frac{\omega_m \sin(2\mu t)}{2\mu} \right) - \frac{\omega_m \sin(2\mu t)}{2\mu} \]

We note that the term containing the spin-spin interaction in the propagator \( \hat{U}(t, 0) \) grows linearly with time and can be identified as the phase of the system evolving with an effective Ising Hamiltonian, \( \hat{H}_{\text{Ising}} = \sum_{j,k} \sigma_j^z \sigma_k^z \), with

\[ J_{j,k} = g^2 \sum_m \frac{\eta_j^{(m)} \eta_k^{(m)}}{\mu^2 - \omega_m^2}. \]

As it is shown in Eq. (4), the interactions between the ions are determined by the structure of the phonon modes. Thus, the ability to engineer these collective vibrational modes of the crystal allows us to realize a wide variety of interaction matrices.

Our method uses local optical potentials to induce additional (anti)confinement of individual ions and frequency state-dependent Raman forces. The result of the additional optical potentials is a change in the phonon mode spectra and of the individual amplitudes of each mode at each ion.

The main result of our work is as follows: Given a target 1D or 2D spin-1/2 Hamiltonian, specified by the interaction matrix \( \mathbf{J} \), of the form

\[ \hat{H}_T = \sum_{\alpha} F_{\alpha} \hat{a}^\dagger \hat{a}, \]

we (a) outline a procedure to determine if the target Hamiltonian can be realized and (b) provide a systematic approach to find the optimal tweezer pattern to realize \( \hat{H}_T \). Here we have used \( F_{\alpha} \) to denote the matrix elements of the target interaction matrix \( \mathbf{J} \) along the Cartesian coordinate \( \alpha = x, y, \) and \( z \).

III. PHONON MODE ENGINEERING

In order to characterize the effect of the tweezer potential on the normal modes, we consider \( N \) ions of mass \( M \) which are confined by the harmonic trapping potential \( V_{tp}(\rho_i) = \frac{1}{2} \sum_{\alpha,\beta} M \omega^2_{\alpha,\beta} (\rho^2_{\alpha,\beta}) \), where \( \rho_i = (\rho^x_i, \rho^y_i, \rho^z_i) \) is the position of the \( i \)th ion and \( \omega_{\alpha,\beta} \) is the trap frequency in the \( \alpha,\beta \) direction. The ions are further confined by the tweezer potential \( V_{tp} \). Thus, the potential energy of the system is given by

\[ V(\rho_i) = V_{tp}(\rho_i) + V_{tp}(\rho_i) + \frac{1}{2} \sum_{\alpha,\beta} \frac{e^2}{4\pi\epsilon_0 |\rho_i - \rho_j|} \]

where the third term is the Coulomb potential between the ions, \( e \) is the Coulomb constant, and \( \epsilon_0 \) is the vacuum permittivity.

In order to find the collective vibrational modes of the ion crystal we follow the procedure described in Ref. [29] and find the equilibrium positions \( r^{(0)}_i \) corresponding to the solutions of \( \nabla V = 0 \). Assuming that the ions perform small oscillations about this equilibrium position, the position of each ion can be written as \( \rho_i = r^{(0)}_i + \phi \), where \( \phi \) are deviations from the equilibrium position. Furthermore, considering the tweezer intensity profile at each ion, \( I(\rho_i) \), being centered at each corresponding equilibrium position \( r^{(0)}_i \), the optical dipole potential can be approximated as harmonic. In this way, the general form of the optical tweezer potential is given as

\[ V_{tp}(\rho_i) = \sum_{\alpha,\beta} M \frac{2}{\pi} \frac{1}{2} \frac{\omega^2_{\alpha,\beta}}{\omega^2_{\alpha,\beta} - \omega^2_{\alpha,\beta}} \Delta \alpha_i \Delta \alpha'_i \]

where \( (\omega^2_{\alpha,\beta})^2 \) denotes the local optical pinning curvature expressed as the trap frequency squared at the \( i \)th ion and \( \Delta \alpha_i = \alpha_i - \alpha^{(0)}_i \) is the displacement of the ion position with respect to the equilibrium position along the corresponding direction. Note that this potential can be made confining or anticongfing by modifying the wavelength of the tweezers.

The addition of \( V_{tp} \) does not modify the equilibrium position of the ions since its gradient vanishes there. However, the collective modes of the crystal are modified by the additional tweezer potentials. We obtain the phonon spectrum by expanding the Coulomb potential to second order in \( r \). The resulting Lagrangian, using the explicit form of \( V_{tp} \) given in Eq. (7), is

\[ L = \frac{M}{2} \left[ \sum_i \sum_{\alpha} (\dot{\alpha}_i)^2 - \frac{1}{2} \sum_i \sum_{\alpha,\alpha'} \frac{\omega^2_{\alpha,\alpha'}}{\omega^2_{\alpha,\alpha'} - \omega^2_{\alpha,\alpha'}} \left( \frac{d^2V}{d\alpha_i d\alpha'_i} \right)_{\alpha,\alpha'\rightarrow 0} \right] \]

\[ = \frac{M}{2} \left[ \sum_i \sum_{\alpha} (\dot{\alpha}_i)^2 - \frac{1}{2} \sum_i \sum_{\alpha,\alpha'} \frac{\omega^2_{\alpha,\alpha'}}{\omega^2_{\alpha,\alpha'} - \omega^2_{\alpha,\alpha'}} \left( \frac{d^2V}{d\alpha_i d\alpha'_i} \right)_{\alpha,\alpha'\rightarrow 0} \right]. \]

The eigenvalues and eigenvectors of the Hessian matrix \( \mathbf{A} \) determine the normal modes of the crystal. The \( k \)th normalized eigenvector corresponds to a normal mode of the crystal, which we denote as \( \mathbf{b}_k \). Its entries represent the amplitude of motion of each ion in each of these modes. The mode frequencies are \( \omega_n = \sqrt{\lambda_n} \), with \( \lambda_n \) being the eigenvalues of \( \mathbf{A} \). In the case of a 1D ion crystal, the eigenmodes separate in
three subclasses, corresponding to the directions of motion $x$, $y$, and $z$ and $k = 1, \ldots, 3N$.

IV. OPTIMIZATION OF NON-NATIVE SPIN-SPIN INTERACTIONS

The realization of the target Hamiltonian, given by $\hat{H}_T$ of the form Eq. (5) with the specified coupling matrix $J_T$, relies on finding the optimal confinement realized by the tweezer at the position of each ion. We solve this problem through three optimization steps.

First, we consider an equidistantly spaced ion crystal with inter-ion distance $d_0$, defined by an effective axial trap frequency, $\omega_{z,\text{eff}}$, as [29–31]

$$d_0 \approx \left( \frac{e^2}{4\pi\epsilon_0 M \omega_{z,\text{eff}}^2} \right)^{\frac{1}{3}} \cdot \frac{2}{N^{0.56}}.$$

In this way we can find an approximation to the optimal trap frequency, without having to solve numerically the equilibrium position of the ions, by optimizing the values of $s' = \{\omega_{x,\text{eff}}, \mu', \{\Omega_i\}\}$ that minimize the error of the matrix of Ising couplings:

$$\epsilon(s) = \frac{\|J_T - \tilde{J}(s)\|}{\|J_T\|}.$$

Here $\tilde{J}(s)$ is the resulting coupling matrix of the pinned crystal, normalized such that the largest entries of $J_T$ and $\tilde{J}$ have the same magnitude. This problem is formulated as constrained optimization of the form

$$\arg\min_{s'} \epsilon(s') : s_{i}^\text{min} \leq s'_{i} \leq s_{i}^\text{max}.$$

We limit the parameter space of the search by first testing a feasibility condition (Fig. 1) for the sign structure of $J_T$ for a particular set of values of $\{\omega_{x,\text{eff}}, \mu'\}$. The idea consists of determining if there is a gradient direction in the parameter manifold of $\Omega = \{\Omega_i\}_{i=1}^N$ along which the sign (and magnitude) of the couplings of the modified system change towards those of the target matrix. For example, taking a single coupling, $J_{l,l}$, and considering optical potentials along a single direction, we evaluate the directional derivative of the value of the coupling at a trial point in $\Omega$, i.e., $\nabla \tilde{J}_{l,l} \cdot \Omega_i = \text{diag}(\tilde{A}_{k,l}) \cdot \Omega_i$. Here $\text{diag}(\tilde{A}_{k,l})$ is the diagonal of the adjoint of $J_{l,l}$ with respect to the system Hessian $A$, and $J^0 = \tilde{J}(\omega_{x,\text{eff}}, \mu', [0])$ is the coupling matrix of the unmodified system (see Appendix). Then, the condition for the existence of this direction can be written as

$$\text{sgn}(\Delta J_{l,l}) \text{diag}(\tilde{A}_{k,l}) \cdot \Omega_i > 0,$$

where $\Delta J = J - J^0$.

Considering $n$ entries of interest of the target coupling matrix, we can define for each of them a constraint like the one above. The test for the feasibility condition consists then of determining the existence of a solution $\Omega$, which satisfies $X\Omega_i > 0$. Here we have defined the defined the matrix of constraints $X = (X^{(1)}, \ldots, X^{(n)})^T$, where $X^{(1)} = \text{sgn}(\Delta J_{l,l}) \times \text{diag}(\tilde{A}_{k,l})$.

If values of $\{\omega_{x,\text{eff}}, \mu'\}$ exist for which a solution is found, we optimize in a second step only the optical potential frequencies:

$$\arg\min_{\Omega_i} \epsilon(s') : \Omega_i^\text{min} \leq \Omega_i' \leq \Omega_i^\text{max}.$$

By setting the appropriate limits $\Omega_i^\text{min/max}$, the optimization can be constrained to only trapping or antitrapping potentials. Furthermore, this optimization step can be simplified by considering the symmetries of $J_T$ in the crystalline lattice. For example, we can reduce the number of optical potential frequencies to be searched for by defining a rotational unit cell for the lattice and optimize only for optical potentials belonging to that cell (Fig. 2).

In a final step, we calculate the actual positions of the ions in a harmonic trap for the optimal value $\omega_{x,\text{eff}}$. With these new positions, we perform a second search of optimal values of $s = \{\mu, \{\Omega_i\}\}$ using as the initial guess the values of $\{\mu', \{\Omega_i\}\}$ found in the previous optimizations.

V. EXAMPLES

For the results presented in this section, we have used a pseudo-Hessian method (L-BFGS) in combination with a line-search scheme (backtracking or Hager Zhang) to perform the optimizations of Eqs. (10) and (12). In general, convergence is obtained in much less than 1 min for the backtracking scheme or in a few minutes for the Hager Zhang scheme using a standard workstation. For the optimizations we used libraries JUMP.jl [32] and OPTIM.jl [33] versions 1.2.0 and 0.21.6, respectively, loaded in JULIA [34] version 1.5.2.

A. 1D crystals

We first consider a linear chain of ions in a Paul trap. A 1D crystal of $N$ ions features $3N$ phonon modes: $N$ axial phonons
modes and $2N$ radial modes. The radial modes are split into two groups of $N$ with an identical set of $N$ eigenvectors $\{b_m^{r+i}\}$. We only consider engineering one group of radial modes, e.g., those along the $y$ direction. However we note that modifying modes belonging to each of the three sets should allow a larger set of possible couplings.

We demonstrate the tunability of interactions using phonon mode engineering by considering a crystal of 12 ions and two target interaction forms: (i) a homogeneous nearest-neighbor interaction (Fig. 3), and (ii) a controllable power-law interaction [Fig. 4(a)], both with antiferromagnetic (AF) couplings. We summarize the relevant experimental parameters for the optimal configuration for both scenarios in 1D in Table I and discuss our choices further in Sec. VI.

A nearest-neighbor (NN) interaction is the antithesis of the phonon-mediated interactions occurring naturally in trapped-phonon quantum simulators. In them, the collective nature of the phonon modes gives rise to effective spin-spin interactions that are long range in character. Methods to obtain these NN couplings have been been proposed using single-ion Raman addressing [35]. Here we show that with our method we can also generate a uniform, nearest-neighbor AF coupling matrix using experimentally accessible parameters (see Fig. 3).

In the case of the power-law couplings, we consider an ion crystal in a segmented Paul trap with almost equidistant ion spacing and compare it against a crystal in a harmonic trap where the spacing between ions decreases away from the center. Finally we compare both scenarios to a crystal in a harmonic trap in the absence of the tweezer potential. For this scenario we use the same trap parameters but vary the beat-note frequency $\mu$ to minimize the error as defined in Sec. IV.

Figure 4(b) shows that, in the presence of the tweezer potential, for both evenly spaced crystals and crystals in harmonic traps, the smallest error of the approximated power-law decay occurs close or at $\xi = 3$, which corresponds to interactions of dipole-dipole nature [15]. Furthermore, we find that for shorter-range interactions with $\xi > 1.5$ the addition of tweezers significantly reduces the error between the target Hamiltonian and the realized Hamiltonian. Importantly, this allows us to reach values of $\xi$ not accessible to existing methods.

**Table I. Summary of frequencies for the homogeneous nearest-neighbor (NN) and two values of power-law couplings in equally (+) and unequally (x) spaced (harmonically trapped) 1D crystals. The highlighted values indicate the direction of the confinement.**

| Frequency (MHz/2$\pi$) | NN | $\xi = 3.5$ | $\xi = 1.5$ |
|-------------------------|----|------------|------------|
| $\omega_{\mu}$ | $+$ | $0.6, 0.6, 0.33$ | $0.6, 0.6, 0.33$ |
| $\max \Omega_{\pi}$ | $+$ | $2.0, 0.6$ | $0.4, 0.6, 0.1$ |
| $\mu$ | $+$ | $0.49$ | $2.9$ |

**B. 2D crystals**

We now consider radial 2D ion crystals in a harmonic Paul trap, with $N$ transverse phonon modes and $2N$ in-plane modes. The presence of micromotion in these crystals has implications for the applicability of the secular approximation, in which the trapping potential is replaced by a static one as described above. This leads to a modification of the mode spectrum as characterized in Ref. [18], but the corrections to the mode spectra are small [17] and can be practically eliminated by the appropriate choice of geometry [36].

We first focus on the planar modes which offer more degrees of freedom and thus allow us to engineer a wider variety of couplings. We illustrate this using the spin ladder with frustration which is shown in Fig. 5(a). Here nearest-neighboring spins interact ferromagnetically along the rungs of the ladder and antiferromagnetically along the legs of ladder. For this specific set of couplings, a mode exits that generates the required sign structure, although the magnitude of the couplings deviate largely from those of the target. Adding optical potentials [Fig. 5(b)] improves these magnitudes while preserving the correct sign of the couplings. However some deviations will still be present which cannot be completely fixed: (i) the
nonuniformity of the nearest-neighbor couplings [Fig. 5(c)] and (ii) residual longer-ranged couplings [Fig. 5(d)].

Considering now couplings generated by transverse modes, we show an example with uniform sign structure which exploits the benefits of larger spacing between mode frequencies of these modes. In Fig. 6 we illustrate the realization of a frustrated triangular lattice with antiferromagnetic nearest-neighbor interactions between 19 ions. We can observe the symmetry of the optical potential frequencies in Fig. 6(b), a property we have exploited to simplify the optimization of these frequencies as described in Sec. IV. The effect of the edges can be seen on the error of the couplings [Figs. 6(c) and 6(d)]. One could think of reducing this effect by increasing the size of the crystal but limiting the spins coupled by the Raman field to the innermost ones, e.g., by adding ions on the edges of the lattice without the appropriate level structure or controlling the shape of the Raman field.

We note that the optimization can be fine-tuned by modifying the error function used for a particular target coupling. For instance, some physical phenomena may be robust to the presence of longer-range interactions but sensitive to the nonuniform couplings. Thus including additional weights to the error of critical couplings or ignoring those of noncritical ones can be used to favor one particular outcome of the optimization.

To conclude this section, we summarize the relevant experimental parameters of the optimal configuration for both scenarios in 2D in Table II.

### VI. EXPERIMENTAL CONSIDERATIONS

The dipole interaction due to the optical tweezers can only effectively alter the phonon spectrum of a trapped ion crystal if it can compete with the monopole interaction due to the Paul trap, which is in general dominating. Therefore, it is beneficial to reduce the strength of the Paul trap as much as possible while maintaining the validity of the LD approximation, \( \eta_j^{(m)} \ll 1 \) for all \( j \) and \( m \). This sets a lower limit on the strength of the Paul trap. For a single \( ^{171}\text{Yb}^+ \) ion excited by a pair of Raman beams near the D1 transition at 369 nm with an angle of 90° between them and 45° with respect to the ion motion, we get \( \eta \sim 0.2 \) at \( \omega_m = 2\pi \cdot 400 \text{ kHz} \). We note that reducing the angle between the Raman beams further allows us to be deep in the LD regime at even lower phonon frequencies. However, this is at the expense of reducing the speed of the quantum simulator in order to eliminate off-resonant coupling. Hence we require optical potentials with local trap frequencies in the 100–400 kHz range to make meaningful changes to the phonon spectrum while maintaining the LD regime.

In order to test the feasibility of changing the local trap frequency on this scale, we estimate the effect of a single tweezer. For \( ^{171}\text{Yb}^+ \), and an experimentally feasible tweezer power of \( P = 1 \text{ W} \), a waist of \( W_0 = 1 \text{ μm} \), and a wavelength of \( \lambda = 1070 \text{ nm} \), we find that the local trap frequencies due to the tweezers are \( \sim 2\pi \cdot 200 \text{ kHz} \) [37,38].

Each optical tweezer will introduce a differential ac-Stark shift between the qubit states of the pinned ions and lead to off-resonant scattering. Both processes can lead to phase shifts...
two qubit states \[^{40}\text{, 43}\]. For fine splitting that causes a difference in detuning between the tweezer polarization and is dominated by the 12.6-GHz hyperstates. The differential Stark shift is almost independent of the the case of 171Yb\[^{+}\], we are concerned about both effects on the qubit states encoded on the hyperfine levels \(|F = 0, m_F = 0\rangle \equiv |0\rangle\) and \(|F = 1, m_F = 0\rangle \equiv |1\rangle\) of the \(^{2}S_{1/2}\) ground state. The photon scattering rate in the center of the Gaussian tweezer beam with waist \(W_0\) and a peak intensity of \(I(0) = 2P/\pi W_0^2\) with total light power \(P\) is approximately \[^{37}\]

\[
\Gamma_{sc}(\omega) = \frac{3\pi^2}{\hbar\omega_0^2} \left( \frac{\omega}{\omega_0} \right)^3 \left( \frac{\Gamma}{\omega_0 - \omega} + \frac{\Gamma}{\omega_0 + \omega} \right)^2 \frac{P}{W_0^2}. \tag{13}
\]

When we only consider contributions from the D1 and D2 transitions in 171Yb\[^{+}\] and \(P = 1\ W, W_0 = 1\ \mu m\), and a wavelength of \(\lambda = 1070\ nm\), we find a photon scattering rate of \(~2\ s^{-1}\). More complete calculations will result in slightly higher scattering rates \[^{41}\]. In Fig. 7(a), we give an overview of the photon scattering rate at various tweezer wavelengths. Our results indicate that it is possible to modify the phonon spectrum of trapped ions within the LD regime and maintain negligible photon scattering probability on timescales of \(~100\ ms\).

For our qubit states, the differential Stark shift is highly suppressed as compared to the common Stark shift \[^{37,42}\]. This is because the huge (100 THz) spin-orbit splitting of the \(P\) states does not play a role for the hyperfine clock states. The differential Stark shift is almost independent of the tweezer polarization and is dominated by the 12.6-GHz hyperfine splitting that causes a difference in detuning between the two qubit states \[^{41,43}\]. For \(P = 1\ W, W_0 = 1\ \mu m\), and \(\lambda = 1070\ nm\), we obtain a differential Stark shift of \(~2\pi \times 10\ kHz\) [see Fig. 7(b)].

Since the tweezer pattern is in general not homogeneous, the differential Stark shift will vary between the ions and will appear as an inhomogeneous additional field in the quantum simulator. The differential Stark shift may be canceled by using pairs of blue- and red-detuned tweezers such that the combined differential Stark shift becomes zero. Unfortunately, the D1 and D2 transitions for most relevant ions lie in the UV range, making this solution technically demanding. Eliminating the variation in differential Stark shifts can be done with a single wavelength. This is because the tweezer trap frequency around the \(i\)th ion, \(\Omega_i = \Omega(t_i)\), scales as \(\Omega_i^2 \propto P_i/w_0^4\), whereas the differential Stark shift scales as \(\Delta_{AC} \propto P_i/w_0^2\). Therefore, we can make the differential Stark shift between the qubit states homogeneous throughout the ion crystal by controlling not only the power \(P_i\) of each tweezer but also each waist \(w_i\) and assuring that \(P_i/w_i^2\) is constant around each ion. While this solution still gives us complete freedom to engineer each local tweezer trap frequency, it comes at the expense of having, in general, stronger laser power requirements.

An additional source of error is the misalignment of the tweezers from the equilibrium positions of the ions. In this situation, the tweezers start to supply local stress to the ion crystal, and for each tweezer setting, new ion equilibrium positions have to be found before the eigenmodes can be obtained. In Fig. 8 we show the effect of this type of error on the nearest-neighbor interaction pattern for 12 ions in a linear crystal as also shown in Fig. 3 for perfect alignment. We conclude that our scheme is robust to such misalignments as only minor deviations from the desired spin-spin interactions occur as long as the alignment can be done to within a resolution of \(~100\ nm\). This will likely require active stabilization in which the effects of the tweezers are periodically measured on the ion crystal, for instance, via laser spectroscopy. Note also that for some of the random misalignments an improvement can even be seen, suggesting that using tweezers to apply local forces to the ion crystal may be another useful way of controlling spin-spin interactions. For these calculations, we approximated the tweezers as harmonic, which is justified as the misalignment \(\ll w_0\).

A final experimental complication will be the presence of micromotion for large ion crystals \[^{17–19,21}\]. This could lead to the ions moving in or out of the tweezer beam or experiencing different tweezer waists (and therefore pinning frequencies) as they oscillate under micromotion. For the case of 2D crystals, we have to make the distinction between couplings generated with in-plane or out-of-plane modes. For the former ones, the same mitigation can be applied as for a linear crystal with the micromotion aligned out-of-plane.
For out-of-plane modes, the micromotion has to be aligned along the plane and the tweezers have to be applied with a small angle with respect to the crystal plane. This could lead however to coupling of in-plane and out-of-plane modes. An alternative is the use of standing wave potentials [20].

While this assures that the effect of micromotion is minimized, a full treatment of the setup, including the interplay of micromotion and the tweezer optical potential, is essential to the successful implementation of our scheme in the experiment. We plan to address this in a future work.

VII. DISCUSSION

In this paper we have shown that engineered phonon modes can be used to create a wide variety of interaction ranges and connectivities in trapped-ion quantum simulators. We have shown how optimal tweezer settings can be found using numerical optimization techniques and have given examples of calculated spin-spin interactions in 1D and 2D ion crystals. We can calculate the gradient of the coupling matrix with respect to the Hessian matrix, i.e., $\tilde{A} = \frac{\partial A}{\partial A}$ using adjoint back-propagation methods [48]. The gradient of each entry $J_{k,l}$ with respect to $A$ is obtained from

$$\tilde{A}_{k,l} = U_{k,l} \left[ \tilde{A}_{k,l} + \frac{F}{2} \left( \sum_{i=1}^{N} |U_{k,l}^{T}|^{2} - U_{k,l}^{T}U_{k,l} \right) \right] U_{k,l}^{T}, \quad (A1)$$

where $\circ$ is the Hadamard product, $U \Lambda U^{T} = A$, $F^{ij} = (\lambda_{j} - \lambda_{i})^{-1}$ if $i \neq j$ and zero otherwise, and the corresponding adjoints of $U$ and $A$ are

$$\tilde{U}^{ij} = \Theta(j)U^{ij}, \quad (k = i \lor l = i),
\tilde{A}^{ij} = \Theta(i)U^{k\cdot l}U^{l\cdot i},$$

where $\Theta(j) = (\mu^{2} - \lambda_{j})^{-1}$. Finally, we write

$$A = \left[ \text{vec}(\tilde{A}_{11}), \ldots, \text{vec}(\tilde{A}_{1N}), \ldots, \text{vec}(\tilde{A}_{NN}) \right]^{T}.$$

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APPENDIX: GRADIENT COUPLING MATRIX

We can calculate the gradient of the coupling matrix with respect to the Hessian matrix, i.e., $\tilde{A} = \frac{\partial A}{\partial A}$ using adjoint back-propagation methods [48]. The gradient of each entry $J_{k,l}$ with respect to $A$ is obtained from

$$\tilde{A}_{k,l} = U_{k,l} \left[ \tilde{A}_{k,l} + \frac{F}{2} \left( \sum_{i=1}^{N} |U_{k,l}^{T}|^{2} - U_{k,l}^{T}U_{k,l} \right) \right] U_{k,l}^{T}, \quad (A1)$$

where $\circ$ is the Hadamard product, $U \Lambda U^{T} = A$, $F^{ij} = (\lambda_{j} - \lambda_{i})^{-1}$ if $i \neq j$ and zero otherwise, and the corresponding adjoints of $U$ and $A$ are

$$\tilde{U}^{ij} = \Theta(j)U^{ij}, \quad (k = i \lor l = i),
\tilde{A}^{ij} = \Theta(i)U^{k\cdot l}U^{l\cdot i},$$

where $\Theta(j) = (\mu^{2} - \lambda_{j})^{-1}$. Finally, we write

$$A = \left[ \text{vec}(\tilde{A}_{11}), \ldots, \text{vec}(\tilde{A}_{1N}), \ldots, \text{vec}(\tilde{A}_{NN}) \right]^{T}.$$
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