

Quantum simulation of small-polaron formation with trapped ions

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We propose a method for simulating polaron physics using a one-dimensional system of trapped ions acted upon by off-resonant standing waves. This system, envisioned as an array of ion microtraps, in the single-excitation case provides a realization of the anti-adiabatic regime of the Holstein model. We show that the strong excitation-phonon coupling regime, characterized by the formation of small polarons, can be reached using realistic values of the relevant system parameters. Finally, we propose measurements of the quasiparticle residue and the average number of phonons in the ground state, experimental probes validating the polaronic character of the phonon-dressed excitation.

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The field of quantum simulation [1], inspired by the ideas of Feynman [2], holds promise to advance our understanding of complex many-body systems [3]. In this context, trapped ions [4] constitute a versatile experimental platform on which to explore a variety of models and phases [5]. Owing to the high degree of control over the internal degrees of freedom and the single-ion addressability, trapped-ion systems allow both analog and digital quantum simulations of quantum spin models [6–8], models with bosonic degrees of freedom [9], and even of phenomena outside the realm of low-energy physics [10].

Electron-phonon (more generally, particle-phonon) coupling, a traditional subject of solid-state physics, has only quite recently attracted interest from the quantum-simulation community [11]. The most striking consequence of this coupling in semiconductors and insulators is small-polaron formation: an excess electron (or a hole) can be severely localized in the potential well that it creates by displacing the surrounding atoms of the host crystal (“self-trapping”) [12]. While the polaron concept was conceived by Landau and Pekar in their studies of polar semiconductors [13], evidence has by now accumulated for small polarons in systems as diverse as amorphous and organic semiconductors, manganites, undoped cuprates, superlattices of graphene, etc. [14]. In particular, studies of small polarons in systems with short-range electron-phonon coupling are typically based on the Holstein molecular-crystal model [15]. The static and dynamical properties of this model, describing purely local interaction of tightly-bound electrons with dispersionless (Einstein) phonons, have been extensively studied [12].

In this Letter, we present a scheme for simulating small-polaron formation using a linear array of trapped ions subject to off-resonant standing light waves. We show that, if the relevant parameters are chosen appropriately, this system is described by an effective model whose single-excitation sector corresponds to the anti-adiabatic regime of the Holstein model (hopping amplitude much smaller than the phonon frequency). Furthermore, we find that with realistic values of experi-

mental parameters (laser intensities, detunings, trap frequencies, etc.) a regime is realized where the dressed single-excitation ground state has polaronic character. Finally, we suggest methods for measuring the quasiparticle spectral residue and the average number of phonons in the single-excitation ground state, quantities that provide typical signatures of small-polaron formation.

System and effective Hamiltonian.— We consider a one-dimensional system of N trapped ions with four internal states ($|\uparrow\rangle_z$, $|\downarrow\rangle_z$, $|e_\uparrow\rangle_z$, $|e_\downarrow\rangle_z$) and a possible physical implementation as an array of microtraps (for an illustration, see Fig. 1). We take the z -axis to be parallel to the direction of the ion chain (longitudinal direction), while x and y will be the radial (transverse) directions.

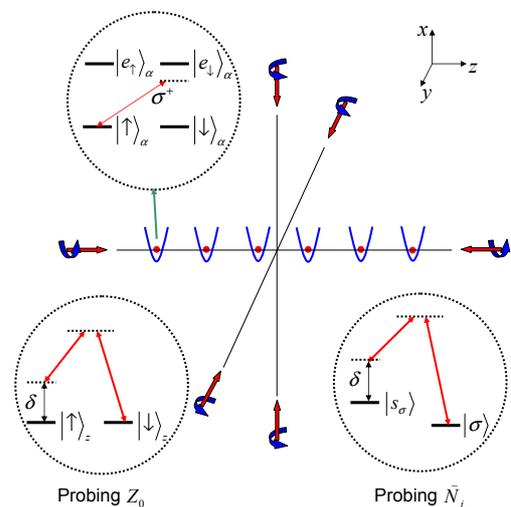


FIG. 1: (Color online) System schematic: Trapped-ion chain subject to three pairs of counterpropagating laser beams giving rise to three standing waves. The standing wave with the polarization σ^+ in the direction α induces the transition from $|\uparrow\rangle_\alpha$ to $|e_\downarrow\rangle_\alpha$, where $|\uparrow, \downarrow\rangle_x = (|\uparrow\rangle_z \pm |\downarrow\rangle_z)/\sqrt{2}$ and $|\uparrow, \downarrow\rangle_y = (|\uparrow\rangle_z \pm i|\downarrow\rangle_z)/\sqrt{2}$.

The total potential felt by an ion consists of the trapping-potential contribution (with trapping frequencies ω_α , $\alpha = x, y, z$) and the Coulomb repulsion between the ions. In the harmonic approximation, the total vibrational Hamiltonian of the system reads (hereafter $\hbar = 1$)

$$H_{\text{ph}} = \sum_{i,\alpha} \frac{(p_i^\alpha)^2}{2m} + \frac{m}{2} \sum_{i,j,\alpha} \mathcal{K}_{ij}^\alpha q_i^\alpha q_j^\alpha. \quad (1)$$

The displacements q_i^α of the i -th ion (mass m) from its equilibrium position z_i^0 (p_i^α are the corresponding momenta) are expressed through the creation and annihilation operators of phonon modes with frequencies $\omega_{s,\alpha}$ as $q_i^\alpha = \sum_s \mathcal{M}_{s,\alpha}^i (2m\omega_{s,\alpha})^{-1/2} (a_{s,\alpha} + a_{s,\alpha}^\dagger)$, such that $H_{\text{ph}} = \sum_{s,\alpha} \omega_{s,\alpha} a_{s,\alpha}^\dagger a_{s,\alpha}$; $\mathcal{M}_{s,\alpha}^i$ is the i -th component of the normalized eigenstate $\mathcal{M}_{s,\alpha}$ of the matrix \mathcal{K}^α : $\sum_{i,j} \mathcal{M}_{s,\alpha}^i \mathcal{K}_{ij}^\alpha \mathcal{M}_{s',\alpha}^j = \omega_{s,\alpha}^2 \delta_{ss'}$. If the trapping potential in a transverse direction α dominates over the Coulomb interaction [the stiff limit: $\beta_\alpha \equiv e^2/(m\omega_\alpha^2 d_0^3) \ll 1$, where d_0 is the mean distance between two adjacent ions], the vibrations in this direction are highly localized in real space (weakly dispersive phonons) [6]. On the other hand, by tuning ω_z one can reach both the weakly-dispersive ($\beta_z \ll 1$) and the strongly-dispersive ($\beta_z \gg 1$) regime for longitudinal phonons.

As shown in Fig. 1, three pairs of counterpropagating laser beams with the polarization σ^+ form three standing waves, which induces the transition from $|\uparrow\rangle_\alpha$ to $|e_\downarrow\rangle_\alpha$ [6]. Under the rotating-wave approximation, the adiabatic elimination of the higher energy states $|e_\uparrow\rangle_z$ and $|e_\downarrow\rangle_z$ leads to the effective interaction

$$H_I = \sum_{i,\alpha} \frac{G_\alpha^2}{2\Delta_\alpha} \cos^2(k_\alpha q_i^\alpha + \phi_\alpha) (1 + \sigma_i^\alpha) \quad (2)$$

between phonons and the pseudo-spins corresponding to the internal states $|\uparrow\rangle_z$ and $|\downarrow\rangle_z$, where $\Delta_\alpha \equiv \omega_{L,\alpha} - \omega_0$ is the detuning between the energy-level spacing ω_0 and the laser frequency along the α direction; σ_i^α is the Pauli matrix in the basis of $|\uparrow\rangle_z$ and $|\downarrow\rangle_z$. These pseudo-spins are simultaneously acted upon by global magnetic fields, as described by the Hamiltonian $H_m \equiv \sum_{i,\alpha} B_\alpha \sigma_i^\alpha$.

In the Lamb-Dicke limit, the ion-position dependent coupling constants can be linearized around the equilibrium position, so that the interaction term becomes $H_I = -\sum_{i,\alpha} F_\alpha q_i^\alpha (1 + \sigma_i^\alpha)$. Here, the effective force F_α is given by $F_\alpha \sim G_\alpha^2 k_\alpha / (2\Delta_\alpha)$. For convenience, we focus on the parameters $F_x = F_y = F$, $\omega_x = \omega_y = \omega_0$, and $\beta_x = \beta_y = \beta$. Given that $F/(\omega_0 \sqrt{2m\omega_0}) \equiv \eta \ll 1$, due to the large transverse-phonon frequencies, one can perturbatively eliminate transverse phonons using a Fröhlich-like canonical transformation [6]. In this manner, we ob-

tain the effective Hamiltonian

$$H_{\text{eff}} = H_L + F_z \sum_i q_i^z (1 + \sigma_i^z) \quad (3)$$

$$+ B_z \sum_i \sigma_i^z + \sum_{i < j, \alpha = x, y} \frac{2\beta\eta^2\omega_0}{|i-j|^3} \sigma_i^\alpha \sigma_j^\alpha,$$

where the external magnetic fields $B_\alpha = F_\alpha^2/m\omega_\alpha^2$ ($\alpha = x, y$) were chosen in order to cancel the effective fields from the adiabatic elimination. The Hamiltonian

$$H_L = \tilde{\omega}_z \sum_i b_i^\dagger b_i - \sum_{i \neq j} \frac{\tilde{\beta}_z \tilde{\omega}_z}{2|i-j|^3} (b_j^\dagger b_i + \text{H.c.}) \quad (4)$$

describes longitudinal phonons in terms of local-phonon operators, where $q_i^z = (2m\tilde{\omega}_z)^{-1/2} (b_i + b_i^\dagger)$ and the renormalized longitudinal-phonon frequency is given by $\tilde{\omega}_z = \omega_z^2 \sqrt{1 + \sum_{j' \neq i} (2\beta_z / |i-j'|^3)}$. The form of the second term in Eq. (4) results from omitting the phonon-number nonconserving terms under the rotating-wave approximation; the corresponding condition coincides with the stiff limit $\tilde{\beta}_z \equiv e^2/(m\tilde{\omega}_z^2 d_0^3) \ll 1$.

By switching to the fermion representation of the effective spin operators [$1 + \sigma_i^z \rightarrow 2c_i^\dagger c_i$; $\sigma_i^x \sigma_j^x + \sigma_i^y \sigma_j^y \rightarrow 2(c_i^\dagger c_j + \text{H.c.})$], the effective Hamiltonian in the *single-excitation* sector of the problem can be written as $H_{\text{se}} = H_e + H_L + H_{\text{e-ph}}$, with

$$H_e = \sum_{i < j} \frac{J}{|i-j|^3} (c_i^\dagger c_j + \text{H.c.}) + 2B_z \sum_i c_i^\dagger c_i,$$

$$H_{\text{e-ph}} = g\tilde{\omega}_z \sum_i c_i^\dagger c_i (b_i + b_i^\dagger). \quad (5)$$

Here $J = 4\beta\eta^2\omega_0$ is the hopping amplitude, while $g = \sqrt{2}F_z/\sqrt{m\tilde{\omega}_z^3}$ is the dimensionless excitation-phonon (e-ph) coupling strength. This coupling, described by $H_{\text{e-ph}}$, has Holstein-like (local) form.

Limits of validity and parameter range.— Let us summarize the conditions of validity of the Hamiltonian H_{se} and specify in which parameter regime it reduces to the Holstein model with dispersionless phonons.

Firstly, the use of perturbation theory for eliminating transverse phonons requires that $\eta \ll 1$, which implies that $J \ll \omega_0$ must be fulfilled. Secondly, while a weak phonon dispersion [here proportional to $\beta_z \tilde{\omega}_z$; cf. Eq. (4)] is inherent to the stiff limit, for our purposes the dispersion should be negligible even compared to the hopping amplitude J . From the condition $\tilde{\beta}_z \tilde{\omega}_z \ll J$ we readily obtain $\omega_0/\tilde{\omega}_z < 4\eta^2 < 1$. Thus our system can simulate the Holstein model with $J \ll \omega_0 < \tilde{\omega}_z$, i.e., in its anti-adiabatic regime. In other words, the effective Hamiltonian of the system then reads $H = H_e + H_{\text{ph}} + H_{\text{e-ph}}$, with $H_{\text{ph}} = \tilde{\omega}_z \sum_i b_i^\dagger b_i$.

Unlike the genuine Holstein model, which only involves nearest-neighbor hopping, the last effective Hamiltonian

also contains long-range hopping terms decaying with the characteristic inverse third power of the distance. However, in the anti-adiabatic regime that we will be solely concerned with these long-range terms are of minor importance.

We now discuss whether one can realize the strong-coupling regime of the Holstein model, characterized by small-polaron formation. To achieve that, a coupling constant g of the order of unity is needed. We first express g in terms of the relevant experimental parameters starting from the expression $F_z \sim (G_z^2/\Delta_z) \times (2\pi/\lambda)$, where λ the laser wavelength, and Δ_z the detuning between the laser and the internal energy-level spacing. Since $g\tilde{\omega}_z = \sqrt{2}F_z/\sqrt{m\tilde{\omega}_z}$ and $a/d \sim 1/(\lambda\sqrt{2m\tilde{\omega}_z})$, where a is the size of the trap ground state (for concreteness, we assumed that $d_0 = \lambda$, while in general d_0 is an integer multiple of λ), we readily obtain

$$g = \frac{4\pi}{\tilde{\omega}_z} \frac{G_z^2}{\Delta_z} \times \frac{a}{d_0}. \quad (6)$$

Thus the value of g can be varied by tuning the ratio G_z^2/Δ_z , for different values of the phonon frequency ω_z .

We choose $\lambda = d_0 = 2\mu\text{m}$, and the typical value of the detuning $\Delta = 1000\text{ GHz}$. With Rabi frequencies $G_z = 10 - 100\text{ GHz}$, the ratio G_z^2/Δ_z is in the range $0.1 - 10\text{ GHz}$. At the same time, the phonon frequency is typically $\omega_z/2\pi = 1 - 20\text{ MHz}$. For example, already for $G_z^2/\Delta_z = 2\text{ GHz}$ and $\tilde{\omega}_z/2\pi = 10\text{ MHz}$ (the ratio $a/d_0 \approx 4.25 \times 10^{-3}$) we obtain $g \approx 1.72$, a value of g that belongs to the strong-coupling regime.

Polaron ground state.— To determine the ground state of the system, we make use of the variational method. Variational approaches, commonly employed in small-polaron studies, have been established to yield results that agree very well with exact-diagonalization results on systems of small size [16–18].

The eigenstates of the total Hamiltonian are good quasi-momentum states, i.e., simultaneous eigenstates of the total momentum operator $K = \sum_k k c_k^\dagger c_k + \sum_q q b_q^\dagger b_q$ (with eigenvalues denoted by κ in what follows). Therefore, variational states must be Bloch-like linear combinations $|\psi_\kappa\rangle = N^{-1/2} \sum_n e^{i\kappa n} |\psi_\kappa(n)\rangle$ of Wannier-like functions $|\psi_\kappa(n)\rangle$. In particular, for the Toyozawa Ansatz states [19]

$$|\psi_\kappa(n)\rangle = \sum_{m=-N/2}^{N/2-1} \Phi_\kappa(m) e^{i\kappa m} c_{n+m}^\dagger |0\rangle_e \otimes |\xi_\kappa(n)\rangle_{\text{ph}}, \quad (7)$$

with $|\xi_\kappa(n)\rangle_{\text{ph}} \equiv \prod_l \exp(v_l^\kappa b_{n+l}^\dagger - v_l^{\kappa*} b_{n+l}) |0\rangle_{\text{ph}}$ being a direct product of phonon coherent states at sites $n+l$ ($l = -N/2, \dots, N/2$). The parameters $\{\Phi_\kappa(m), v_l^\kappa\}$, in total $2N$ of them, are complex valued. The normalization is given by $\langle\psi_\kappa|\psi_\kappa\rangle = \sum_{m,m'} \Phi_\kappa^*(m') \Phi_\kappa(m) S_{m'-m}^\kappa$, where $S_{n-n'}^\kappa \equiv \exp[-\frac{1}{2} \sum_p (|v_{p-n'}^\kappa|^2 + |v_{p-n}^\kappa|^2 - 2v_{p-n'}^{\kappa*} v_{p-n}^\kappa)]$.

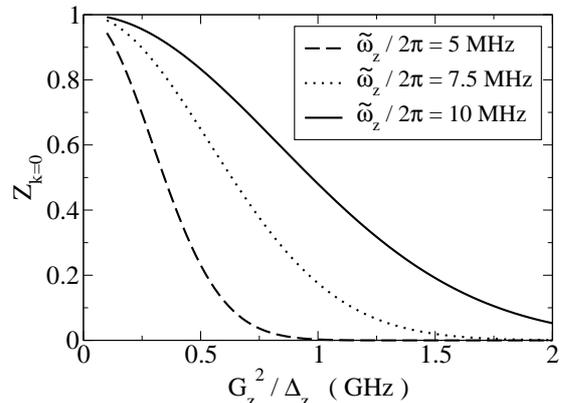


FIG. 2: Calculated quasiparticle residue at $k = 0$ for different values of the renormalized longitudinal-phonon frequency $\tilde{\omega}_z$. All three curves correspond to the hopping amplitude $J = 25\text{ KHz}$.

In the limit $\tilde{\omega}_z/J \rightarrow \infty$ the Toyozawa Ansatz yields (for $\kappa = 0$) the exact ground state of the Holstein model, given by $a_{n_0}^\dagger |0\rangle_e \otimes |v_{n_0}^{\kappa=0} = g\rangle_{\text{ph}}$ (where $v_l^{\kappa=0}$ at sites $l \neq n_0$ are equal to zero) [17]. The last statement holds true not only for the genuine Holstein model with nearest-neighbor hopping J , but also for our model with long-range hoppings, as the latter have amplitudes proportional to J . This makes the Toyozawa Ansatz particularly appropriate for the problem at hand.

The ground-state energy E_{GS} is obtained by minimizing the expectation value $\langle\psi_{\kappa=0}|H|\psi_{\kappa=0}\rangle$ with respect to $4N$ variational parameters, the modules and phases of the complex parameters $\Phi_{\kappa=0}(m)$ and $v_l^{\kappa=0}$. While there is no principal obstacle to treating even larger system, in the following we present results obtained for $N = 32$.

Characterization of the polaron crossover.— The quasiparticle residue at quasi-momentum k is defined as $Z_k \equiv |\langle\Psi_k|\psi_k\rangle|^2 / \langle\Psi_k|\Psi_k\rangle$, the overlap squared of the bare-excitation Bloch state $|\Psi_k\rangle \equiv c_k^\dagger |0\rangle = N^{-1/2} \sum_n e^{ikn} c_n^\dagger |0\rangle$ and the corresponding (dressed-excitation) Bloch state $|\psi_k\rangle$ of the coupled excitation-phonon system. For the Toyozawa Ansatz state, we find

$$Z_k = \frac{\left| \sum_m \Phi_k(m) \right|^2}{\sum_{m,m'} \Phi_k^*(m') \Phi_k(m) S_{m'-m}^k} \prod_l e^{-|v_l^k|^2}. \quad (8)$$

The quasiparticle residue $Z_{k=0}$, when evaluated for optimal values of the variational parameters, characterizes the ground state of the system. The change of this quantity from unity (non-interacting system) to values very close to zero (Fig. 2) illustrates the crossover from a quasi-free excitation to a small polaron.

Another quantity characterizing the polaron crossover

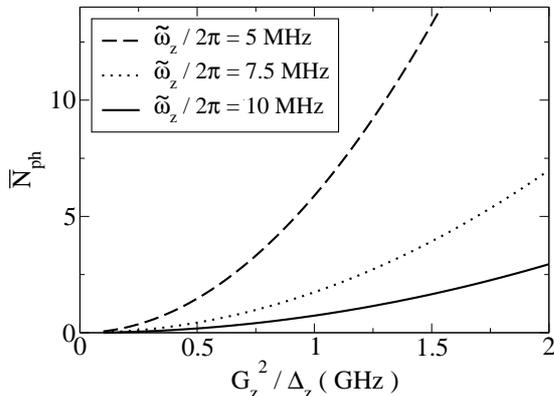


FIG. 3: Average number of phonons in the single-excitation ground state. All three curves correspond to $J = 25$ KHz.

is the average number of phonons in the ground state

$$\begin{aligned} \bar{N}_{\text{ph}} &\equiv \langle \psi_{\kappa=0} | \sum_i b_i^\dagger b_i | \psi_{\kappa=0} \rangle \\ &= \sum_{m, m', p} \Phi_{\kappa=0}^*(m') \Phi_{\kappa=0}(m) S_{m'-m}^{\kappa=0} v_{p+m'}^{\kappa=0*} v_{p+m}^{\kappa=0}. \quad (9) \end{aligned}$$

As illustrated in Fig. 3, this quantity varies from $\bar{N}_{\text{ph}} \approx 0$ (quasi-free excitation) to values $\bar{N}_{\text{ph}} \gtrsim 3$ (small polarons) with increasing coupling strength.

Our analysis indeed shows that the effect of the fast-decaying long-range hopping on the quantities characterizing the polaron crossover is very small in the anti-adiabatic regime. This is consistent with a recent study of the Holstein model with next-nearest-neighbor hopping which established that such hopping is significant only in the opposite, adiabatic regime [20].

Experimental validation.— We propose two experimental methods, as illustrated in Fig. 1, to detect the quasiparticle residue $Z_{k=0}$ and the average number of phonons \bar{N}_{ph} in the single-excitation ground state.

To probe $Z_{k=0}$, we first prepare the system in the ground state (without a polaronic excitation), namely, the vacuum state of the longitudinal phonons and the internal states $|\downarrow\rangle$ of all the ions. Then, all the laser beams are turned on. At the same time, an additional Raman laser with the detuning δ is used for generating an excitation (polaron). The latter is described by the Hamiltonian $H_{\text{detect}} = \xi N^{-1/2} \sum_i (\sigma_i^+ e^{-i\delta t} + \text{H.c.})$, where ξ is the effective Rabi frequency. After the evolution time T , we switch off the laser beams and measure $O = N^{-1/2} \sum_i \sigma_i^x$ [4]. By repeating the measurement one can determine the mean-value $\langle O \rangle$. For short times $T \ll 1/\xi$, near the resonance frequency $\delta \sim E_{\text{GS}}$ of the ground state in the single-polaron space, first-order perturbation theory yields

$$\langle O \rangle \sim 2\xi Z_{k=0} \frac{\sin(\delta T) - \sin(E_{\text{GS}}T)}{\delta - E_{\text{GS}}}. \quad (10)$$

Thus measurements of $\langle O \rangle$ provide a direct access to the quasiparticle residue $Z_{k=0}$, the quantity whose strongly reduced values indicate the presence of small polarons.

For detecting the mean phonon number \bar{N}_{ph} , we first prepare the system in the single-polaron ground state $|E_{\text{GS}}\rangle \equiv |\psi_{\kappa=0}\rangle$ and switch off all laser beams. Then, we detect the internal state of the ion on the site j . If the internal state is $|\downarrow\rangle_j$, the Raman laser is turned on to induce the transition between $|\downarrow\rangle_j$ to another state $|s_\downarrow\rangle_j$; if the internal state is $|\uparrow\rangle_j$, the Raman laser is turned on to induce the transition between $|\uparrow\rangle_j$ to the state $|s_\uparrow\rangle_j$, as shown in Fig. 1. Here, each Raman laser is turned to the lower sideband detuning $\delta = \omega_z$. Thus, in the interaction picture the time evolution of the system is described by the Hamiltonian $H_{\sigma=\uparrow,\downarrow} = \xi(b_j |s_\sigma\rangle_j \langle\sigma| + \text{H.c.})$. After the evolution time T , we detect the probability $p_{\sigma,j}$ of the transition to $|s_\sigma\rangle_j$. For the short-time evolution, first-order perturbation theory leads to $p_{\sigma,j} = \xi^2 T^2 \langle E_{\text{GS}} | b_j^\dagger b_j P_\sigma^{(j)} | E_{\text{GS}} \rangle$, where $P_\sigma^{(j)} = |\sigma\rangle_j \langle\sigma|$ is the projection operator. Finally, the average number of phonons at site j is $\bar{N}_j = \sum_\sigma p_{\sigma,j} / (\xi^2 T^2)$. Therefore, measurements of the transition probabilities $p_{\sigma,j}$ ($j = 1, \dots, N$) allow us to extract the average number of phonons at each site (microtrap). Large values of $\bar{N}_{\text{ph}} = \sum_j \bar{N}_j$ represent a signature of small polarons.

Conclusions.— To conclude, we have suggested a scheme for the quantum simulation of polaron physics with trapped ions. We have shown that with realistic values of the relevant experimental parameters one can reach the strong-coupling regime of the Holstein model, characterized by small-polaron formation. An experimental realization of our suggested scheme in an array of ion microtraps is clearly called for. The scheme proposed here opens up new possibilities to analyze polaron physics with trapped ions. For instance, one may go beyond to the single-excitation regime, and thus study the interactions among polaronic excitations. Furthermore, with the advent of surface traps [4, 21], it should be possible to extend the study to two dimensions, and also to engineer other kinds of interactions. Experiments with trapped ions may allow us to better understand polaron physics in these circumstances, and to develop new theoretical tools to describe the resulting phenomena.

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