

# Spin-Holstein models in trapped-ion systems

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In this work, we highlight how trapped-ion quantum systems can be used to study generalized Holstein models, and benchmark expensive numerical calculations. We study a particular *spin*-Holstein model that can be implemented with arrays of ions confined by individual microtraps, and that is closely related to the Holstein model of condensed matter physics, used to describe electron-phonon interactions. In contrast to earlier proposals, we focus on realizing many-electron systems and inspect the competition between charge-density wave order, fermion pairing and phase separation. In our numerical study, we employ a combination of complementary approaches, based on non-Gaussian variational ansatz states and matrix product states, respectively. We demonstrate that this hybrid approach outperforms standard density-matrix renormalization group calculations.

Electron-phonon interactions lie at the heart of several phenomena in condensed matter physics, including Cooper pairing [1] and the formation of polarons [2]. Generally, the low-energy excitations of electrons in solids are modified by their coupling to lattice vibrations, which alters their transport and thermodynamic behaviour. Often simplified toy models can be employed to study those essential properties. As a complementary approach to traditional solid-state methods, quantum simulations utilize the rich toolbox of atomic physics to provide a characterization of equilibrium and dynamical properties of paradigmatic quantum many-body models.

The Holstein model is one such paradigmatic model that features a local coupling between the electron density and optical phonons on a lattice [3]. Despite its apparent simplicity, it hosts rich physics, giving rise to superconducting (SC) phases, charge-density wave (CDW) order and phase separation (PS) at strong coupling [4, 5]. Yet, notwithstanding recent progress, its numerical treatment is often costly, especially when interactions become increasingly strong or of long-range character. As a tantalizing prospect, trapped-ion quantum simulators may help to gain new insights into the underlying physical mechanisms [6, 7]. Their spin and motional degrees of freedom can be harnessed to realize a quantum-optics analogue of the electron-phonon system [8–11], which enables access to a variety of system observables. Moreover, their key parameters may be tuned *in-situ* to explore different regions of the phase diagram. Currently available setups may thus be utilized to benchmark analogue quantum simulators against numerical computations.

In this Letter, we theoretically investigate such trapped-ion systems and derive an effective model that contains strong and highly non-local interactions be-

tween effective spins and lattice phonons. We highlight its similarities and differences with the Holstein model and develop a powerful numerical toolbox to thoroughly characterize its ground-state properties. Our numerical method combines density matrix renormalization group (DMRG) calculations [12] and computations based on non-Gaussian variational ansatz states (NGS) [13, 14]. We define spin and phonon observables motivated by the physics of the Holstein model and study their characteristics. Using these observables, we identify SC and CDW phases and their relation to the ion-trap parameters, thus demonstrating the rich Holstein-like physics of the trapped-ion system. Finite-temperature and finite-size calculations show that our results can be expected to be robust against thermal excitations in state-of-the-art setups.

*Setup and model.*—We consider a physical system of  $N$  ions with mass  $m$ , each confined to a harmonic microtrap. All of the ions' equilibrium positions are assumed to be aligned along the  $\hat{z}$  axis and equidistantly spaced, see Fig. 1(a). The vibrations of ions in a microtrap array can be described by ( $\hbar = 1$ )

$$H_{\text{ph}} = \sum_{\substack{i=1, \\ \alpha=x,y,z}}^N \frac{(p_i^\alpha)^2}{2m} + \frac{m}{2} \sum_{i,j,\alpha} \mathcal{K}_{ij}^\alpha r_i^\alpha r_j^\alpha, \quad (1)$$

where  $p_i^\alpha$  denotes the momentum and  $r_i^\alpha = 1/\sqrt{2m\omega_\alpha}(b_{i,\alpha} + b_{i,\alpha}^\dagger)$  is the displacement of the  $i$ th ion from its equilibrium position in the  $\alpha$  ( $= x, y$  or  $z$ ) direction, with the trap frequencies  $\omega_\alpha$  and local phonon ladder operators  $b_{i,\alpha}^{(\dagger)}$ .  $\mathcal{K}^\alpha$  denotes the elasticity matrix of the ion chain in the  $\alpha$  direction, and its eigenvectors describe the chain's normal modes [8].

In the setup we consider (see Fig. 1), a laser beam

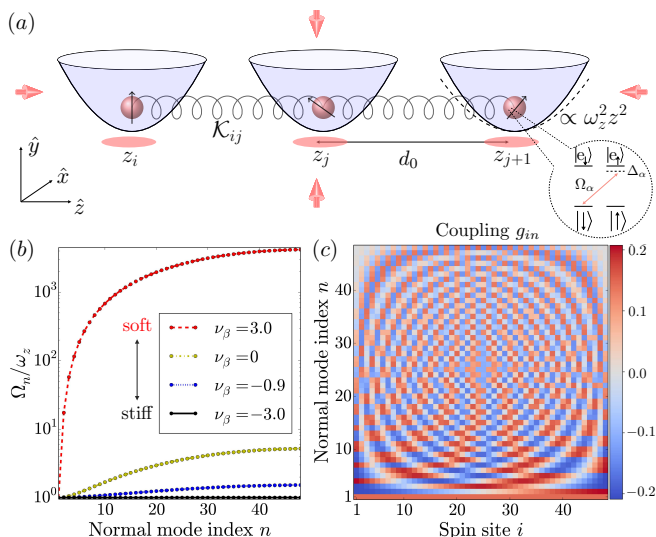


FIG. 1. Schematic illustration of setup. (a) Trapped-ion chain subject to three counter-propagating laser beams. The microtraps are aligned along the  $\hat{z}$  direction at a distance  $d_0$ . Ions are coupled to each other via their mutual Coulomb interaction, indicated by springs. The inset shows an exemplary level scheme with four internal states  $|\uparrow\rangle, |\downarrow\rangle, |e_\downarrow\rangle, |e_\uparrow\rangle$ , and a  $\sigma^+$  transition with laser parameters  $\Omega_\alpha$  and  $\Delta_\alpha$ . (b) Normal-mode frequencies  $\Omega_n/\omega_z$  for different values of  $\nu_\beta$ .  $\omega_z$  is fixed while  $d_0$  is varied. (c) Coupling  $g_{in}$  for  $\nu_\beta = 0$  exemplarily shows long-range interactions between spins and phonons.

configuration is chosen to host three standing waves along the  $\hat{x}, \hat{y}$  and  $\hat{z}$  axes. Light that is off-resonant with chosen hyperfine-state transitions of the ions can be harnessed to introduce a coupling between the motional and spin degrees of freedom of the ions [8, 9]. Within the rotating-wave approximation, we obtain an effective spin-phonon coupling of the form

$$H_{\text{int}} = \sum_{\substack{i=1, \\ \alpha=x,y,z}}^N \frac{\Omega_\alpha^2}{2\Delta_\alpha} \cos^2(k_\alpha r_i^\alpha + \phi_\alpha) (1 + \sigma_i^\alpha), \quad (2)$$

where  $\Omega_\alpha$  denotes the Rabi frequency,  $\Delta_\alpha$  is the qubit-laser detuning,  $k_\alpha$  the wavenumber,  $\phi_\alpha$  the relative phase of counterpropagating lasers and  $\sigma_i^\alpha$  denotes the Pauli matrix associated with the internal spin states  $|\uparrow\rangle$  and  $|\downarrow\rangle$  at site  $i$  and direction  $\alpha$ . In the Lamb-Dicke regime, characterized by a small parameter  $\eta_\alpha = k_\alpha/\sqrt{2m\omega_\alpha} \ll 1$ , Eq. (2) can be linearized around the ions' equilibrium positions, so that the interaction Hamiltonian takes the simplified form  $H_{\text{int}} = -F_\alpha \sum_{i,\alpha} r_i^\alpha (1 + \sigma_i^\alpha)$ , with a coupling strength  $F_\alpha \sim \Omega_\alpha^2 k_\alpha / (2\Delta_\alpha)$  that can be controlled by laser parameters.

We assume large transverse trap frequencies and eliminate the motional degrees of freedom along  $\hat{x}$  and  $\hat{y}$  via a polaron transformation, such that two pseudospins of distance  $r$  become effectively coupled through an effective dipolar interaction  $J/r^3$  [8]. Thus we obtain an effective

description of our system  $H_{\text{eff}} = U_{\text{pol}}(H_{\text{ph}} + H_{\text{int}})U_{\text{pol}}^\dagger$ , which takes the form (see [15] for more details)

$$H_{\text{eff}} = \sum_n \Omega_n a_n^\dagger a_n + \sum_{\substack{i \neq j, \\ \alpha=x,y}} \frac{J}{|i-j|^3} \sigma_i^\alpha \sigma_j^\alpha + H_{\text{int}} \quad (3)$$

where  $a_{n=1,\dots,N}$  are annihilation operators of the  $N$  collective phonon normal modes with frequencies  $\Omega_n$  (see Fig. 1(b)). In terms of the mode expansion  $r_i = \sum_n g_{in}(a_n + a_n^\dagger)$  the interaction  $H_{\text{int}} = -F_z \sum_i r_i (1 + \sigma_i^z)$  of spins and local longitudinal phonons becomes

$$H_{\text{int}} = -F_z \sum_{i,n} g_{in}(a_n + a_n^\dagger)(1 + \sigma_i^z), \quad (4)$$

where  $g_{in}$  describes the non-local coupling between phonon normal modes and spins (see Fig. 1(c)).

Our effective model in Eq. (3) contains several key parameters that determine its behaviour. In the following, we set  $\omega_z/J = 1$  for all microtraps, and focus on the rich physics left to explore with the remaining free parameters. In particular, the system can now be described by (i) the spin-phonon coupling  $F_z$  and (ii) the ion trap stiffness  $\beta = e^2/(m\omega_z^2 d_0^3)$  along the  $\hat{z}$  direction. Throughout this work, we will use  $\nu_\beta = \log \beta$ . Typically, in trapped-ion physics, the limit  $\nu_\beta \lesssim -1$  ( $\nu_\beta \gtrsim 1$ ) is referred to as the stiff (soft) limit, in which the phonon dispersion is weak (strong) (see Fig. 1(b)). The ion-trap setup therefore allows us to switch between the adiabatic (small phonon frequency) and anti-adiabatic (large phonon frequency) regimes of the spin-Holstein model (3).

*Numerical approach.*—In our numerical study of Eq. (3), we complement DMRG simulations with numerical calculations based on NGS,  $|\Psi_{\text{NGS}}\rangle$ , that can be written in the form [13]

$$|\Psi_{\text{NGS}}\rangle = U_S |\Psi_{\text{GS}}\rangle \quad (5)$$

where  $U_S$  is a unitary operator and  $|\Psi_{\text{GS}}\rangle$  an arbitrary Gaussian state, both of which depend on a set of variational parameters (see Eqs. (S15) and (S17)). We derive and solve the equations of motion for these variational parameters to obtain the many-body ground state of  $H_{\text{eff}}$ , see [15] for more details. In order to treat the model in Eq. (3) with the NGS, we employ a Jordan-Wigner transformation and map  $H_{\text{eff}}$  onto a fermionic model via

$$\sigma_i^z = 2c_i^\dagger c_i - 1, \quad \sigma_i^+ = e^{i\pi \sum_{l < i} c_l^\dagger c_l} c_i^\dagger. \quad (6)$$

Expressing the Hamiltonian (3) in terms of fermionic operators by means of (6) shows the similarity with the Holstein model, as studied in condensed matter physics. However the models are not equivalent. One key difference originates from the long-range hopping terms  $\propto P_{ij}/|i-j|^3 c_i^\dagger c_j$  (with the string operator  $P_{ij}$ , see [15] for more details) present in our effective fermionic model, which stems from the dipolar decay of interactions in

Eq. (3). Moreover, in contrast to the genuine Holstein model which features a purely local coupling of electron and Einstein phonon, the phonon described by Eq. (3) is dispersive and its bandwidth may be tuned by means of  $\beta$ .

While NGS excel at numerical efficiency and capture the essential physics well, DMRG yields higher numerical accuracy. However the DMRG study of Eq. (3) faces several technical challenges. Arguably two of the most relevant practical obstacles are associated with (i) not getting stuck in a local energy minimum during the algorithm, and (ii) avoiding truncation errors introduced by working with finite local phonon Hilbert spaces. In our numerical treatment, we find that (i) NGS can provide an excellent educated guess for the initial state fed into the DMRG algorithm, thus lowering the chances for getting stuck with a metastable solution. Moreover, (ii) the truncation error associated with finite local Hilbert spaces can be significantly lowered by employing a unitary displacement transformation on Eq. (3) (see [15]). Note that more general approaches exist to tackle this issue and have been applied to problems with fermion-phonon coupling [16–21].

*Phase diagram.*—Equipped with our numerical toolbox, we study the ground-state properties of  $H_{\text{eff}}$  and calculate several spin and phonon observables. Especially, we introduce the CDW order parameter

$$O_{\text{CDW}} = \frac{1}{2N} \sum_{n=1}^N (-1)^n (1 + \langle \sigma_n^z \rangle), \quad (7)$$

and the four-point spin correlator

$$O_{\text{SC}} = \langle \sigma_i^+ \sigma_{i+1}^+ \sigma_{i+\delta}^- \sigma_{i+1+\delta}^- \rangle, \quad (8)$$

with which we identify the superconducting ground state by calculating its decay as a function of  $\delta$  for fixed  $i$ . The order parameters that we compute with the NGS approach for the fermionic model are derived in the Supplemental Material [15].

We study the phase diagram for different filling factors  $\nu = (\sum_i 1 + \langle \sigma_i^z \rangle)/(2N)$ . In Fig. 2, we show the result for  $N = 48$  spins at  $\nu = 1/2$  (left panel) and  $\nu = 1/4$  (right panel) as a function of  $F_z$  and  $\nu_\beta$ . The phase boundaries obtained with both numerical methods quantitatively agree with each other.

At half filling ( $\nu = 1/2$ ), and at sufficiently large spin-phonon coupling  $F_z \gtrsim 1$ , we find three distinct phases, that display charge-density wave order, quasi-long range superconducting order of  $p$ -wave pairing, and phase separation into two regions, in which the spins are pointing either up or down, respectively: (i) In the stiff limit ( $\nu_\beta \lesssim -1$ ), where the harmonic trapping potential dominates the Coulomb interaction, the phonons are more localized than in the soft limit. As a result, the mediated interactions are short-ranged, and in the regime  $\nu_\beta \lesssim -1$

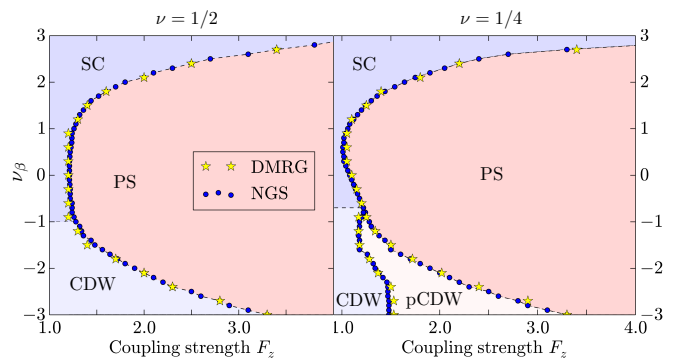


FIG. 2. Phase diagram of spin-Holstein model.  $\nu_\beta \gtrsim 1$  ( $\nu_\beta \lesssim -1$ ) corresponds to the soft (stiff) limit. *Left panel:* At filling factor  $\nu = 1/2$ , there exist three distinct phases at sufficiently large  $F_z$ , in a charge-density wave (CDW), a superconducting (SC) and a phase-separated (PS) regime. *Right panel:* At  $\nu = 1/4$ , there exists an additional pCDW phase (discussed in the main text). Numerical parameters:  $N = 48$ ,  $\omega_z/J = 1$ .

we discover a CDW state as the preferred ground state at moderate  $F_z$ . It is characterized by an alternating spin configuration  $\langle \sigma_n^z \rangle \propto (-1)^n$  ( $n = 1, \dots, N$ ) and a large order parameter  $O_{\text{CDW}} \sim 0.5$ . (ii) In the soft limit ( $\nu_\beta \gtrsim 1$ ), where the phonon modes mediate long-range interactions between spins, we find a superconducting ground state that exhibits a slow power-law decay  $O_{\text{SC}} \sim \delta^{-\alpha}$ , with  $\alpha \approx 2$ . (iii) At sufficiently large  $F_z$ , the ground state displays phase separation into two regions with opposite polarization, both in the stiff and in the soft limit. The size of the domain wall between those regions decreases, as  $F_z$  is increased (see [15] for details).

At quarter filling ( $\nu = 1/4$ ), we map out a similar phase diagram, and find an additional phase in the stiff limit ( $\nu_\beta \lesssim -1$ ), which we refer to as the pCDW phase, see Fig. 2. It is prevalent in an intermediate coupling-strength regime between the CDW and PS regions, and it is characterized by the coexistence of phase separation and an enhanced CDW order parameter. The pCDW phase is characterized by half of the spin chain being polarized and a staggered magnetization in the other half. Representative results for the spin configurations of different phases at  $\nu = 1/4$  are shown in Fig. 3(e)–(h). As we increase  $F_z$  in the stiff limit, first the CDW order emerges, as can be seen in Fig. 3(g), where  $\nu_\beta = -2.1$ ,  $F_z = 1.2$  and  $O_{\text{CDW}} \approx 0.14$ . In this case, the structure factor  $S(q) \sim \sum_{i,j} \langle \sigma_i^z \sigma_j^z \rangle \exp(iq|i-j|)$  features two pronounced peaks at  $q = \pi/2$  and  $q = 3\pi/2$  [15]. At intermediate  $F_z$ , we find a pCDW ground state as depicted in Fig. 3(h), where  $\nu_\beta = -2.1$ ,  $F_z = 1.5$  and  $O_{\text{CDW}} \approx 0.20$ . Again, at large  $F_z$  the ground state displays phase separation into two regions of opposite polarization. In all cases, we find excellent agreement between the DMRG and NGS numerical results.

*Spin-phonon correlations.*—To study the correlation

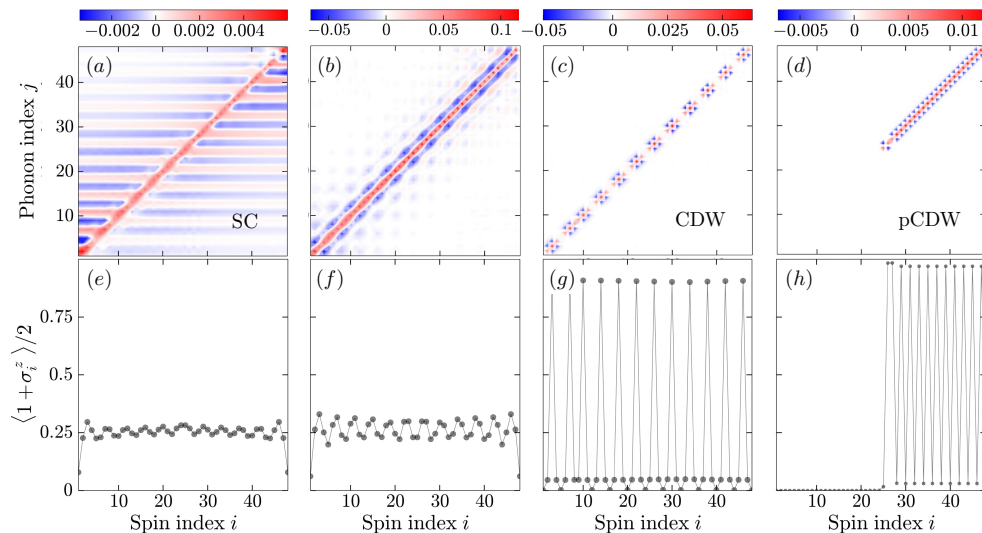


FIG. 3. Spin phonon correlator  $\Pi_{ij}$  and spin configuration for different ground states at quarter filling  $\nu = 1/4$  as obtained with DMRG. *Upper panel*: Spin-phonon correlator  $\Pi$  as defined in Eq. (9). *Lower panel*: Site-dependent spin expectation value  $(1 + \langle \sigma_i^z \rangle)/2$ . The four columns correspond to particular choices for  $F_z$  and  $\nu_\beta$  (compare right panel of Fig. 2). (a) and (e):  $F_z = 1.6$ ,  $\nu_\beta = 2.1$  (SC regime). (b) and (f):  $F_z = 0.6$ ,  $\nu_\beta = -2.1$  (precursor of CDW regime). (c) and (g):  $F_z = 1.2$ ,  $\nu_\beta = -2.1$  (CDW regime). (d) and (h):  $F_z = 1.5$ ,  $\nu_\beta = -2.1$  (pCDW regime). Other numerical parameters:  $N = 48$ ,  $\omega_z/J = 1$ .

between spins and phonons, we calculate the observable

$$\Pi_{ij} = \langle \sigma_i^z r_j \rangle - \langle \sigma_i^z \rangle \langle r_j \rangle. \quad (9)$$

In Figs. 3(a)-(d) we show the DMRG results at  $\nu = 1/4$  which agree very well with the corresponding results obtained with the NGS. In the superconducting regime, cf. Fig. 3(a), the stripe pattern of  $\Pi_{ij}$  demonstrates the presence of non-local spin-phonon correlations. For a fixed spin index  $i$ , it displays oscillations with a period four near the center of the chain. In contrast, the correlations decay quickly in the CDW and pCDW regimes and are symmetric about  $i = j$ . In the stiff limit, at small couplings we find a precursor of the CDW state, where  $\Pi_{ij}$  decays more slowly away from  $i = j$  than deep in the CDW regime, compare Figs. 3(b) and (c). A representative result for  $\Pi_{ij}$  for the pCDW ground state is shown in Fig. 3(d). As expected, the spin-phonon correlations vanish in one half of the system, while in the other they feature oscillations with a period two along the diagonal  $i = j$ , as would be expected for a CDW state at half filling. In the pCDW regime, the magnitude of the spin-phonon correlator is smaller than in the charge-density wave phase. At even larger coupling  $F_z$ , i.e. in the presence of phase separation,  $\Pi_{ij}$  vanishes almost everywhere, except for small contributions close to the domain wall.

*Experimental considerations.*—Trapped-ion experiments benefit from well-developed readout techniques. Ions can be excited from one spin state to another with single-site resolution, and subsequent fluorescence imaging allows the extraction of local expectation values  $\langle \sigma_i^z \rangle$ . Repeated measurements at different sites enable

access to spin-spin correlation functions like  $\langle \sigma_i^z \sigma_j^z \rangle$  and  $O_{SC}$ . Spin-phonon correlations may be probed with only spin measurements and additional lasers that locally couple spins and phonons. All observables of our numerical study may thus be probed experimentally.

While we have only shown numerical results for a system with  $N = 48$  ions, we also study how the phase boundary in Fig. 2 shifts in the  $(F_z, \nu_\beta)$  plane with respect to the system size  $N$  using NGS. We choose  $N = 24$  and  $N = 96$  and compare the results with those obtained for  $N = 48$ . Deep in the stiff limit ( $\nu_\beta = -3$ ), we find that there is no noticeable influence of the system size on the phase boundaries both at half and quarter filling factors. However in the soft limit, we find that the phase boundary moves to smaller (larger)  $F_z$  as  $N$  is increased (decreased). At half filling,  $\nu = 1/2$ , and  $\nu_\beta = 3$ , we find the SC-to-PS transition near  $F_z = 2.6$  for  $N = 96$  and  $F_z = 4.5$  for  $N = 48$ . For  $N = 24$ , the phase boundary disappears, i.e., we do not find any critical point numerically for  $F_z \leq 16$ . Similarly, at quarter filling and  $\nu_\beta = 3$ , we find the SC-to-PS transition near  $F_z = 2.5$  for  $N = 96$  and  $F_z = 5.9$  for  $N = 48$ . Again, for  $N = 24$  there is no transition for  $F_z \leq 16$ . To summarize, for larger systems and in the soft limit, smaller coupling strengths are thus sufficient to induce phase separation. A scaling analysis of the NGS results obtained for larger systems with up to  $N = 400$  shows that the SC phase survives in the thermodynamic limit. For example, at  $\nu_\beta = 3$  the SC-to-PS boundary moves to  $F_z \approx 1$  for  $N \rightarrow \infty$ .

We perform finite-temperature calculations using the NGS to confirm that the predicted phases survive at  $T > 0$  and may actually be observed in state-of-the-

art experiments. At temperatures up to  $T \sim J/k_B$ , we find that the  $T = 0$  ground states are robust and the phase diagrams in Fig. 2 change only insignificantly. For  $^{40}\text{Ca}^+$  ions at an effective temperature  $T = 1\mu\text{K}$  and with our choice  $\omega_z/J = 1$ , this corresponds to trap distances  $d_0 \approx 5\mu\text{m}$  deep in the soft limit ( $\nu_\beta = 3$ ) and larger separations in the stiff limit. This shows that our results are consistent with the parameters of typical trapped-ion setups.

*Conclusions.*—To conclude, we have studied a generalized Holstein model that can be implemented in state-of-the-art trapped-ion experiments. In our numerical study, we have demonstrated that it can be useful to choose a hybrid approach in which calculations based on non-Gaussian variational ansatz states and density-matrix renormalization group complement each other. This allowed us to map out the phase diagram of the trapped-ion spin system, which is governed solely by tunable laser and ion trap parameters. While we have concentrated on  $\nu = 1/2$  and  $\nu = 1/4$ , other filling factors may be explored in future work, and could give rise to an even richer hierarchy of phases in the stiff limit. As a future prospect, also more exotic models could be investigated that include higher-order interactions between the spins and phonons. While they would be harder to tackle with classical methods, in a trapped-ion quantum simulator, they may be implemented by driving higher-order sidebands with a laser. A straightforward extension of our work is the consideration of well-established Paul trap setups instead of microtrap arrays, in which the ions are not perfectly equidistantly spaced.

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- [1] L. N. Cooper, Phys. Rev. **104**, 1189 (1956).
- [2] H. Fröhlich, Adv. Phys. **3**, 325 (1954).
- [3] T. Holstein, Ann. Phys. **8**, 325 (1959).
- [4] R. T. Scalettar, N. E. Bickers, and D. J. Scalapino, Phys. Rev. B **40**, 197 (1989).
- [5] F. Marsiglio, Phys. Rev. B **42**, 2416 (1990).
- [6] J. I. Cirac, and P. Zoller, Nat. Phys. **8**, 264 (2012).
- [7] R. Blatt, and C. F. Roos, Nat. Phys. **8**, 277 (2012).
- [8] D. Porras, and J. I. Cirac, Phys. Rev. Lett. **92**, 207901 (2004).

- [9] X.-L. Deng, D. Porras, and J. I. Cirac, Phys. Rev. A **72**, 063407 (2005).
- [10] V. M. Stojanovic, T. Shi, C. Bruder, and J. I. Cirac, Phys. Rev. Lett. **109**, 250501 (2012).
- [11] K. Jachymski, and N. Negretti, Phys. Rev. Research **2**, 033326 (2020).
- [12] S. R. White, Phys. Rev. Lett. **69**, 2863 (1992).
- [13] T. Shi, E. Demler, and J. I. Cirac, Ann. Phys. **390**, 245 (2018).
- [14] T. Shi, E. Demler, and J. I. Cirac, Phys. Rev. Lett. **125**, 180602 (2020).
- [15] See Supplemental Material of this work.
- [16] E. Jeckelmann, and S. R. White, Phys. Rev. B **57**, 6376 (1998).
- [17] C. Zhang, E. Jeckelmann, and S. R. White, Phys. Rev. Lett. **80**, 2661 (1998).
- [18] C. Guo, A. Weichselbaum, J. von Delft, and M. Vojta, Phys. Rev. Lett. **108**, 160401 (2012).
- [19] C. Brockett, F. Dorfner, L. Vidmar, F. Heidrich-Meisner, and E. Jeckelmann, Phys. Rev. B **92**, 241106 (2015).
- [20] J. Stolpp, J. Herbrych, F. Dorfner, E. Dagotto, and F. Heidrich-Meisner, Phys. Rev. B **101**, 035134 (2020).
- [21] T. Köhler, J. Stolpp, and S. Paecckel, SciPost Phys. **10**, 058 (2021).
- [22] M. Fishman, S. R. White, and E. M. Stoudenmire, *The ITensor Software Library for Tensor Network Calculations*, arXiv:2007.14822 (2020).

## Supplemental Materials: Spin-Holstein models in trapped-ion systems

This Supplemental Material is structured as follows. Sec. S1 summarizes the derivation of the effective Hamiltonian used in the main text. In Sec. S2 we discuss the displacement transformation employed for the DMRG simulations. Numerical convergence of these simulations is discussed in Sec. S3. We discuss the fermionic model and non-Gaussian state ansatz in Sec. S4. In Sec. S5, we complement the results from the main text with additional numerical data on the structure factor  $S(q)$ , phonon observables and the domain wall in the phase-separated regime.

### S1. DERIVATION OF EFFECTIVE HAMILTONIAN $H_{\text{eff}}$

For completeness, we sketch here the derivation of our effective model. We refer to the existing trapped-ion literature for more details, cf. Refs. [S8, S9]. We start from Eqs. (1) and (2) in the main text and an additional external magnetic-field term,

$$H = \sum_{i=1}^N \sum_{\alpha=x,y,z} \frac{(p_i^\alpha)^2}{2m} + \frac{m}{2} \sum_{i,j=1}^N \sum_{\alpha=x,y,z} \mathcal{K}_{ij}^\alpha r_i^\alpha r_j^\alpha + \sum_{i=1}^N \sum_{\alpha=x,y,z} \frac{\Omega_\alpha^2}{2\Delta_\alpha} \cos^2(k_\alpha r_i^\alpha) (1 + \sigma_i^\alpha) + \sum_{i=1}^N \sum_{\alpha=x,y,z} B_\alpha \sigma_i^\alpha, \quad (\text{S1})$$

where the elasticity matrix is given by [S8]

$$\mathcal{K}_{ij}^\alpha = \omega_z^2 \times \begin{cases} 1 + c_\alpha \sum_{k \neq i} \frac{\beta_\alpha}{|i-k|^\beta}, & i = j, \\ -c_\alpha \frac{\beta_\alpha}{|i-j|^\beta}, & i \neq j, \end{cases} \quad (\text{S2})$$

with  $c_{x,y} = 1$  and  $c_z = -2$ . Now we apply a unitary transformation  $U_{\text{pol}}$  to Eq. (S1),

$$U_{\text{pol}} = \exp \left( \sum_{i=1}^N \sum_{n=1}^N \sum_{\alpha=x,y,z} \eta_{i,n}^\alpha (1 + \sigma_i^\alpha) (a_{n,\alpha}^\dagger - a_{n,\alpha}) \right), \quad (\text{S3})$$

where

$$\eta_{i,n}^\alpha = \frac{F_\alpha}{\Omega_{n,\alpha} \sqrt{2m\Omega_{n,\alpha}}} \mathcal{M}_{i,n}^\alpha, \quad \sum_{i,j=1}^N \mathcal{M}_{i,n}^\alpha \mathcal{K}_{ij}^\alpha \mathcal{M}_{j,m}^\alpha = \Omega_{n,\alpha}^2 \delta_{mn}. \quad (\text{S4})$$

Denoting with  $H_{\text{eff}} = U_{\text{pol}} H U_{\text{pol}}^\dagger$  our effective Hamiltonian, to first order in  $\eta_{i,n}^\alpha$  we eliminate the transverse ( $\alpha = x, y$ ) phonons and interaction terms from the description, and introduce effective spin-spin interaction terms. The Hamiltonian takes the form

$$H_{\text{eff}} = \sum_n \Omega_n a_n^\dagger a_n - F_z \sum_{i=1}^N \sum_{n=1}^N g_{in} (a_{n,z} + a_{n,z}^\dagger) (1 + \sigma_i^z) + \sum_{i \neq j} \sum_{\alpha=x,y} J_{ij}^\alpha \sigma_i^\alpha \sigma_j^\alpha + \sum_{i=1}^N \sum_{\alpha=x,y,z} \left( B_\alpha - \frac{F_\alpha^2}{m\omega_\alpha^2} \right) \sigma_i^\alpha, \quad (\text{S5})$$

where  $g_{in} = \mathcal{M}_{in} / \sqrt{2m\Omega_n}$ .

The last term in Eq. (S5) shows why we introduced external magnetic fields in Eq. (S1). The global force term stemming from the transformation can be canceled by appropriately choosing  $B_\alpha$  along all directions. Note that in the main text we focus on the case where  $B_\alpha - F_\alpha^2/(m\omega_\alpha^2) = 0$  along all three directions.

In order to obtain the effective model (??) from the main text, we use that  $J_{ij} \equiv J_{ij}^x = J_{ij}^y \sim 1/|i-j|^3$ . In general, the interaction can be derived from the elasticity matrix,

$$J_{ij}^\alpha = -\frac{F_\alpha^2}{m} \left[ (\mathcal{K}^\alpha)^{-1} \right]_{ij}. \quad (\text{S6})$$

Since we have assumed large transverse trap frequencies to adiabatically eliminate transverse phonons, the transverse traps are operated in the stiff limit. In this case, the dipolar scaling  $J_{ij} = 1/|i-j|^3$  follows directly from (S6). Fig. S1 demonstrates the scaling for decreasing  $\beta_{x,y}$  in the stiff limit.

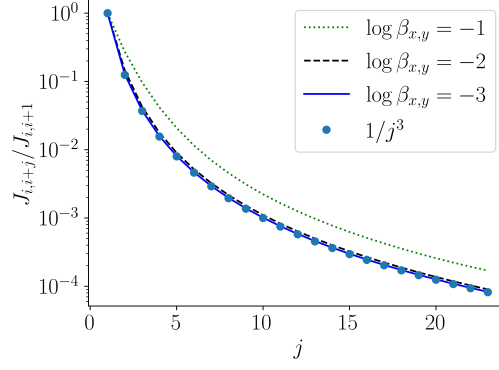


FIG. S1. Scaling  $J_{ij} \sim 1/|i-j|^3$  in the stiff limit. Result shown for chain of length  $N = 48$  and distance from central spin at site  $i = 24$ .

## S2. DISPLACEMENT TRANSFORMATION

In our numerical simulations, it is often more convenient to remove the phononic displacement term  $\sim F_z \sum_{i,n} g_{in}(a_n + a_n^\dagger)$  from the description at the cost of a spin-dependent shift. It renders the DMRG calculations more efficient, especially at strong coupling  $F_z$ . To this aim, we introduce the displaced phonon operators

$$\hat{\alpha}_n := \hat{a}_n - F_z \sum_i \frac{\mathcal{M}_{in}}{\sqrt{2m\Omega_n^{3/2}}} \equiv \hat{a}_n - c_n. \quad (\text{S7})$$

As the displacement transformation only affects the phonons, we denote the spin Hamiltonian by  $H_s = \sum_{i,j,\alpha} J_{ij} \sigma_i^\alpha \sigma_j^\alpha$  and rewrite Eq. (??) as

$$\begin{aligned} H_{\text{eff}} &= \sum_n \Omega_n a_n^\dagger a_n - F_z \sum_{i,n} \frac{\mathcal{M}_{in}}{\sqrt{2m\Omega_n}} (a_n + a_n^\dagger)(1 + \sigma_i^z) + H_s \\ &= \sum_n \Omega_n \alpha_n^\dagger \alpha_n + \sum_n \Omega_n c_n (\alpha_n + \alpha_n^\dagger) + \sum_n \Omega_n c_n^2 \\ &\quad - F_z \sum_{i,n} \frac{\mathcal{M}_{in}}{\sqrt{2m\Omega_n}} (\alpha_n + \alpha_n^\dagger) - F_z \sum_{i,n} \frac{\mathcal{M}_{in}}{\sqrt{2m\Omega_n}} (\alpha_n + \alpha_n^\dagger) \sigma_i^z - 2F_z \sum_{i,n} \frac{\mathcal{M}_{in}}{\sqrt{2m\Omega_n}} c_n - 2F_z \sum_{i,n} \frac{\mathcal{M}_{in}}{\sqrt{2m\Omega_n}} c_n \sigma_i^z + H_s \\ &= \sum_n \Omega_n \alpha_n^\dagger \alpha_n - F_z \sum_{i,n} g_{in} (\alpha_n + \alpha_n^\dagger) \sigma_i^z + H_s + H_R, \end{aligned} \quad (\text{S8})$$

with the residual phonon-independent contribution

$$H_R = -F_z^2 \sum_n \frac{1}{2m\Omega_n^2} \left( \sum_i \mathcal{M}_{in} \right)^2 - 2F_z^2 \sum_{i,n} \frac{\mathcal{M}_{in}}{2m\Omega_n^2} \sigma_i^z \left( \sum_j \mathcal{M}_{jn} \right). \quad (\text{S9})$$

## S3. CONVERGENCE ANALYSIS

We benchmark our numerical calculations against each other and compare the ground state energies obtained with DMRG and the NGS method outlined in Sec. S4. Most importantly, we make sure that the ground state energies are close to each other, see Fig. S2. Typically the energies obtained with DMRG are slightly lower. However, the runtime of the simulation is decreased significantly if we first perform the NGS calculation and then feed a good initial seed into the DMRG simulation.

In the derivation of the phase diagram (see Fig. 2) we explore the ground states in  $(F_z, \beta)$  space using an adaptive grid with a higher resolution closer to the phase boundary. Slight deviations between the NGS and DMRG results can partially be explained by the fact that the maximal resolution used within the NGS calculations can be as small as

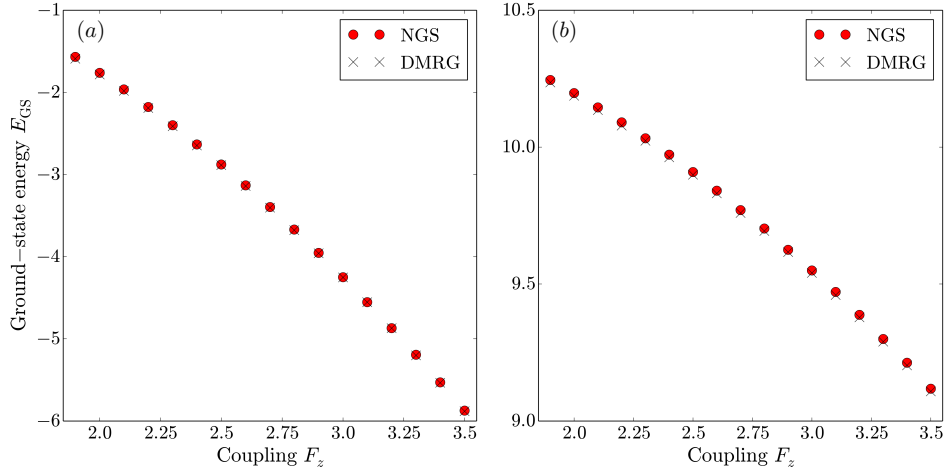


FIG. S2. Ground-state energies obtained with DMRG and NGS methods. (a)  $\beta = -3.0$  (stiff) and (b)  $\beta = 3.0$  (soft). Other numerical parameters:  $N = 48$ ,  $\omega_z/J = 1$ .

$\Delta F_z \sim 10^{-4}$ , while in the DMRG simulations we limit ourselves to  $\Delta F_z \sim 10^{-2}$ . Similarly, with DMRG we discretize the possible values for the stiffness parameter and choose a resolution  $\Delta\nu_\beta = 0.3$ . In our numerical calculations based on non-Gaussian ansatz states we choose  $\Delta\nu_\beta = 0.1$  instead, as they are less costly.

#### S4. NON GAUSSIAN STATES AND EQUATIONS OF MOTION

In this section, we study the ground state and thermal properties of a 1D array of ions with the lattice spacing  $d$  and mass  $m$ , which is described by the 1D spin-Holstein model

$$H = \sum_{i \neq j, \alpha = x, y} J_{ij} \sigma_i^\alpha \sigma_j^\alpha + \frac{B}{2} \sum_i \sigma_i^z \quad (\text{S10})$$

$$+ \sum_i \frac{p_i^2}{2m} + \frac{m}{2} \sum_{ij} \mathcal{K}_{ij} r_i r_j - \sum_i F_z r_i (1 + \sigma_i^z).$$

The long-range interaction  $J_{ij} = J_{\text{dd}}/|i-j|^3$  between ions at sites  $i$  and  $j$  is induced by the transverse phonon modes, where the exchange interaction strength  $J_{\text{dd}} = F_0^2 e^2 / (2m^2 \omega_0^4 d^3)$  is determined by the ion charge  $e$ , the frequency  $\omega_0$  of the microtrap and the force  $F_0$  generated by the laser along the transverse directions  $\alpha = x, y$ . The longitudinal mode is described by

$$\mathcal{K}_{ij} = (\omega_z^2 + \sum_{l \neq i} \frac{\omega_{\text{dd}}^2}{|i-l|^3}) \delta_{ij} - \frac{\omega_{\text{dd}}^2}{|i-j|^3} (1 - \delta_{ij}), \quad (\text{S11})$$

where  $\omega_{\text{dd}} = \sqrt{2e^2/(md^3)}$ . The laser along the longitudinal direction induces the local Holstein interaction between the internal state and the longitudinal mode with strength  $F_z$ .

Via the Jordan-Wigner transformation

$$\begin{aligned} \sigma_i^z &= 2c_i^\dagger c_i - 1, \\ \sigma_i^+ &= e^{i\pi \sum_{l < i} c_l^\dagger c_l} c_i^\dagger, \end{aligned} \quad (\text{S12})$$

we rewrite the Hamiltonian

$$\begin{aligned} H &= \sum_{i \neq j} \frac{1}{|i-j|^3} P_{ij} c_i^\dagger c_j + B \sum_i c_i^\dagger c_i \quad (\text{S13}) \\ &+ \frac{1}{4} \sum_i \bar{p}_i^2 + \frac{1}{4} \sum_{ij} \mathcal{K}_{ij} \bar{r}_i \bar{r}_j - 2 \sum_i \bar{F}_z \bar{r}_i c_i^\dagger c_i, \end{aligned}$$



where  $t_0 = 4J_{\text{dd}}$  is chosen as the unit,  $\bar{F}_z = F_z/\sqrt{2m}$ , and

$$\bar{r}_i = \sqrt{2mr_i}, \bar{p}_i = \sqrt{\frac{2}{m}}p_i \quad (\text{S14})$$

satisfy the canonical commutation relation  $[\bar{r}_i, \bar{p}_i] = 2i$ . The operator  $P_{ij} = e^{i\pi \sum_{l \in \mathcal{S}_{ij}} c_l^\dagger c_l}$  is defined on the string  $\mathcal{S}_{ij}$  connecting sites  $i$  and  $j$  (without points  $i$  and  $j$ ).

We employ the variational ansatz

$$|\Psi_{\text{NGS}}\rangle = U_S |\Psi_{\text{GS}}\rangle, \quad (\text{S15})$$

$$\rho_{\text{NGS}} = U_S \rho_{\text{GS}} U_S^\dagger, \quad (\text{S16})$$

combining the generalized Lang-Firsov transformation

$$U_S = e^{i \sum_{nl} \lambda_{ln} \bar{p}_l c_n^\dagger c_n} \quad (\text{S17})$$

and the Gaussian states

$$|\Psi_{\text{GS}}\rangle = e^{-\frac{1}{2}R^T \sigma^y \Delta_R} e^{-i\frac{1}{4}R^T \xi_b R} e^{i\frac{1}{2}C^\dagger \xi_f C} |0\rangle, \quad (\text{S18})$$

$$\rho_{\text{GS}} = e^{-\frac{1}{2}R^T \sigma^y \Delta_R} \frac{1}{Z_b} e^{-\Omega_b} e^{\frac{1}{2}R^T \sigma^y \Delta_R} \frac{1}{Z_f} e^{-\Omega_f} \quad (\text{S19})$$

to study the ground state and the thermal state, where the partition functions  $Z_{b,f} = \text{tr} e^{-\Omega_{b,f}}$ . The Gaussian state  $|\Psi_{\text{GS}}\rangle$  and  $\rho_{\text{GS}}$  is completely characterized by the covariance matrices  $\Gamma_f = \langle CC^\dagger \rangle$  (equivalently,  $\Gamma_m = i(W_f \Gamma_f W_f^\dagger - 1)$  in the Majorana basis  $A = W_f C$ ) and  $\Gamma_b = \langle \{R, R^T\} \rangle / 2$  defined in the basis  $C = (c_i, c_i^\dagger)^T$  and  $R = (\bar{r}_i, \bar{p}_i)^T$ , where  $W_f = \begin{pmatrix} 1 & 1 \\ -i & i \end{pmatrix}$ .

For the imaginary time evolution, the projections of

$$\partial_\tau |\Psi_{\text{NGS}}\rangle = -\mathbf{P}(H - \langle H \rangle) |\Psi_{\text{NGS}}\rangle, \quad (\text{S20})$$

$$\partial_\tau |\Psi_\rho\rangle = -\mathbf{P}(F - f) |\Psi_\rho\rangle, \quad (\text{S21})$$

on the tangential space result in the EOM of variational parameters  $\lambda_{ln}$ ,  $\Delta_R$ , and  $\Gamma_{f,b}$ , which in the limit  $\tau \rightarrow \infty$  give rise to the ground state and thermal state, respectively. Here,  $|\Psi_\rho\rangle = U_S \otimes I |\rho_{\text{GS}}\rangle$  is determined by the purification  $|\rho_{\text{GS}}\rangle = \sqrt{\rho_{\text{GS}}} \otimes I |\phi^+\rangle$  of the Gaussian state  $\rho_{\text{GS}}$  via the maximal entangled state  $|\phi^+\rangle$  between the physical space and the fiducial space, and the free energy  $f$  is the average value of the free energy operator  $F = H + T \ln \rho_{\text{GS}}$ .

The flow equations of variational parameters are

$$\partial_\tau \Delta_x = -(\Gamma_b^{-1})_{\text{phys},x}^{-1} (\mathcal{K} \Delta_x - 2 \sum_n G_{ln} \langle c_n^\dagger c_n \rangle) + 2 \sum_n \partial_\tau \lambda_{ln} \langle c_n^\dagger c_n \rangle, \quad (\text{S22})$$

$$\partial_\tau \Gamma_b = \sigma^y \Omega \sigma^y - \Gamma_b \Omega \Gamma_b, \quad (\text{S23})$$

$$\partial_\tau \Gamma_f = \{\mathcal{F}_f, \Gamma_f\} - 2\Gamma_f \mathcal{F}_f \Gamma_f, \quad (\text{S24})$$

and

$$\partial_\tau \lambda_{ln} = \sum_{n' \neq m} w_{l,n'm} \frac{e^{-\frac{1}{2}w_{n'm}^T \Gamma_b w_{n'm}}}{|n' - m|^3} \langle P_{n'm} c_{n'}^\dagger c_m \rangle D_{n'n}^{-1} - (\Gamma_{b,p}^{-1} G)_{ln} \quad (\text{S25})$$

with  $D_{nm} = \langle c_n c_m^\dagger \rangle \langle c_n^\dagger c_m \rangle + \langle c_n^\dagger c_m^\dagger \rangle \langle c_m c_n \rangle$  and  $G_{ln} = 2F_z \delta_{ln} + (\mathcal{K} \lambda)_{ln}$ , where for phonons the effective mean-field matrix

$$\Omega = \begin{pmatrix} \mathcal{K} & 0 \\ 0 & \Omega_p \end{pmatrix} - T \sigma^y \ln \frac{\Gamma_b \sigma^y + 1}{\Gamma_b \sigma^y - 1} \quad (\text{S26})$$

is determined by

$$\Omega_p = 1 - \sum_{n \neq m} \frac{2e^{-\frac{1}{2}w_{nm}^T \Gamma_p w_{nm}}}{|n - m|^3} \langle P_{nm} c_n^\dagger c_m \rangle w_{nm} w_{nm}^T \quad (\text{S27})$$

and  $w_{l,nm} = \lambda_{ln} - \lambda_{lm}$ , while for fermions the effective mean-field matrix

$$\begin{aligned} \mathcal{F}_f = 2i \sum_{n \neq m} \frac{e^{-\frac{1}{2}w_{nm}^T \Gamma_p w_{nm}}}{|n-m|^3} W_f^\dagger \frac{\delta}{\delta \Gamma_m} \langle P_{nm} c_n^\dagger c_m \rangle W_f \\ + \begin{pmatrix} \mathcal{E}_{\text{HF}} & \Delta_{\text{F}} \\ \Delta_{\text{F}}^\dagger & -\mathcal{E}_{\text{HF}}^T \end{pmatrix} + T \ln\left(\frac{1}{\Gamma_f} - 1\right) \end{aligned} \quad (\text{S28})$$

is determined by

$$\begin{aligned} \mathcal{E}_{\text{HF}} = [B + \frac{1}{2}V_{nn} + \sum_{n'} V_{nn'} \langle c_n^\dagger c_{n'} \rangle - (\Delta_x^T G)_n] \delta_{nm} - V_{nm} \langle c_m^\dagger c_n \rangle, \\ \Delta_{\text{F}} = V_{nm} \langle c_m c_n \rangle, V_{nm} = 2[(\lambda^T \mathcal{K} \lambda)_{nm} + 2F_z(\lambda_{nm} + \lambda_{mn})]. \end{aligned} \quad (\text{S29})$$

The average value

$$\langle P_{nm} c_n^\dagger c_m \rangle = -\frac{1}{4} \langle P_{nm} \rangle [(1, i) \mathcal{S} \Theta \begin{pmatrix} 1 \\ -i \end{pmatrix}]_{mn} \quad (\text{S30})$$

of the string operator on the Gaussian state is determined by

$$\begin{aligned} \langle P_{nm} \rangle &= (-1)^N s_f \text{Pf}\left(\frac{\Gamma_F}{2}\right), \\ \Gamma_F &= \sqrt{1 - \Theta} \Gamma_m \sqrt{1 - \Theta} - i\sigma^y (1 + \Theta), \\ \mathcal{S} &= (i\sigma^y \Gamma_m - 1) \mathcal{T}, \Gamma_m = i(W_f \Gamma_f W_f^\dagger - 1), \\ \mathcal{T} &= \frac{1}{1 + \frac{1}{2}(1 - \Theta)(i\sigma^y \Gamma_m - 1)}, \\ \Theta &= I_2 \otimes e^{i\pi \mathcal{N}}, (\mathcal{N}_{l \notin \mathcal{S}_{nm}} = 0, \mathcal{N}_{l \in \mathcal{S}_{nm}} = 1), \end{aligned} \quad (\text{S31})$$

where  $s_f = (-1)^{N/2}$  and  $(-1)^{(N-1)/2}$  for the system with even and odd modes, respectively. The functional derivatives are

$$\frac{\delta}{\delta \Gamma_{m,ij}} \text{Pf}\left(\frac{\Gamma_F}{2}\right) = -\frac{1}{2} \text{Pf}\left(\frac{\Gamma_F}{2}\right) (\sqrt{1 - \Theta} \frac{1}{\Gamma_F} \sqrt{1 - \Theta})_{ij}, \quad (\text{S32})$$

and

$$\begin{aligned} \frac{\delta}{\delta \Gamma_{m,ij}} \langle P_{nm} c_n^\dagger c_m \rangle &= -\frac{1}{2} \langle P_{nm} c_n^\dagger c_m \rangle (\sqrt{1 - \Theta} \frac{1}{\Gamma_F} \sqrt{1 - \Theta})_{ij} \\ &\quad + i \frac{1}{4} \langle P_{nm} \rangle [\mathcal{T} \Theta \begin{pmatrix} 1 \\ -i \end{pmatrix}]_{jn} [(1, i) \mathcal{T}^T]_{mi}. \end{aligned} \quad (\text{S33})$$

The free energy

$$\begin{aligned} f &= \frac{1}{4} \text{tr}(\mathcal{K} \Gamma_{b,x} + \Gamma_{b,p}) + \frac{1}{4} \Delta_x^T \mathcal{K} \Delta_x + \sum_{n \neq m} \frac{e^{-\frac{1}{2}w_{nm}^T \Gamma_p w_{nm}}}{|n-m|^3} \langle P_{nm} c_n^\dagger c_m \rangle \\ &\quad + \sum_n [B + \frac{1}{2}V_{nn} - (\Delta_x^T G)_n + \frac{1}{2} \sum_m V_{nm} \langle c_m^\dagger c_m \rangle] \langle c_n^\dagger c_n \rangle \\ &\quad - \frac{1}{2} \sum_{nm} V_{nm} \langle c_m^\dagger c_n \rangle \langle c_n^\dagger c_m \rangle + \frac{1}{2} \sum_{nm} V_{nm} \langle c_m^\dagger c_n^\dagger \rangle \langle c_n c_m \rangle \\ &\quad - \sum_j \frac{d_j^b}{e^{\beta d_j^b} - 1} + T \sum_j \ln(1 - e^{-\beta d_j^b}) - \sum_j \frac{d_j^f}{e^{\beta d_j^f} + 1} - T \sum_j \ln(1 + e^{-\beta d_j^f}) \end{aligned} \quad (\text{S34})$$

monotonically decreases in the imaginary time evolution, where  $d_j^b$  and  $d_j^f$  are the positive eigenvalues of  $T\sigma^y \ln \frac{\Gamma_b \sigma^y + 1}{\Gamma_b \sigma^y - 1}$  and  $-T \ln(\frac{1}{\Gamma_f} - 1)$ , respectively.

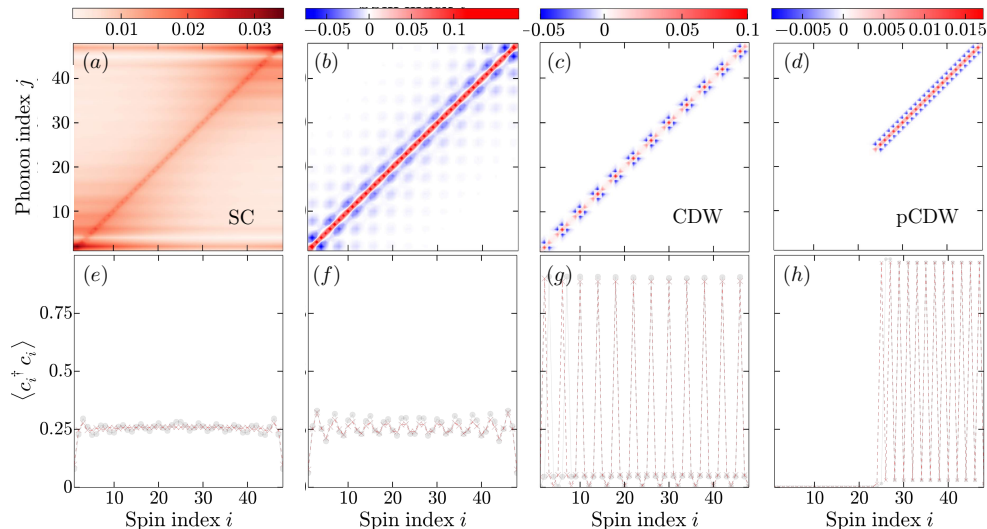


FIG. S3. Spin phonon correlator  $\Pi_{ij}$  and spin configuration for different ground states at quarter filling  $\nu = 1/4$  as obtained with NGS. *Upper panel*: Spin-phonon correlator  $\Pi$  as defined in Eq. (S39). *Lower panel*: Site-dependent density  $\langle c_i^\dagger c_i \rangle$ . The grey dots indicate the DMRG result. The four columns correspond to particular choices for  $F_z$  and  $\nu_\beta = \log \beta$  (compare right panel of Fig. 2). (a) and (e):  $F_z = 1.6$ ,  $\nu_\beta = 2.1$  (SC regime). (b) and (f):  $F_z = 0.6$ ,  $\nu_\beta = -2.1$  (precursor of CDW regime). (c) and (g):  $F_z = 1.2$ ,  $\nu_\beta = -2.1$  (CDW regime). (d) and (h):  $F_z = 1.5$ ,  $\nu_\beta = -2.1$  (pCDW regime). Other numerical parameters: equivalent to Fig. 3 in the main text.

To characterize the SC, CDW, and PS phases, we calculate the displacement

$$\langle r_l \rangle = \Delta_{x,l} - 2 \sum_n \lambda_{ln} \langle c_n^\dagger c_n \rangle, \quad (\text{S35})$$

of phonons, and the order parameters

$$\begin{aligned} O_{\text{CDW}} &= \frac{1}{N} \sum_n (-1)^n \langle c_n^\dagger c_n \rangle, \\ O_{\text{SC}} &= \langle \sigma_m^- \sigma_n^- \rangle. \end{aligned} \quad (\text{S36})$$

The SC order parameter

$$O_{\text{SC}} = e^{-\frac{1}{2} \bar{w}_{nm}^T \Gamma_p \bar{w}_{nm}} \langle P_{nm} c_m c_n \rangle \text{sgn}(m - n), \quad (\text{S37})$$

is determined by the phonon dressing factor  $\bar{w}_{l,nm} = \lambda_{ln} + \lambda_{lm}$  and the average value

$$\langle P_{nm} c_m c_n \rangle = -\frac{1}{4} \langle P_{nm} \rangle [(1, i) \mathcal{S} \left( \begin{matrix} 1 \\ i \end{matrix} \right)]_{nm}. \quad (\text{S38})$$

The connected correlation function  $\Pi_{ln} = \langle \bar{r}_l c_n^\dagger c_n \rangle - \langle \bar{r}_l \rangle \langle c_n^\dagger c_n \rangle \equiv \langle \bar{r}_l c_n^\dagger c_n \rangle_c$  between the spin at the site  $n$  and the phonon at the site  $l$  reads

$$\Pi_{ln} = -2 \sum_m \lambda_{lm} D_{mn}. \quad (\text{S39})$$

In Fig. S3, we show the numerical results obtained with the NGS ansatz for the same numerical parameters used to obtain Fig. 3 in the main text. We find that the results agree well, both qualitatively and quantitatively. The only quantitatively different result concerns the SC regime. Here we find that the NGS ansatz overestimates the spin-phonon correlation, cf. Fig. S3(a). The stripe pattern from Fig. 3(a) is still present, but less pronounced.

## S5. OTHER OBSERVABLES

Here we discuss additional observables that are not shown in the main text.

### A. Structure factor

We study the structure factor via the spin-spin correlations as

$$S(q) = \frac{1}{N} \sum_{i,j} \langle \sigma_i^z \sigma_j^z \rangle e^{iq|i-j|}, \quad (\text{S40})$$

and show results for the CDW state in Fig. S4 that correspond to the cases studied in the main text. At half filling ( $\nu = 1/2$ ), the structure factor displays a peak at  $q = \pi$  as expected, and shows two additional peaks nearby. Figs. S4(b) and (c) show the structure factor in the stiff limit ( $\beta \ll 1$ ) at quarter filling  $\nu = 1/4$ . At a comparatively small coupling  $F_z = 0.6$  (compare Figs. 3(b) and (f) from the main text), two peaks start to evolve at  $q = \pi/2$  and  $q = 3\pi/2$ . Only when  $F_z$  is increased,  $S(q)$  features two prominent peaks at  $q = \pi/2$  and  $q = 3\pi/2$ , and another peak at  $q = \pi$ . The latter is related to the non-vanishing background of the CDW state with period 4 shown in Fig. 2(g).

### B. Phonon observables

We study the staggered phonon parameter

$$m_{\text{ph}} = \frac{1}{N} \sum_{n=1}^N (-1)^n \langle b_n + b_n^\dagger \rangle. \quad (\text{S41})$$

In the soft limit ( $\beta \gg 1$ ), we find that  $m_{\text{ph}}$  suddenly increases from zero to a finite value at the phase transition from SC to PS. This is a contribution from the domain wall in the phase-separated regime and approaches a constant finite value as  $F_z$  is increased and the width of the domain wall tends to zero.

### C. Width of domain wall

In the case of phase separation, the domain wall separating the two phases shrinks as  $F_z$  increases. We calculate the width of the domain wall and define

$$W_z = \sum_{n=1}^N \frac{(z_n - z_c)^2}{2} (1 - |1 - |\langle \sigma_n^z \rangle - 1||), \quad (\text{S42})$$

where  $z_n$  denotes the  $n$ th ion position and  $z_c$  is the center of the domain wall. An exemplary result is shown in Fig. S5.

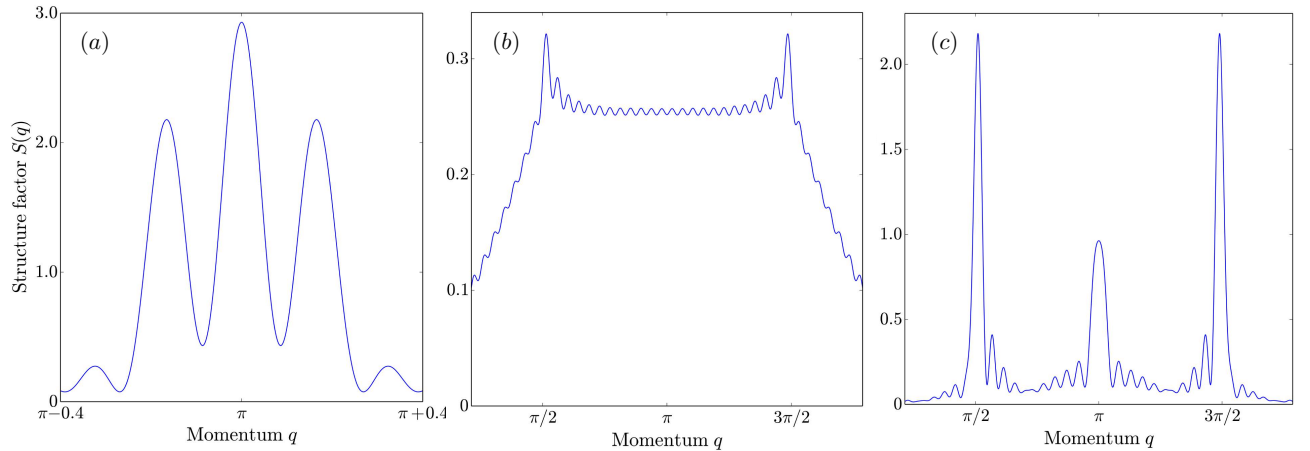


FIG. S4. Structure factor  $S(q)$ . (a) Half filling  $\nu = 1/2$ ,  $\beta = -2.4$ ,  $F_z = 2.1$ , (b) quarter filling  $\nu = 1/4$ ,  $\beta = -2.1$ ,  $F_z = 0.6$ , (c) quarter filling  $\nu = 1/4$ ,  $\beta = -2.1$ ,  $F_z = 1.2$ . Other numerical parameters:  $N = 48$ ,  $\omega_z/J = 1$ .

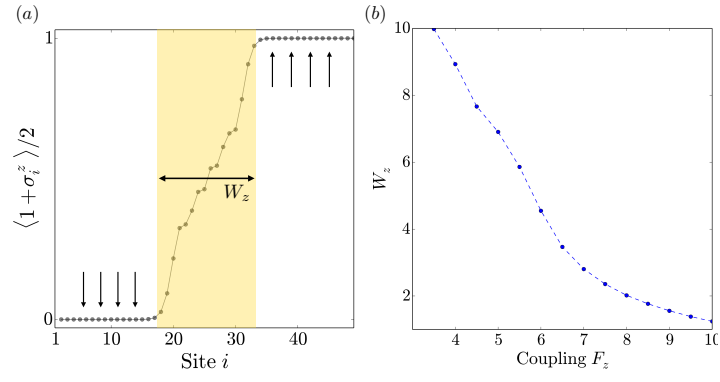


FIG. S5. Width of domain wall  $W_z$  in the case of phase separation. (a) Sketch of domain wall and width  $W_z$  at half filling  $\nu = 1/2$ . (b) Width  $W_z$  as a function of coupling  $F_z$  in soft limit at  $\nu_\beta = 3$  and at  $\nu = 1/2$ .