## Spin Peierls Quantum Phase Transitions in Coulomb Crystals

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The spin Peierls instability describes a structural transition of a crystal due to strong magnetic interactions. Here, we demonstrate that cold Coulomb crystals of trapped ions provide an experimental test bed in which to study this complex many-body problem and to access extreme regimes where the instability is triggered by quantum fluctuations alone. We present a consistent analysis based on different analytical and numerical methods, and we provide a detailed discussion of its experimental feasibility.

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The beauty of low-dimensional quantum many-body systems (QMBS) lies in the complexity born of the combination of interactions, disorder, and quantum fluctuations. However, these ingredients also conspire to render perturbative techniques inefficient, posing thus a fundamental challenge that has inspired the development of a variety of analytical [[1\]](#page-4-0) and numerical [\[2\]](#page-4-1) tools. Moreover, the synthesis of low-dimensional materials has upgraded these challenges from a theoretical endeavor into a discipline that underlies some of the most exciting recent discoveries in condensed-matter physics, such as the fractional quantum Hall effect. The recent progress in the field of atomic, molecular, and optical (AMO) physics presents a promising alternative to these solid-state realizations of low-dimensional QMBS. This field, which was originally devoted to the study of light-matter interactions at the scale of a single or few atoms, is progressively focusing on the many-body regime in platforms such as neutral atoms in optical lattices [\[3](#page-4-2)], cold Coulomb crystals of trapped ions [\[4\]](#page-4-3), or coupled cavity arrays [\[5](#page-4-4)]. The possibility of designing the Hamiltonians microscopically to target various many-body models yields a novel approach to explore QMBS in a controlled fashion, the so-called ''quantum simulations'' (QSs) [[6](#page-4-5)]. Some remarkable QSs are the optical-lattice realization of Mott [[7](#page-4-6)] and Anderson [\[8\]](#page-4-7) insulators, and the recent efforts toward a quantum-Hall insulator [[9](#page-4-8)]. More specific to this manuscript is the QS of quantum magnetism [\[10](#page-4-9)[,11\]](#page-4-10).

In this Letter, we explore the capabilities of AMO setups for the QS of interaction-mediated instabilities in QMBS. The standard playground for these phenomena is the so-called metal-insulator transition [[12](#page-4-11)], which has been investigated for a variety of transition-metal compounds in the field of strongly correlated electrons. A paradigmatic case is the one-dimensional metal, where either the electron-electron interactions destabilize the metal toward a superconducting state, or the electron-phonon coupling leads to a charge-density-wave condensate [[13\]](#page-4-12). The latter instability is a consequence of the so-called "Peierls transition" [[14](#page-4-13)], where the electron-phonon interactions induce a periodic distortion of the ionic lattice and open an energy gap in the conduction band of the metal. By virtue of the Jordan-Wigner transformation [\[15\]](#page-4-14), this phenomenon finds a magnetic counterpart: the "spin Peierls transition"  $[16]$  $[16]$  $[16]$ , whereby a spin-phononcoupled antiferromagnet (AFM) becomes unstable with respect to a dimerization of the lattice. This creates an alternating pattern of weak and strong spin interactions, which in turn opens an energy gap in the spectrum of collective excitations. We note that this instability has turned out to be important for different compounds, such as organic molecular crystals and transition-metal oxides [\[17\]](#page-4-16). From a theoretical perspective, the complete understanding of such a complex many-body system, treating the dynamics of the spins and phonons on the same footing, is still considered to be an open problem [\[17,](#page-4-16)[18\]](#page-4-17). From an experimental perspective, the spin Peierls instabilities observed so far [\[17](#page-4-16)[,19\]](#page-4-18) are limited to the Heisenberg model at finite temperatures. Hence, the realization of a spin Peierls transition only driven by quantum fluctuations, and also capable of exploring different magnetic interactions, remains an experimental challenge.

We hereby present a theoretical proposal for a trappedion QS to tackle both problems. In particular, by building on the recent experiments [[10](#page-4-9)] on the quantum Ising model (QIM) [[20\]](#page-4-19), we describe how to tailor a spin Peierls instability. We show that (i) the disordered paramagnet in a linear ion chain changes into an ordered antiferromagnet in a zigzag crystal [Figs.  $1(a)$  and  $1(b)$ ], and (ii) the spin Peierls transition can be driven only by the quantum fluctuations introduced by the transverse field of the QIM. Let us remark that, in comparison to neutral atoms in optical lattices or coupled arrays of cavities, trapped ions seem to be the best candidates to realize the spin Peierls quantum simulator. One of the main reasons is that the underlying lattice is not externally fixed, but rather results from the self-assembling dynamics of the ions.

The system.—The advent of experimental techniques for the confinement, cooling, and coherent manipulation of atomic ions has recently been exploited for QS purposes [\[4\]](#page-4-3), in which the controlled increase of the number of trapped ions yields a genuine bottom-up approach to the

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<span id="page-1-6"></span>

<span id="page-1-0"></span>FIG. 1 (color online). Scheme of the spin Peierls instability: (a) In the paramagnetic phase  $|P\rangle = | \uparrow \uparrow \cdots \uparrow \rangle$ , all the spins are parallel to a transverse field  $g > \tilde{g}_c$  along the z axis, and form an ion string. (b) The antiferromagnetic phase  $g < \tilde{g}_c$  corresponds to the two Néel states  $|AFM\rangle \in \{ | + - \cdots + - \rangle, | - + \cdots - + \rangle \}$ where the spins are antiparallel in the x basis  $|\pm\rangle = (|\uparrow\rangle \pm \langle\downarrow\rangle)$  $| \downarrow \rangle / \sqrt{2}$ , and form a zigzag ladder. (c) Laser wave vector  $\mathbf{k}_L$ <br>in the xy plane in the xy plane.

many-body regime. We consider a Coulomb gas formed by an ensemble of N trapped ions of mass  $m$  and charge  $e$ , which are described by the Hamiltonian

<span id="page-1-2"></span>
$$
H_0 = \frac{\omega_0}{2} \sum_i \sigma_i^z + \sum_{i,\alpha} \left( \frac{1}{2m} p_{i\alpha}^2 + \frac{1}{2} m \omega_\alpha^2 r_{i\alpha}^2 \right) + \frac{e^2}{2} \sum_{i \neq j} \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|},\tag{1}
$$

where  $\{\omega_{\alpha}\}_{{\alpha}={x,y,z}}$  are the effective trapping frequencies of a linear Paul trap. Here,  $\omega_{\alpha}$  is the energy difference bea linear Paul trap. Here,  $\omega_0$  is the energy difference be-<br>tween two electronic ground states of the atomic structure tween two electronic ground states of the atomic structure  $|\uparrow\rangle_i, |\downarrow\rangle_i$ , where  $\hbar = 1$  and  $\sigma_i^z = |\uparrow_i\rangle\langle\uparrow_i| - |\downarrow_i\rangle\langle\downarrow_i|$ . This Hamiltonian must be complemented by the laser-ion inter-Hamiltonian must be complemented by the laser-ion interaction responsible for coupling the electronic and motional degrees of freedom. We consider a pair of laser beams with  $\{\omega_l\}_{l=1,2}$ , wave vectors  $\{k_l\}_{l=1,2}$ , and phases  $\{\phi_l\}_{l=1,2}$ , tuned close to the atomic transition. In the dipolar approximation, the laser-ion Hamiltonian is

<span id="page-1-1"></span>
$$
H_{\rm L} = \sum_{l,i} (\Omega_l \sigma_i^+ + \Omega_l^* \sigma_i^-) \cos(\mathbf{k}_l \cdot \mathbf{r}_i - \omega_l t + \phi_l), \quad (2)
$$

where  $\Omega_l$  stands for the Rabi frequency of the transition,<br>and we have introduced the spin raising and lowering and we have introduced the spin raising and lowering operators  $\sigma_i^+ = |\uparrow_i\rangle\langle\downarrow_i| = (\sigma_i^-)^\dagger$ . To proceed further, we make some assumptions about the ion dynamics operators  $\sigma_i = \frac{1}{i} \sqrt{4} i = (\sigma_i)^T$ . To proceed furthermake some assumptions about the ion dynamics.

As evidenced in early experiments [[21](#page-4-20)], a laser-cooled ensemble of ions self-assembles in a Coulomb crystal, which undergoes a series of structural phase transitions (SPTs) as the trapping conditions are modified. In particular, when  $\omega_y \gg \omega_x$ ,  $\omega_z$  and the ratio  $\kappa_x = (\omega_z/\omega_x)^2$  is<br>tuned across a critical value  $\kappa$  [22] the geometry of the tuned across a critical value  $\kappa_c$  [[22](#page-4-21)], the geometry of the crystal changes from a linear string to a zigzag ladder. Note that this SPT displays a rich phenomenology that has recently revived interest in the subject [\[23–](#page-4-22)[28](#page-4-23)]. Here, we focus on the linear regime close to the critical point  $\kappa_x \leq \kappa_c$ , where the vibrations of the ions along each of the confining axes are decoupled. We consider that the laser wave vectors in [\(2\)](#page-1-1) lie within the xy plane [Fig. [1\(c\)](#page-1-0)],  $\mathbf{k}_l =$  $k_{lx}\mathbf{e}_x + k_{ly}\mathbf{e}_y$ , such that their frequencies are tuned close to the resonance of the vibrational sidebands  $\omega_l \approx \omega_0 \pm \omega_v$ . Since these sidebands correspond to the strongly confining y axis,  $\omega_{y} \gg \omega_{z}$ ,  $\omega_{z}$ , the coupling of the laser beams to the x and z vibrational modes becomes far off-resonant and can be neglected. Let us remark that this argument has one possible exception: there might be a vibrational soft mode where the phonons condense at the SPT. As identified in Ref. [[23](#page-4-22)], this soft mode corresponds precisely to the zigzag mode along the  $x$  axis, which affects the laser-ion coupling [\(2](#page-1-1)) regardless of the soft-mode frequency [[17](#page-4-16)].

The above considerations allow us to extract the relevant part of the Hamiltonian ([1](#page-1-2)) after introducing  $\mathbf{r}_i = l_z(\tilde{z}_i^0 \mathbf{e}_z + q_{ix} \mathbf{e}_x + q_{iy} \mathbf{e}_y + q_{iz} \mathbf{e}_z)$ , where  $\tilde{z}_i^0$  are the equilibrium positions in units of  $l_z = (e^2/m\omega_z^2)^{1/3}$ , and  $a_{\text{max}}$  are the small displacements along the corresponding  $\alpha$  are the small displacements along the corresponding axes. Following Ref.  $[27]$  $[27]$ , the displacements along the  $x$  axis have been adapted to the aforementioned zigzag mode  $q_{ix} = (-1)^i \delta q_{ix}$ , such that  $\delta q_{ix}$  is a smooth function<br>that allows a gradient expansion. The Hamiltonian then that allows a gradient expansion. The Hamiltonian then becomes  $H_0 = \frac{1}{2} \sum_i \omega_0 \sigma_i^z + H_x + H_y$ , where

<span id="page-1-3"></span>
$$
H_{x} = \sum_{i} \left( \frac{m l_{z}^{2}}{2} (\partial_{t} \delta q_{ix})^{2} + \frac{r_{i}^{x}}{2} \delta q_{ix}^{2} + \frac{u_{i}^{x}}{4} \delta q_{ix}^{4} \right) + \sum_{i \neq j} \frac{K_{ij}^{x}}{2} (\partial_{j} \delta q_{ix})^{2}
$$
  
\n
$$
H_{y} = \sum_{i} \left( \frac{m l_{z}^{2}}{2} (\partial_{t} q_{iy})^{2} + \frac{r_{i}^{y}}{2} q_{iy}^{2} \right) + \sum_{i \neq j} \frac{K_{ij}^{y}}{2} (\partial_{j} q_{iy})^{2},
$$
\n(3)

and we have introduced the gradient  $\partial_i f_i = f_i - f_i$ . In these expressions, the vibrational couplings are

<span id="page-1-5"></span>
$$
r_i^x = m\omega_x^2 l_z^2 \bigg(1 - \frac{1}{2} \kappa_x \zeta_i(3)\bigg), \quad u_i^x = m\omega_x^2 l_z^2 \bigg(\frac{3}{4} \kappa_x \zeta_i(5)\bigg),
$$
  
\n
$$
K_{ij}^x = m\omega_x^2 l_z^2 \bigg(\sum_{l \neq i} \frac{(-1)^{l+i+1} \kappa_x}{2|\tilde{z}_i^0 - \tilde{z}_l^0|}\bigg)\delta_{j,i+1},
$$
\n(4)

along the x axis, expressed in terms of the inhomogeneous<br>function  $\mathcal{L}(n) = \sum_{n=1}^{\infty} [(-1)^i - (-1)^i]^{n-1} \xi^0 - \xi^0$ function  $\zeta_i(n) = \sum_{l \neq i} [(-1)^i - (-1)^l]^{n-1} \left[\tilde{z}_i^0 - \tilde{z}_l^0\right]^{-n}$  with  $n \in \mathbb{Z}$  and the Kronecker delta  $\delta$ . In the limit of tight  $\frac{1}{2}$  ive  $\frac{1}{2}$  in the limit  $n \in \mathbb{Z}$ , and the Kronecker delta  $\delta_{lm}$ . In the limit of tight<br>confinement along the vaxis  $\kappa = (\omega / \omega)^2 \ll 1$  we find confinement along the y axis,  $\kappa_y = (\omega_z/\omega_y)^2 \ll 1$ , we find  $r_i^y = m\omega_y^2 l$  $Z_z$ ,  $K_{ij}^y = \frac{m\omega_y^2 l_z^2 \kappa_y}{2|\bar{z}_i^0 - \bar{z}_j^0|^3}$ . Accordingly,  $H_y$  corresponds to a set of dipolarly coupled harmonic oscillators, whereas  $H_x$  describes a set of nearest-neighbor-coupled anharmonic oscillators.

The coupled harmonic oscillators [\(3](#page-1-3)) are diagonalized, yielding a set of collective modes with frequencies  $\omega_n$ , whose excitations, created and annihilated by  $a_n^{\dagger}$ ,  $a_n$ , shall<br>be referred to as the "hard phonons". This vields the be referred to as the ''hard phonons.'' This yields the quadratic Hamiltonian  $H_y = \sum_n \omega_n a_n^{\dagger} a_n$ . By setting the laser frequencies to the red and blue vibrational sidebands laser frequencies to the red and blue vibrational sidebands of the atomic transition,  $\omega_1 \approx \omega_0 - \omega_n$  and  $\omega_2 \approx \omega_0 + \omega_n$ , we express the laser-ion interaction  $(2)$  as  $[17]$ 

<span id="page-1-4"></span>
$$
H_{\rm L} = \sum_{\rm in} (\mathcal{F}_{\rm in}^r e^{i\theta_r q_{ix}} \sigma_i^+ a_n + \mathcal{F}_{\rm in}^b e^{i\theta_b q_{ix}} \sigma_i^+ a_n^{\dagger} + \text{H.c.}), \tag{5}
$$

where we have introduced the sideband coupling strengths  $\mathcal{F}_{\text{in}}^r = \frac{i}{2} \Omega_1 \eta_{1n} \mathcal{M}_{\text{in}} e^{i\phi_1}$ ,  $\mathcal{F}_{\text{in}}^b = \frac{i}{2} \Omega_2 \eta_{2n} \mathcal{M}_{\text{in}} e^{i\phi_2}$ , the

Lamb-Dicke parameters  $\eta_{\text{ln}} = k_{ly} / \sqrt{2m\omega_n} \ll 1$ , the normal-mode amplitudes  $M_{\text{ln}}$  and  $\theta_{\text{ln}} = k_{\text{ln}} / \theta_{\text{ln}} = k_{\text{ln}} / \theta_{\text{ln}}$ normal-mode amplitudes  $\mathcal{M}_{\text{in}}$ , and  $\theta_r = k_{1x}l_z$ ,  $\theta_b = k_{2x}l_z$ .

In contrast, the anharmonic oscillators  $(3)$  $(3)$  correspond to an inhomogeneous version of the  $\phi^4$  model on a lattice, namely, an interacting scalar field theory that cannot be exactly diagonalized. This model yields a SPT that can be understood as follows. The regime  $r_i^x > 0$ ,  $u_i^x > 0$ , corresponding to trapping-frequency ratios fulfilling  $\kappa_x$  <  $\kappa_{c,i} = 2/\zeta_i(3)$ , yields the linear ion configuration, which respects the  $\mathbb{Z}_2$  symmetry of the model. Conversely, when  $r_i^x < 0$ ,  $u_i^x > 0$  for  $\kappa_x > \kappa_{c,i}$ , the ions self-organize in the troken-symmetry the zigzag ladder corresponding to the broken-symmetry phase, whereby  $\langle \delta q_{ix} \rangle \neq 0$  signals the condensation of the "soft phonons" in the zigzag mode. We note that the  $\phi^4$ model fulfills  $r_i^x \neq r_j^x$ , which leads to an inhomogeneous<br>SPT extinct at the contex of the transless  $\Delta \varepsilon$  outlined SPT setting at the center of the trap [[25](#page-4-25)]. As outlined previously, when the soft phonons condense  $\langle \delta q_{ix} \rangle \neq 0$ , there is a nontrivial effect in the laser-ion Hamiltonian [\(5\)](#page-1-4) that must be considered. We show below that, in this case, the hard phonons mediate a spin-spin interaction, whereas the soft condensed phonons are responsible for a dimerization of the coupling strengths. This condensation turns out to be the key ingredient for a zero-temperature spin Peierls transition. Let us also emphasize that this model, which is a cornerstone in the microscopic description of SPTs [\[29\]](#page-4-26), has not been combined with a spin Peierls distortion, to the best of our knowledge.

Dimerized quantum spin model.—The spin phonon model in Eqs. [\(3\)](#page-1-3) and ([5\)](#page-1-4) yields an extremely complex QMBS. We analyze the onset of a spin Peierls quantum phase transition by performing a series of simplifications. First, we neglect the time-dependence of the zigzag distortion ([3](#page-1-3)). This adiabatic approximation, which is standard in the treatment of spin Peierls phenomena [[16](#page-4-15)], is justified if the zigzag mode is much slower than the effective spin dynamics, which is valid close to the critical point. Hence, we treat the SPT classically by setting  $q_{ix}$  =  $(-1)^i \langle \delta q_{ix} \rangle$  self-consistently. Second, we consider a ho-<br>mogeneous zigzag distortion, which amounts to neglecting mogeneous zigzag distortion, which amounts to neglecting the nearest-neighbor couplings in Eq. ([3](#page-1-3)). Third, when the coupling of the spins to the hard phonons ([5](#page-1-4)) is weak, they can be integrated out, yielding an effective quantum spin model. In the linear string, this process leads to a dipolar version of the celebrated QIM [[30](#page-4-27)], whereas the frustrated  $J_1-J_2$  QIM arises in the zigzag configuration [[31](#page-4-28)]. In this Letter, we show that, in the vicinity of the critical point  $\kappa_{x} \approx \kappa_{c,i}$ , the quantum spin model corresponds to a dipolar QIM with additional spin-spin couplings whose sign alternates periodically when the soft phonons condense.

In analogy to the Sørensen-Mølmer gates [\[32\]](#page-4-29), we consider that the red- and blue-sideband terms [\(5\)](#page-1-4) have opposite detunings  $\delta_{nr} = -\delta_{nb} =: \delta_n$ , where  $\delta_{nr} = \omega_1 - (\omega_0 - \omega_n)$  and  $\delta_{nb} = \omega_2 - (\omega_0 + \omega_n)$ . Also, their Rabi  $(\omega_0 - \omega_n)$  and  $\delta_{nb} = \omega_2 - (\omega_0 + \omega_n)$ . Also, their Rabi<br>frequencies fulfill  $Q_k k^2 = Q_k k^2$  and attain values such frequencies fulfill  $\Omega_1 k_{1y}^2 = \Omega_2 k_{2y}^2$  and attain values such that  $|\mathcal{F}^r| = |\mathcal{F}^b| \ll \frac{8}{5}$ . In this limit, the sidebands (5) that  $|\mathcal{F}_{\text{in}}^r| = |\mathcal{F}_{\text{in}}^b| \ll \delta_n$ . In this limit, the sidebands [\(5\)](#page-1-4) create a virtual hard phonon that is then reabsorbed by a distant ion, leading thus to the aforementioned effective spin-spin interaction. The above constraints are responsible for the destructive interference of the processes where a phonon is created and then reabsorbed by the same ion, a crucial property that underlies the availability of an effective spin Hamiltonian that is decoupled from the hard phonons. Finally, by considering that the pair of laser beams are counterpropagating  $\mathbf{k}_1 = -\mathbf{k}_2 =: \mathbf{k}$ , which implies that the parameters are  $\theta_r = -\theta_b = \theta$ , it is possible to obtain the spin Hamiltonian [\[17\]](#page-4-16)

$$
H_{\text{eff}} = \sum_{i \neq j} (J_{ij}^{xx} \sigma_i^x \sigma_j^x + J_{ij}^{yy} \sigma_i^y \sigma_j^y + J_{ij}^{xy} \sigma_i^x \sigma_j^y + J_{ij}^{yx} \sigma_i^y \sigma_j^x),
$$

where the coupling strengths are

$$
J_{ij}^{xx} = J_{ij}\{\cos[\theta(q_{ix} - q_{jx})] + \cos[\theta(q_{ix} + q_{jx}) + \phi_{-}]\},
$$
  
\n
$$
J_{ij}^{yy} = J_{ij}\{\cos[\theta(q_{ix} - q_{jx})] - \cos[\theta(q_{ix} + q_{jx}) + \phi_{-}]\},
$$
  
\n
$$
J_{ij}^{xy} = J_{ij}\{\sin[\theta(q_{ix} - q_{jx})] - \sin[\theta(q_{ix} + q_{jx}) + \phi_{-}]\},
$$
  
\n
$$
J_{ij}^{yx} = -J_{ij}\{\sin[\theta(q_{ix} - q_{jx})] + \sin[\theta(q_{ix} + q_{jx}) + \phi_{-}]\},
$$

and the relative laser phase is  $\phi_{-} = \phi_1 - \phi_2$ . Here, the spin-spin couplings are  $J_{ij} = \frac{J_{\text{eff}}}{2|\bar{z}_i^0 - \bar{z}_j^0|^3}$ ,  $J_{\text{eff}} = \frac{\Omega_L^2 \eta_y^2 \kappa_y}{16 \delta_y^2} (1 + \delta_y)$  $\frac{\delta_y}{\omega_y}$ , where we made an expansion for  $\kappa_y \ll 1$  and introduced the bare detuning  $\delta_y = \omega_1 - (\omega_0 - \omega_y) =$ <br>=  $(\omega_1 + (\omega_2 + \omega_1))$  the bare I amb-Dicke parameter  $-\omega_2 + (\omega_0 + \omega_2)$ , the bare Lamb-Dicke parameter  $\eta_y = k_y / \sqrt{2m\omega_y}$ , and the common Rabi frequency  $\Omega_L :=$ <br> $\Omega = \Omega$ . Hence, the spin-phonon interaction leads to a  $\Omega_1 = \Omega_2$ . Hence, the spin-phonon interaction leads to a generalization of the famous XY quantum spin model [[33\]](#page-4-30). In order to obtain the promised dimerized spin model, one has to phase-lock the laser beams  $\phi = 0$ , and consider the critical region where the zigzag distortion is small enough  $\theta \langle \delta q_i \rangle \ll 1$ . Then, we can Taylor-expand and obtain an antiferromagnetic Ising interaction characterized by  $J_{ij}^{xx} = 2J_{ij}$  and  $J_{ij}^{yy} = 0$ , but also  $J_{ij}^{xy}$ <br>2J  $(-1)^{j+1} \theta(\delta \sigma) = J^{yx}$  which give rise to the quanti  $2J_{ij}(-1)^{j+1}\theta(\delta q_{jk}) = J_{ji}^{yx}$ , which give rise to the quantum<br>dimension  $\delta q_{jk}$  = means is interestion that does not dimerization [i.e., a magnetic interaction that does not commute with the Ising coupling, and alternates between a ferromagnetic-antiferromagnetic sign  $J_{ij}^{xy}$ ,  $J_{ji}^{yx}$ <br> $(-1)^{i+1}$  . Also, we consider a transverse field h that can  $(-1)^{i+1}$ . Also, we consider a transverse field h that can be<br>obtained from a microwave that is far off-resonant with obtained from a microwave that is far off-resonant with respect to the atomic transition. Altogether, the spin Hamiltonian becomes  $H_{\text{eff}} = H_{\text{Ising}} + H_{\text{dimer}}$ , where

$$
H_{\text{Ising}} = \sum_{i \neq j} \frac{J_{\text{eff}}}{|\tilde{z}_{i}^{0} - \tilde{z}_{j}^{0}|^{3}} \sigma_{i}^{x} \sigma_{j}^{x} - h \sum_{i} \sigma_{i}^{z},
$$
  

$$
H_{\text{dimer}} = \sum_{i \neq j} \frac{J_{\text{eff}}(-1)^{j+1} \xi_{j}}{|\tilde{z}_{i}^{0} - \tilde{z}_{j}^{0}|^{3}} \sigma_{i}^{x} \sigma_{j}^{y} + \frac{J_{\text{eff}}(-1)^{i+1} \xi_{i}}{|\tilde{z}_{i}^{0} - \tilde{z}_{j}^{0}|^{3}} \sigma_{i}^{y} \sigma_{j}^{x},
$$

and we have introduced  $\xi_i = \theta \langle \delta q_i \rangle \ll 1$ . Let us remark that the couplings of the dimerization Hamiltonian depend on the condensation of the soft phonons  $\langle \delta q_{ix} \rangle$ , which is in

turn described by the  $\phi^4$  theory. Below, we show how this model leads to the desired spin Peierls instability.

Spin Peierls quantum phase transition.—To demonstrate that the introduced scheme yields a QS of the spin Peierls instability, we simplify the model by neglecting its longrange interactions and inhomogeneities. The spin model can be solved by a Jordan-Wigner transformation with  $\xi = \xi_i \forall i$ , later used as input to the  $\phi^4$  model selfconsistently. For  $\xi \ll 1$ , the ground-state energy is

<span id="page-3-1"></span>
$$
E_g(\xi) \approx E_g(0) - \frac{2JN}{\pi} \varphi(g)\xi^2 < E_g(0),\tag{6}
$$

where  $J > 0$  is the nearest-neighbor antiferromagnetic coupling,  $g = h/J$ , and we have introduced a monotonically decreasing positive-definite function  $\varphi(g)$  that depends on the complete elliptic integrals (see Supplemental Material [[17](#page-4-16)]). We have compared this expression to numerical density matrix renormalization group (DMRG) [\[34\]](#page-4-31) calculations [see Fig.  $2(a)$  and Supplemental Material [\[17](#page-4-16)] ], which support our claim for small dimerizations. The above lowering of the ground-state energy pinpoints the instability toward the lattice distortion. Also, the spectrum of magnetic excitations displays the following energy gap  $\Delta \propto |g - \sqrt{1 + 4\xi^2}|$ . With respect to the paramagnetic-to-antiferromagnetic quantum phase transiparamagnetic-to-antiferromagnetic quantum phase transition of the standard QIM at  $g_c = 1$  [\[20\]](#page-4-19), the dimerization breaks the self-duality of the model leading to

$$
g_c \to \tilde{g}_c(\xi) = \sqrt{1 + 4\xi^2}.\tag{7}
$$

<span id="page-3-3"></span>In Fig.  $2(b)$ , we corroborate this flow of the critical point from the divergence of the magnetic susceptibility  $\chi_m \propto$  $\tilde{\chi}_m = -\partial^2 E_g / \partial g^2.$ 

Therefore, the paramagnet close to  $g_c < g \le \tilde{g}_c$  will be unstable toward the antiferromagnet if the lowering of the energy ([6\)](#page-3-1) compensates the structural change. For selfconsistency, we incorporate this energy change in the  $\phi^4$ model. Since  $E_g(\xi) - E_g(0) \propto \sum_i \delta q_{ix}^2$ , it becomes clear<br>how to modify the parameters of (4). In analogy to the how to modify the parameters of [\(4\)](#page-1-5). In analogy to the magnetic phase transition, the SPT is also displaced, but toward a smaller value:



<span id="page-3-0"></span>FIG. 2 (color online). Spin Peierls transition: (a) Scaling of the ground-state energy with the lattice dimerization. (b) Displacement of the critical point calculated from the divergence of the magnetic susceptibility.

$$
\kappa_{c,i} \to \tilde{\kappa}_{c,i} = \left(\frac{\zeta_i(3)}{2} + \frac{2J}{m\omega_z^2 l_z^2} \frac{\theta^2 \varphi(g)}{\pi}\right)^{-1}.\tag{8}
$$

<span id="page-3-4"></span>Therefore, the linear ion string close to criticality  $\tilde{\kappa}_{c,i} \leq \kappa < \kappa$ , is unstable toward the zigzag phase  $\kappa_{x} < \kappa_{c,i}$  is unstable toward the zigzag phase.

We have thus proved our claim (i) that the paramagnetic phase in the linear ion string will be unstable toward the antiferromagnetic zigzag ladder (Fig. [1\)](#page-1-6). Moreover, by fixing the ratio of the trapping frequencies in the linear regime,  $\kappa_x < \kappa_{c,i}$ , we can drive both the structural and the magnetic phase transitions by only modifying the transverse magnetic field g across  $\tilde{g}_c$ . The necessary condition for the trapping frequencies is

$$
m\omega_z^2 l_z^2 = \frac{2J\theta^2 \varphi(\tilde{g}_c)}{\pi[\kappa_x^{-1} - \frac{1}{2}\zeta_i(3)]}.
$$
 (9)

<span id="page-3-2"></span>Hence, the zigzag AFM  $g < \tilde{g}_c$  transforms onto a linear<br>paramagnet by increasing  $g > g$ . This supports our claim paramagnet by increasing  $g > g_c$ . This supports our claim (ii) that the spin Peierls transition can be driven by quantum fluctuations alone.

Experimental considerations.—We focus on  $^{25}Mg^{+}$ and select two hyperfine levels for the spin states  $|\uparrow_i\rangle$  =  $|F = 2, m_F = 2, |\downarrow_i\rangle = |3, 3\rangle$ , such that the resonance fre-quency in [\(1](#page-1-2)) is  $\omega_0/2\pi = 1.8$  GHz. We consider a  $N = 30$ <br>ion register with transing frequencies  $\omega_0/2\pi \approx 300$  kHz. ion register with trapping frequencies  $\omega_z/2\pi \approx 300 \text{ kHz}$ ,<br>  $\omega_z/2\pi \approx 7 \text{ MHz}$  and  $\omega_z/2\pi = 10 \text{ MHz}$ . The phase- $\omega_x/2\pi \approx 7$  MHz, and  $\omega_y/2\pi = 10$  MHz. The phase-<br>locked laser beams leading to (2) are blue-detuned locked laser beams leading to ([2](#page-1-1)) are blue-detuned  $\delta_y/2\pi \approx 1$  MHz, such that the two-photon Rabi frequen-<br>ciss are  $\Omega_z/2\pi \approx 1$  MHz, and the Lamb-Dicke parameter cies are  $\Omega_L/2\pi \approx 1$  MHz, and the Lamb-Dicke parameter  $n \approx 0.2$  With these values the required constraints de- $\eta_y \approx 0.2$ . With these values, the required constraints detailed in the Supplemental Material [\[17\]](#page-4-16) are fulfilled, and we obtain a nearest-neighbor spin coupling with the typical strength  $J = 2J_{\text{eff}}/|\tilde{z}_i^0 - \tilde{z}_{i+1}^0|^3 \approx 1$  kHz observed in ex-<br>periments [10] By considering these parameters the conperiments [[10](#page-4-9)]. By considering these parameters, the condition ([9](#page-3-2)) imposes the following constraint over the anisotropy  $(\kappa_{c,i} - \kappa_x)/\kappa_{c,i} \sim 10^{-4} \eta_y^2$ , which requires the transference to the structural trap frequency to be sufficiently close to the structural phase transition. In practice, the soft radial trapping frequency must be controlled with an accuracy of  $\Delta \omega_x \sim 10^{-6} \omega_x \approx 1 - 10$  Hz, which coincides with the precision required to observe quantum effects in the SPT [27] cision required to observe quantum effects in the SPT  $\left[\frac{27}{27}\right]$ . Provided that this precision is achieved in the experiments, one could optically pump the linear ion register to  $|\psi(0)\rangle = \otimes |\uparrow_{i}\rangle$  and then study its adiabatic evolution towards the AFM phase as the transverse field  $g(t)$  is decreased. The corresponding AFM order can be measured by fluorescence techniques, whereas the structural phase transition could be directly observed in a CCD camera, or inferred from spectroscopy of the vibrational modes. A simpler experiment would require setting the anisotropy parameter within the instability regime given by the dis-placements in Eqs. ([7](#page-3-3)) and ([8\)](#page-3-4), which leads to  $(\kappa_{c,i} - \kappa_x)/\kappa_{c,i} \approx n^2 \approx 10^{-2}$  and  $h/L \approx 10^{-2}$ . The linear parameter would be directly unstable toward the zigzag AFM without  $\sim \eta_y^2 \approx 10^{-2}$  and  $h/J \approx 10^{-2}$ . The linear paramagnet<br>ld be directly unstable toward the zigzao AEM without adiabatically tuning the transverse field  $g(t)$  and the demanding constraints on the trap frequencies.

Conclusions and outlook.—A sensible QS must address questions that are difficult to assess by other analytical or numerical methods. In this Letter, we have proposed a trapped-ion QS that fulfills this requirement. In particular, in the regime where nonadiabatic effects of the zigzag distortion become relevant, the complexity of the manybody model in Eqs.  $(3)$  $(3)$  $(3)$  and  $(5)$  $(5)$  compromises the efficiency of existing numerical methods. Also, this QS may address the effects of the inhomogeneities, the long-range dipolar tail of the spin-spin interactions, and the dynamics across such a magnetic structural quantum phase transition. We emphasize that the incorporation of all these effects make our QS of the utmost interest, which may also find an application in the context of other Wigner crystals [\[35\]](#page-4-32), such as electrons in quantum wires or liquid helium.

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