



The physics of Ion Coulomb Crystals: Thermodynamics, Quantum control, and Quantum Simulators

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Theoretical characterization of structural phase transitions of ICC in the quantum regime

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Title: Theoretical characterization of structural phase transitions of ICC in the quantum regime

Short Description: Report on the theoretical characterization of the quantum ground state of ion Coulomb crystals at structural phase transitions for two models: (i) ions in a ring trap, with transverse harmonic confinement, and (ii) ions in a linear Paul trap.

Work achieving the deliverable: Refs.[1,2] constitute the main contribution to the deliverable and fulfill its central goal. In these papers, the mapping of the structural phase transition linear-zigzag to an Ising model with a transverse field is performed. This mapping gives the properties of the quantum ground state and of the low-energy spectrum of the crystal at ultralow temperatures across the critical point. This theory, moreover, allows for the estimation of the critical point and predicts the critical exponents. The mapping in [1,2], in particular, allows one to determine the phase diagram of the crystal as a function of the experimental parameter. We note that in these works an appropriate thermodynamic limit is defined for ions in a ring trap and in a linear Paul trap, so that the predictions of the model apply for both systems. The finite-size effects can be determined by means of finite-size scaling techniques. An important verification of this theory has been provided by the numerical results of UULM.QIV, who developed a unique code combining DMRG and Matrix-Product- State types of programs for describing the linear-zigzag quantum phase transition, see [3]. The numerical study provides moreover a more precise determination of the critical point. A draft summarizing the numerical results and comparing them with the theoretical prediction is in preparation.

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- [2] "Quantum structural phase transition in chains of interacting atoms", E. Shimshoni, G. Morigi, and S. Fishman, Phys. Rev. A 83, 032308 (2011); arxiv:1012.4332
- [3] DMRG program developed by UULM.QIV. The program is available to the referees and to the project officer upon request for the purpose of project review but is not for public dissemination. The contact persons are Tommaso Calarco, Simone Montangero, and Pietro Silvi of the University of Ulm, Germany (email: Tommaso.Calarco(at)uni-ulm.de).

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Quantum Zigzag Transition in Ion Chains

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A string of trapped ions at zero temperature exhibits a structural phase transition to a zigzag structure, tuned by reducing the transverse trap potential or the interparticle distance. The transition is driven by transverse, short wavelength vibrational modes. We argue that this is a quantum phase transition, which can be experimentally realized and probed. Indeed, by means of a mapping to the Ising model in a transverse field, we estimate the quantum critical point in terms of the system parameters, and find a finite, measurable deviation from the critical point predicted by the classical theory. A measurement procedure is suggested which can probe the effects of quantum fluctuations at criticality. These results can be extended to describe the transverse instability of ultracold polar molecules in a one-dimensional optical lattice.

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Crystals of singly-charged ions, ion Coulomb crystals, constitute a fascinating physical realization of the phenomenon discussed by Wigner for electrons in metals [1]. These crystals result from the combined Coulomb repulsive force and the restoring force of an external potential, usually a harmonic trap [2]. The strongly correlated regime, leading to long-range order, is accessed by means of laser cooling, allowing one to obtain samples at temperatures T ranging from few mK to hundreds of μK [3].

Ion chains have been most discussed in the literature focused on quantum technological applications [4,5]. They are realized in potentials with an enhanced elliptical geometry, so that the charges align along the trap axis [6–8]. Strictly speaking, in one dimension there is no crystalline order even at ultralow temperatures. However the Coulomb interaction gives rise to very slowly decaying density-density correlations, such that quasi long-range order is generally warranted [9]. At a given interparticle distance the stability of the ion chain is determined by the strength of the transverse potential: if the corresponding frequency ν_t is below a critical value ν_c , a planar, zigzag structure is observed [6,7,10,11]. In Refs. [12,13] it was shown that the classical structural transition linear zigzag is of second order. A Landau model was derived, proving that the soft mode of the phase transition is the zigzag mode of the linear chain (the transverse mode with the shortest wavelength) which drives the instability and determines the new structure [13]. The corresponding Ginzburg-Landau equation in the continuum limit is reported in [14]. The results of these studies are strictly valid in the classical regime, when quantum and thermal fluctuations can be neglected.

A question naturally emerges whether and how quantum fluctuations modify the behavior at the linear-zigzag instability. Theoretical studies on ion systems so far focused on

small samples [15]. In this Letter it is argued that the linear-zigzag transition is a quantum phase transition, which can be mapped to the one of an Ising chain in a transverse field, describing a quantum ferromagnetic transition at $T = 0$ [16]. This equivalence was previously proposed in a theoretical study of linear-zigzag structures for electrons in quantum wires [17]. Here we outline a mapping which allows us to estimate the quantum critical point in terms of the system parameters, and determine the experimental conditions required to observe it. The phase diagram is sketched in Fig. 1. We find a finite, measurable

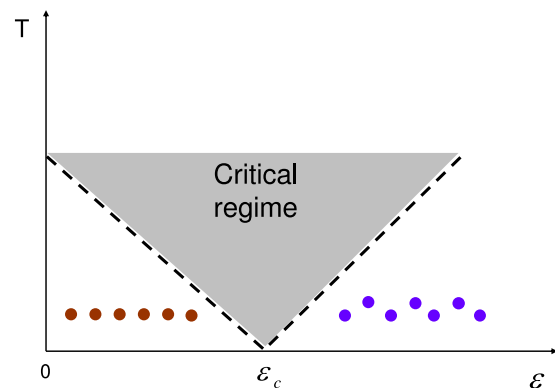


FIG. 1 (color online). Phase diagram for a linear-zigzag transition, according to the mapping to the quantum Ising transition in 1D, where T is the sample temperature and the dimensionless parameter ε is tuned by the confining potential or the interparticle distance. The classical instability of the linear chain [13] occurs at $\varepsilon = 0$. The quantum critical point, at $\varepsilon_c > 0$, separates the linear from the zigzag phase at $T = 0$. For $0 < \varepsilon < \varepsilon_c$ quantum fluctuations dominate, and the crystal is in the linear (disordered) phase. The dashed lines indicate the boundaries of the quantum critical region.

deviation from the critical point predicted by the classical theory [13].

The system we consider is composed of N ions of mass m and charge Q . The ions mutually repel via the Coulomb interaction and are confined in the transverse plane ($y-z$) by an anisotropic harmonic potential, while periodic boundary conditions are assumed in the x direction. The ions experience the potential $V_{\text{tot}} = V_t + V_{\text{int}}$, which is the sum of the transverse harmonic trap, $V_t = m\nu_t^2 \sum_{j=1}^N y_j^2/2$, and the Coulomb repulsion, $V_{\text{int}} = (Q^2/2) \sum_{i \neq j} 1/\sqrt{(x_i - x_j)^2 + (y_i - y_j)^2}$, while the motion in the z direction is frozen out by a tight confining potential, so that the system is essentially two dimensional. The parameters of the potential are such that the particles are aligned along the x axis with uniform interparticle distance a , and their equilibrium positions are $x_j^{(0)} = ja$, $y_j^{(0)} = 0$, with $j = 1, \dots, N$. This configuration can be realized in a ring trap under the condition that one ion is pinned [6], or in an anharmonic trap [18]. It also approximates the ion's distribution at the center of a long chain in a linear Paul trap [6,8,13,19].

At ultralow temperatures the ions perform harmonic vibrations about the mechanically stable equilibrium positions. The linear chain is stable against longitudinal displacements from the equilibrium positions $x_j^{(0)}$, while a soft mode in the transverse direction drives a structural transition into a zigzag configuration. This mode has wavelength $\lambda = 2a$, such that in the classical harmonic crystal the corresponding displacements are $y_j^{\text{soft}} = (-1)^j y_0$ with y_0 the amplitude of the oscillations. We focus on the dynamics of the transverse phonon modes of the linear chain close to the instability, and expand V_{int} to fourth order in $|y_j| \ll a$. Our starting point is the Landau model derived in Ref. [13]. Close to the instability the displacement along y can be rewritten as $y_j = (-1)^j a \phi_j$, where ϕ_j is a dimensionless field which varies slowly with the ion position. To leading order in a gradient expansion, we obtain an effective potential for the field ϕ_j

$$V[\{\phi_j\}] \approx \sum_{j=1}^N V_0(\phi_j) + \frac{1}{2}K \sum_{j=1}^N (\phi_j - \phi_{j+1})^2, \quad (1)$$

where V_0 is a local potential of the form

$$V_0(\phi) = -\frac{1}{2}m(\nu_c^2 - \nu_t^2)a^2\phi^2 + \frac{1}{4}ga^4\phi^4, \quad (2)$$

and the second term in Eq. (1) describes nearest-neighbor interaction at strength $K = (Q^2/a) \ln 2$. The other parameters are $\nu_c = \sqrt{4Q^2/ma^3} \sqrt{C_3}$ and $g = 24C_5 Q^2/a^5$, with $C_\alpha = \sum_{j \geq 1} 1/(2j+1)^\alpha$. Note that ν_c is the frequency at which the linear chain is unstable and a transition to the zigzag configuration occurs within the classical theory [11,13]. It is remarkable that the Coulomb repulsion is mapped to a short-range potential close to the linear-zigzag

instability. This property is clearly visible in the spectrum of the transverse excitations: $\omega_\perp^2(k) \sim \nu_t^2 - \nu_c^2 + (K/m)k^2$ [13], characteristic of a chain with nearest-neighbor coupling and sound velocity $c = \sqrt{K/m}$.

We next define a parameter $\varepsilon \equiv (\nu_c^2 - \nu_t^2)/\nu_c^2$. Classically, the chain is stable for $\varepsilon < 0$ [13]. For $\varepsilon > 0$, the local potential V_0 in Eq. (2) has minima at $\phi_\pm = \pm \phi_0$, with $\phi_0 \equiv (\nu_c/a)\sqrt{m\varepsilon/g}$; the ions therefore order in a zigzag structure at either one of the configurations with $y_j^{(\pm)} = (-1)^j \phi_\pm a$, thereby breaking the reflection symmetry at the x axis. This calculation, however, neglects quantum fluctuations, which induce tunneling between the minima and tend to destroy the zigzag order.

Quantum fluctuations are included in the model of the structural transition by means of a 1 + 1-dimensional quantum field theory [20]. To this end, we write the partition function as

$$Z = \int \mathcal{D}\phi e^{-S[\phi]/\hbar} \quad (3)$$

with the Euclidean action

$$S[\phi] = \int_0^\beta d\tau \sum_{j=1}^N \left[\frac{ma^2}{2} (\partial_\tau \phi_j)^2 + V_0(\phi_j) + \frac{K}{2} (\phi_j - \phi_{j+1})^2 \right] \quad (4)$$

where $\beta = \hbar/k_B T \rightarrow \infty$ for $T \rightarrow 0$. This model describes the quantum dynamics of the zigzag phonon mode in terms of a real continuous scalar field, $-\infty < \phi_j(\tau) < \infty$. We now express it in a form which allows its mapping onto an effective model for the *discrete* field $\sigma_j(\tau) \equiv \text{sgn}[\phi_j(\tau)]$. We first divide the imaginary time (τ) axis into M discrete steps separated by an infinitesimal interval of size $\delta\tau = \beta/M$. The partition function is then cast in the form $Z = \text{Tr}\{\hat{T}^M\}$, where $\hat{T}$ is a transfer matrix describing the time evolution from τ to $\tau' = \tau + \delta\tau$, whose elements read

$$T[\{\phi_j\}, \{\phi'_j\}] = \prod_{j=1}^N T_{\text{loc}}(\phi_j, \phi'_j; \delta\tau) \exp \left\{ -\frac{\delta\tau}{4\hbar} K \sum_{j=1}^N [(\phi_j - \phi_{j+1})^2 + (\phi'_j - \phi'_{j+1})^2] \right\}. \quad (5)$$

Here, $T_{\text{loc}}(\phi_j, \phi'_j; \delta\tau) = \langle \phi'_j | e^{-\hat{H}_j \delta\tau/\hbar} | \phi_j \rangle$ is the propagator describing the quantum dynamics of a particle subject to the local Hamiltonian $\hat{H}_j = p_j^2/(2m) + V_0(\phi_j)$, with $V_0(\phi)$ the double-well potential, Eq. (2), and ϕ_j, p_j canonical conjugate variables. We now write the continuous field as $\phi_j = \phi_0 \sigma_j^z + \delta\phi_j$, where σ_j^z is the Pauli matrix, which can take values ± 1 corresponding to the minima of the double-well potential, and $\delta\phi_j$ are the fluctuations. We then integrate over $\delta\phi_j$, obtaining an effective transfer matrix in terms of Ising fields. When the system is well inside the zigzag phase, the typical frequency of tunnel

splitting in the double wells, $\Delta\omega$, is much smaller than ω_0 , the frequency of the oscillations about the well minima. Under this approximation, we obtain

$$T_{\text{eff}}[\{\sigma_j\}, \{\sigma'_j\}] = \prod_{j=1}^N T_{\text{loc}}[\sigma_j, \sigma'_j] \times \exp\left\{\frac{K\phi_0^2\delta\tau}{2\hbar}(\sigma_j\sigma_{j+1} + \sigma'_j\sigma'_{j+1})\right\} \quad (6)$$

where the 2×2 matrix $\hat{T}_{\text{loc}}$ encodes the single particle dynamics within the double-well potential. The propagator $\hat{T}_{\text{loc}}$ obeys the symmetry $T_{\text{loc}}[\sigma, \sigma'] = T_{\text{loc}}[-\sigma, -\sigma']$, and can therefore be written as

$$\hat{T}_{\text{loc}} = \text{const} \times (A\sigma^0 + B\sigma^x), \quad (7)$$

where σ^α are Pauli matrices in the basis where $\{\sigma = \pm 1\}$ denote the eigenvalues of σ^z , and σ^0 is the 2×2 unit matrix. The coefficients A and B acquire a simple form in the zigzag phase, when the ion wave functions are relatively well localized near $\pm\phi_0$ and can be approximated by Gaussians of width l . In this limit, using the inequality $e^{-2\phi_0^2/l^2} \ll \tanh\{\Delta\omega\delta\tau/2\} \ll 1$, we obtain

$$\hat{T}_{\text{loc}} \approx T_0 \exp\{\Delta\omega\sigma^x\delta\tau/2\} \quad (8)$$

with T_0 a constant prefactor. As a result, the partition function reduces to the form $Z \approx Z_0 \int \mathcal{D}\sigma \exp(-S_I[\sigma]/\hbar)$, in which Z_0 is a constant and S_I the action of an Ising chain in a transverse field [16] subject to the Hamiltonian

$$H_I = - \sum_{j=1}^N (J\sigma_j^z\sigma_{j+1}^z + h\sigma_j^x). \quad (9)$$

Here, the parameters are the fictitious exchange coupling

$$J = K\phi_0^2 = C_J U_P \varepsilon, \quad (10)$$

with $U_P = Q^2/a$ the strength of the interaction and $C_J = C_3 \ln 2 / (6C_5)$, while the transverse field $h = \hbar\Delta\omega/2$ is proportional to the splitting energy. Its dependence on the physical parameters can be estimated by means of a variational calculation [20], which gives

$$h \approx C_h (U_P U_K^2)^{1/3} \quad (11)$$

where $U_K = \hbar^2/ma^2$ is the typical kinetic energy scale of the atoms in the chain and $C_h = (9C_5/2)^{1/3}$. Equation (11) was obtained assuming $U_K/U_P \gg \varepsilon^3$, which holds close to the critical points, where quantum fluctuations dominate.

The model described by Hamiltonian (9) is known to exhibit a quantum phase transition at $h/J = 1$ and $T = 0$, separating an ordered phase at $J > h$ (in our case, the stable zigzag configuration) from a disordered phase at $J < h$ (the linear chain). In both phases the spectrum of excitations is characterized by a gap with energy $\Delta = 2|J - h|$. The

corresponding phase diagram, showing the critical behavior as a function of ε (and hence ν_t) and T is sketched in Fig. 1. The critical regime ($k_B T > \Delta$) is characterized by universal power law T dependence of correlation functions with the critical exponents of the quantum transition [16].

The mapping to the Ising model, here presented, is strictly valid as long as the lowest energy levels of the local, double-well potential are below the barrier. In this regime, the tunneling between the wells is small and hence necessarily $h \ll J$, which is satisfied deep in the zigzag phase. The symmetry of the ordered phase was used to identify the effective model and estimate its parameters. This procedure is strictly valid only in a higher dimension ($4 - \epsilon$). Nevertheless, from conformal symmetry arguments [21] it is reasonable to assume that a quantum Ising model is the appropriate field theory for the $(1+1)\text{D}$ ϕ^4 model describing the present system, and qualitatively describes its critical behavior at $h \sim J$. This hypothesis is further supported by numerical studies [22]. Under this assumption we estimate the quantum critical point in the regime of parameters where classical zigzag order is suppressed by quantum tunneling, and observe that it belongs to a universality class [16,21] that differs from the one of the classical Landau model.

The critical value of ε , and thus of the transverse frequency ν_t , is dictated by the condition $h = J$, yielding

$$\varepsilon_c \approx C_c (U_K/U_P)^{2/3}, \quad C_c \equiv C_h/C_J \sim 10. \quad (12)$$

Hence, for given $U_K/U_P \ll 1$, a quantum critical point is expected at $\varepsilon_c \gg U_K/U_P$.

We now discuss what are the experimental conditions which are required in order to observe the quantum critical point. Chains with dozens of ions are usually realized in linear Paul traps [6–8], where the ion distribution along the chain is inhomogeneous. The considerations here reported apply in the center of the chain, when the chain contains several dozens of ions. More regular distributions are expected in linear traps where the axial potential is anharmonic [18]. Here, one can tune through the critical point by either controlling the transverse frequency ν_t (typically in the MHz regime), or the spacing between neighboring ions a (typically several μm) by means of the axial confinement. To be able to distinguish the quantum disordered phase from the ordered (zigzag) phase, the frequency difference $\delta\nu = \nu_c - \nu_t$ should exceed the experimentally accessible resolution. In order to estimate the required resolution, we write $\varepsilon_c \approx 2\delta\nu/\nu_c$ in terms of $a = a_0 \times 1 \mu\text{m}$ and of the ion mass $m = n_A m_p$, with m_p the proton mass and n_A the atomic number, and find $\varepsilon_c \approx 10^{-4}/(n_A a_0)^{2/3}$, leading to an upper bound on the frequency resolution

$$\delta\nu \approx 10^{-4}(\nu_c/2)(n_A a_0)^{-2/3} \quad (13)$$

ranging from kHz (for protons with $a_0 \sim 1$) to several Hz for, e.g., $^{24}\text{Mg}^+$ ions. This bound must also be compared

with the heating time scale T_h in ion traps, such that $\delta\nu T_h \ll 1$ should be satisfied, which leads to demanding conditions for the existing trapping setups [5]. A larger value $\delta\nu$, and hence less restrictive conditions on observing the quantum critical point, could be reached in presence of screening, when the chain is embedded in a crystal of another ion species [8]. It is also essential to reduce T below the energy scale characteristic of the gap away from criticality, i.e., $\Delta \sim \hbar$, resulting in $T[\text{mK}] \ll 10^3 C_h (U_K^2 U_P)^{1/3} / k_B$, which corresponds to

$$T[\text{mK}] \ll 0.25(n_A^2 a_0^5)^{-1/3}, \quad (14)$$

implying an upper bound of order ~ 0.1 mK for protons to several μK for Mg^+ ions.

The quantum critical point could be more easily observed in a quasi one-dimensional array of ultracold polar molecules, interacting via dipole-dipole repulsion, when the dipoles are aligned by an external field in a direction perpendicular to the plane where their motion takes place [23,24]. Numerical simulations show that quantum tunneling clearly modifies the behavior at the linear-zigzag transition predicted by the classical theory [25]. Assuming the dipoles are pinned by an optical lattice at fixed interparticle position, then the potential for the phononic modes at the instability is given by Eq. (1), and the mapping to the Ising model in the transverse field can be performed, where now $U_P = C_{dd}/(4\pi a^3)$, with C_{dd} the dipole interaction strength [25], while $C_c \sim 10$. Using typical numbers for the dipolar strength [23] one finds $\delta\nu \sim \nu_c$, showing that quantum fluctuations are significant at the linear-zigzag transition.

The phase transition can be experimentally measured by light scattering via the structure factor $S(k)$ [25]. In the critical region $S(k) = S_f(k) + S_0 \delta(k - k_0)$, where $k_0 = \pi/a$ is the wave number of the zigzag, S_0 is proportional to the squared order parameter, $S_0 \propto \phi_0^2$, while S_f is proportional to the isothermal susceptibility χ of the corresponding Ising system [16]. Approaching the quantum critical point in the zigzag phase ($\epsilon > \epsilon_c$) and for $T \ll \Delta$, one has $\chi \sim |\epsilon_c - \epsilon|^{-\gamma}$ and $\phi_0^2 \sim |\epsilon_c - \epsilon|^{2\beta}$ where $\beta = 1/8$ and $\gamma = 7/4$ are the exponents of the classical two-dimensional Ising model. In the critical region $T \gg \Delta$ [shaded area in Fig. 1], $\chi \sim T^{-7/4}$ and $\phi_0^2 \sim T^{1/4}$ [16]. Note that this critical behavior is strictly valid for an infinite system and assumes a uniform density of ions. It is expected to be approximately valid in an ion chain, when the variation of the density in a large region is negligible within a correlation length.

To conclude, we argue that the linear-zigzag instability in two-dimensional systems of trapped ions or polar molecules can be mapped to the one-dimensional Ising model in a transverse field. This result demonstrates once more the potentialities offered by these systems as quantum simulators [5,23,26], and more generally for quantum technological applications.

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Quantum structural phase transition in chains of interacting atoms

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A quasi-one-dimensional system of trapped, repulsively interacting atoms (e.g., an ion chain) exhibits a structural phase transition from a linear chain to a zigzag structure, tuned by reducing the transverse trap potential or increasing the particle density. Since it is a one-dimensional transition, it takes place at zero temperature and therefore quantum fluctuations dominate. In Fishman *et al.* [*Phys. Rev. B* **77**, 064111 (2008)] it was shown that the system close to the linear-zigzag instability is described by a ϕ^4 model. We propose a mapping of the ϕ^4 field theory to the well-known Ising chain in a transverse field, which exhibits a quantum critical point. Based on this mapping, we estimate the quantum critical point in terms of the system parameters. This estimate gives the critical value of the transverse trap frequency for which the quantum phase transition occurs and which has a finite, measurable deviation from the critical point evaluated within the classical theory. A measurement is suggested for atomic systems which can probe the critical trap frequency at sufficiently low temperatures T . We focus in particular on a trapped-ion system and estimate the implied limitations on T and on the interparticle distance. We conclude that the experimental observation of the quantum critical behavior is, in principle, accessible.

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I. INTRODUCTION

The structural transition from a linear chain of repulsively interacting particles to a planar configuration, in the form of a zigzag structure, has been often discussed in theoretical studies on atomic and condensed-matter systems. Examples include electrons in nanowires [1], ultracold dipolar gases [2], vortex lines in Bose-Einstein condensates [3,4], and ion Coulomb crystals in traps [5–7]. Specifically, in ion Coulomb crystals this transition has been experimentally observed and characterized [8–10], thereby determining a phase diagram of the ionic structures as a function of the trap aspect ratio and of the mean interparticle distance [9].

Theoretical studies demonstrated that the transition from the string to the zigzag chain is associated with a symmetry breaking. More specifically, if the Hamiltonian is invariant under rotation about the string axis, it is the rotational symmetry around the chain which is broken in the zigzag phase. If instead the motion of the interacting particles is confined to the plane, the zigzag phase breaks the symmetry by reflection about the chain axis. The phase transition predicted by the classical theory is hence second order [11,12]. It can be described by a Landau model, of which critical values and exponents are well known [12] and where the soft mode is the zigzag mode of the linear chain—namely, the transverse mode with the shortest wavelength—which drives the instability and determines the new structure. The corresponding Ginzburg-Landau equation in the continuum limit and in presence of damping was reported in Ref. [13], where special focus was given on creation of defects when quenching the value of the transverse trap frequency across the mechanical instability. Further works discussed the structural transitions when the external potential is not harmonic [14], showing that the statistical mechanics of the system at the instability may be profoundly modified. The results of these studies are strictly valid in the classical regime, when the thermal fluctuations can be neglected.

In Ref. [15] we addressed the question, whether quantum fluctuations significantly modify the location of the critical point and the behavior in its vicinity, focusing on ion Coulomb crystals. This question draws on numerical studies in low-dimensional dipolar systems, which showed a significant contribution of quantum fluctuations at the transition from a string to a zigzag order [16]. In this article we provide the detailed calculations at the basis of the results presented in Ref. [15] and extend the treatment to interacting atomic chains, with repulsive interaction potential scaling as $1/x^\alpha$ with $\alpha \geq 1$. We focus on the case where the motion of the particles is confined to a plane. As argued below, the string-to-zigzag transition is indeed a quantum phase transition analogous to the ferromagnetic transition of an Ising chain in a transverse field [17]. A phase diagram summarizing the behavior in its vicinity is depicted in Fig. 1. Note that a similar mapping to the Ising model was argued in the context of electronic systems in quantum wires [1]. However, the validity of the assumed equivalence between a continuous-field theoretical model and a discrete (Z_2) field theory cannot be justified on the basis of classification into universality classes below three space dimensions [18].

In the present study we develop a quantum field theoretical approach, which allows a direct mapping to the quantum one-dimensional Ising model under plausible assumptions. On this basis we determine the quantum critical point at which the transition occurs and identify the experimental parameters, for which it can be distinguished from the value predicted by the classical theory [12]. In particular, we relate the critical value of the transverse trap frequency ν_t to the ratio of the typical kinetic energy scale U_K and interaction energy U_P . Defining a parameter $\epsilon = 1 - \nu_t^2/\nu_c^2$, which describes the deviation of the transverse confinement from its stability point, we find that the critical point is given by $\epsilon_c \sim (U_K/U_P)^{2/3}$. A measurement is suggested that can demonstrate transverse

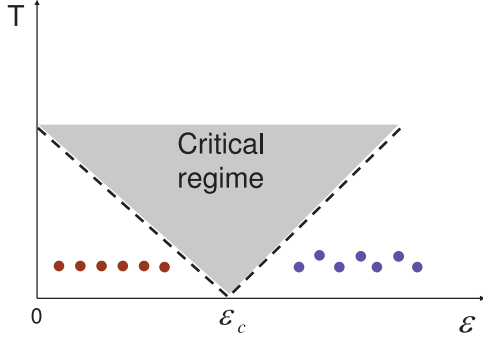


FIG. 1. (Color online) Sketch of the phase diagram exhibiting a linear-zigzag transition, according to the mapping to the one-dimensional model of a quantum Ising transition. Here T is the temperature of the sample and the dimensionless parameter ϵ is tuned by the confining potential or the interparticle distance. The value $\epsilon = 0$ corresponds to the value of the transverse frequency, where the linear chain is classically unstable [12]. The quantum critical point, at $\epsilon_c > 0$, separates the linear chain from the zigzag phase at $T = 0$. For $0 < \epsilon < \epsilon_c$ quantum fluctuations dominate, and the crystal is in the linear (disordered) phase. The dashed lines indicate the boundaries of the quantum critical region, where thermal fluctuations dominate.

quantum fluctuations in a long chain of trapped ions (composed of hundreds of ions) and probe the different regimes in the phase diagram.

This paper is organized as follows. In Sec. II we derive a quantum field theory for the zigzag phonon mode. The mapping to the quantum Ising model is described in Sec. III. In Sec. IV we derive expressions for the Ising model parameters, and in particular their critical values, in terms of microscopic parameters of the interacting atoms system. In Sec. V we discuss an experimental realization in trapped-ion systems, and specify the conditions under which the quantum phase transition is likely to be observable. Finally, our conclusions and outlook are summarized in Sec. VI.

II. QUANTUM FIELD THEORY FOR THE ZIGZAG MODE

We start by considering a linear array of particles with mass m , which are confined in the x - y plane. The system is at low temperature, and the particles at equilibrium are aligned along the x axis and equidistant, with interparticle distance a such that their equilibrium position is $x_j^{(0)} = ja$ and $y_j^{(0)} = 0$, while the motion along the z axis is assumed to be frozen out. Periodic boundary conditions are assumed at the chain edges and one ion of the chain is assumed to be pinned. The particles can oscillate around the equilibrium positions in the x and y directions, where they are confined by a harmonic potential of the form

$$V_t = \frac{1}{2} m v_t^2 \sum_{j=1}^N y_j^2; \quad (1)$$

here y_j is the displacement of the j th atom from the chain axis and v_t the trap frequency. Finally, they interact by means of the repulsive power-law potential,

$$V_{\text{int}} = \frac{A^2}{2} \sum_{i \neq j} \frac{1}{[(x_i - x_j)^2 + (y_i - y_j)^2]^{\alpha/2}}, \quad (2)$$

where $\{\mathbf{r}_j = (x_j, y_j)\}$ denotes the atomic position in the plane, A^2 is the strength of the interaction, and $\alpha \geq 1$.

This model includes the Coulomb interaction when $\alpha = 1$ and the dipolar interaction when $\alpha = 3$, assuming that the dipoles are polarized along the z axis, such that in the x - y plane they experience an isotropic repulsive force. We also note that in the case of the Coulomb interaction the strength is such that $A = Q$, where Q is the charge of the particle. In this case the array can result from the self-organization of the atoms, since quasi-long-range order can be assumed as long as one particle in the chain is pinned. The configuration, in which the particles are aligned along the x axis with uniform interparticle distance, could be realized in a ring trap at ultralow temperatures under the condition that one ion is pinned [9], or in an anharmonic linear Paul trap [19]. It also corresponds with good approximation to the ion distribution at the center of a long chain in a linear Paul trap [9,12,20,21].

For $\alpha > 1$, on the other hand, particle-particle correlations decay at $T = 0$ with a power-law dependence on the distance [22], and long-range order may be only assumed in the presence of an additional periodic potential along x , which localizes the particles at the positions $x_j^{(0)}$. For dipolar atoms or molecules with an electric dipole moment D , this configuration could be realized by means of an optical lattice [23] with periodicity a . Here the dipole-dipole interaction can be made repulsive in the x - y plane when a static electric field along the z axis aligns the dipole. Then the strength of the interaction is such that $A \propto D$.

We assume temperatures such that the atoms crystallize and their motion is well approximated by harmonic vibrations about the equilibrium positions when the configuration is mechanically stable. While the linear chain is stable against longitudinal displacements from the equilibrium positions, a soft mode in the transverse direction drives a structural phase transition of the linear chain into a zigzag configuration, as shown in Ref. [12]. This mode has wavelength $\lambda = 2a$, such that in the classical harmonic crystal the corresponding displacements are described by the function $y_j = (-1)^j y_0$ with y_0 the amplitude of the oscillations. We therefore focus on the dynamics of the transverse phonon modes close to the instability and expand V_{int} to fourth order in $|y_j| \ll a$. Moreover, we introduce the field ϕ_j , which describes a transverse excitation close to the instability and is slowly varying with respect to the length scale a ; that is,

$$\phi_j = (-1)^j y_j / a. \quad (3)$$

Using a gradient expansion to leading order [12], we obtain the effective potential

$$\begin{aligned} V[\{\phi_j\}] &= V_t + V_{\text{int}} \approx \frac{1}{2} m v_t^2 a^2 \sum_{j=1}^N \phi_j^2 + \frac{A^2}{2a^\alpha} \sum_{i \neq j} \frac{\alpha}{2} \\ &\times \left\{ -\frac{(\phi_i - (-1)^{i-j} \phi_j)^2}{|i - j|^{\alpha+2}} + \frac{(\alpha + 2)(\phi_i - (-1)^{i-j} \phi_j)^4}{4|i - j|^{\alpha+4}} \right\}. \end{aligned} \quad (4)$$

Terms describing the coupling between the axial and transverse modes have not been reported because they give rise to

higher-order corrections in the gradient expansion. The latter is defined by the small parameter $\delta ka \ll 1$, with $\delta k = |k - k_0|$ the typical deviation between the wave vector k of the excited mode and the wave vector $k_0 = \pi/a$ of the soft mode. An extensive discussion on the derivation of the effective potential for the soft mode can be found in Ref. [12]. The ordered, zigzag phase is established when ϕ_j acquires a finite, constant expectation value, as we show below. To leading order in a gradient expansion, the potential in Eq. (4) can be mapped to the dynamics described by a potential of the form

$$V[\{\phi_j\}] \approx \sum_{j=1}^N V_0(\phi_j) + \frac{1}{2}K \sum_{j=1}^N (\phi_j - \phi_{j+1})^2, \quad (5)$$

where the interaction is now nearest neighbors. Here V_0 is a local potential,

$$V_0(\phi) = -\frac{1}{2}m(v_c^2 - v_t^2)a^2\phi^2 + \frac{1}{4}ga^4\phi^4, \quad (6)$$

and the parameters K , v_c , and g are given by

$$K = \frac{C_1[\alpha]\alpha A^2}{a^\alpha}, \quad v_c^2 = \frac{4C_2[\alpha + 2]\alpha A^2}{ma^{\alpha+2}}, \quad (7)$$

$$g = \frac{8C_2[\alpha + 4]\alpha(\alpha + 2)A^2}{a^{\alpha+4}},$$

with

$$C_1[\alpha] \equiv \sum_{j=1}^N \frac{(-)^{j+1}}{j^\alpha}, \quad C_2[\alpha] \equiv \sum_{j \geq 1, \text{ odd}} \frac{1}{j^\alpha}.$$

A classical theory, which neglects quantum fluctuations (i.e., valid in the limit $\hbar = 0$), predicts a transition from a linear to a zigzag chain at $T = 0$ when the transverse confining frequency v_t is reduced below the critical value v_c [12]. For later convenience we define a dimensionless parameter describing the deviation of the transverse trap frequency from this classical transition point:

$$\epsilon \equiv \frac{v_c^2 - v_t^2}{v_c^2}. \quad (8)$$

For $\epsilon > 0$, the local potential V_0 [Eq. (6)] has minima at

$$\phi_{\pm} = \pm\phi_0, \quad \phi_0 \equiv \frac{1}{a}\sqrt{\frac{m\omega^2}{g}}, \quad (9)$$

where the frequency ω is given by the relation

$$\omega^2 = v_c^2 - v_t^2 = \epsilon v_c^2 \quad (10)$$

and is associated with the curvature of V_0 at the top of the barrier between the minima of the double-well potential, as one can observe from Eq. (6).

We note that the mapping to Eq. (5) is valid for a power-law interaction with $\alpha \geq 1$ [for which the relevant sums $C_l[\alpha]$ in Eq. (7) converge], hence including the case of the Coulomb interaction at $\alpha = 1$. Therefore, for the linear-zigzag instability the Coulomb interaction effectively belongs to the class of short-range potentials. Indeed, one finds that the spectrum of the transverse excitations close to the instability (approaching from the side where the chain is stable classically) behaves as

$$\omega^2 \sim v_t^2 - v_c^2 + (K/m)k^2$$

for $\alpha \geq 1$ (see, for instance, Ref. [12] for the case $\alpha = 1$). This behavior is markedly different from that of the long-wavelength, axial excitations: For $\alpha > 1$ the axial frequency $\omega \sim ck$, with c sound velocity, while for $\alpha = 1$ there exists no sound velocity, and $\omega \sim k\sqrt{|\log k|}$ [20,24,25].

These considerations on the structure, which are based on identifying the minima of the potential energy, do not account for the contribution of the kinetic energy. Thermal effects are expected to modify the behavior at the critical point. Moreover, even at temperatures $T \rightarrow 0$, when thermal fluctuations are small, quantum fluctuations will become relevant. Sufficiently close to the value v_c , that is, for sufficiently small values of the parameter ϵ (where the classical zigzag ordering is expected), quantum fluctuations will induce tunneling between degenerate minima of the potential and are expected to destroy the zigzag ordering. A true phase transition will therefore occur at a smaller value of v_t , corresponding to a *quantum* critical point, such that $v_t < v_c$, that is, at $\epsilon_c > 0$.

In order to investigate the quantum critical behavior, one has to introduce a 1 + 1-dimensional quantum field theory for the system. To this end, we write the partition function as

$$Z = \int \mathcal{D}\phi e^{-S[\phi]/\hbar}, \quad (11)$$

with the Euclidean action

$$S[\phi] = \int_0^{\hbar\beta} d\tau \sum_{j=1}^N \left[\frac{1}{2}ma^2(\partial_\tau \phi_j)^2 + V_0(\phi_j) + \frac{1}{2}K(\phi_j - \phi_{j+1})^2 \right], \quad (12)$$

where $\beta = 1/k_B T$ and $\beta \rightarrow \infty$ for $T \rightarrow 0$. Below we demonstrate the mapping of this model to the Ising chain in a transverse field, and derive approximate expressions for its parameters in terms of microscopic parameters of the interacting particles system. This will facilitate the study of the conditions under which the phase transition can be observable in such systems.

III. MAPPING TO THE QUANTUM ISING CHAIN

The low-energy model derived in the previous section [Eqs. (11) and (12)] describes the quantum dynamics of the zigzag phonon mode in terms of a real continuous scalar field $-\infty < \phi_j(\tau) < \infty$. We now express it in a form which will allow its mapping onto an effective model for the discrete field $\sigma_j(\tau) \equiv \text{sgn}[\phi_j(\tau)]$. As a starting point, we perform the standard procedure of dividing the imaginary time (τ) axis into discrete time steps $\{\tau_m\}$ separated by an infinitesimal interval of size $\delta\tau$, with $m = 0, \dots, M$ and $M = \hbar\beta/\delta\tau$. The partition function is then cast in the form

$$Z = \text{Tr} \{ \hat{T}^M \}, \quad (13)$$

where $\hat{T}$ is a transfer matrix describing the time evolution from τ_m to τ_{m+1} . Using the notation $\phi_j = \phi_j(\tau_m)$, $\phi'_j = \phi_j(\tau_{m+1})$,

the matrix elements of $\hat{T}$ are given by

$$T[\{\phi_j\}, \{\phi'_j\}] = \exp \left\{ -\frac{\delta\tau}{2\hbar} \sum_{j=1}^N \left[ma^2 \left(\frac{\phi_j - \phi'_j}{\delta\tau} \right)^2 + V_0(\phi_j) + V_0(\phi'_j) + \frac{1}{2} K ((\phi_j - \phi_{j+1})^2 + (\phi'_j - \phi'_{j+1})^2) \right] \right\} \quad (14)$$

$$= \prod_{j=1}^N G(\phi_j, \phi'_j; \delta\tau) \exp \left\{ -\frac{\delta\tau}{4\hbar} K \sum_{j=1}^N [(\phi_j - \phi_{j+1})^2 + (\phi'_j - \phi'_{j+1})^2] \right\}. \quad (15)$$

Here the propagator $G(\phi_j, \phi'_j; \delta\tau)$ is given by

$$G(\phi_j, \phi'_j; \delta\tau) = \langle \phi'_j | e^{-\hat{H}_j \delta\tau / \hbar} | \phi_j \rangle, \quad (16)$$

in which the local Hamiltonian $\hat{H}_j = p_j^2 / (2m) + V_0$ describes the quantum dynamics of a particle in the double-well potential $V_0(\phi)$, where p_j is the momentum conjugate to ϕ_j . The symmetry of the potential implies that the exact eigenstates of $\hat{H}_j$ consist of pairs of states with well-defined symmetry under $\phi \rightarrow -\phi$: symmetric ($|S_n\rangle$) and antisymmetric ($|A_n\rangle$). The corresponding energy eigenvalues can be expressed as $\hbar(\bar{\omega}_n - \Delta\omega_n/2)$ and $\hbar(\bar{\omega}_n + \Delta\omega_n/2)$, respectively, where the splitting energy $\hbar\Delta\omega_n$ is associated with the overlap of wave functions centered in either of the two wells. The propagator $G(\phi, \phi'; \delta\tau)$ (the index j is dropped to simplify the notation) therefore acquires the form

$$G(\phi, \phi'; \delta\tau) = \sum_n e^{-\bar{\omega}_n \delta\tau} \{ \langle \phi' | S_n \rangle \langle S_n | \phi \rangle e^{\Delta\omega_n \delta\tau / 2} + \langle \phi' | A_n \rangle \langle A_n | \phi \rangle e^{-\Delta\omega_n \delta\tau / 2} \}. \quad (17)$$

We now change basis into wave functions centered at the right and left potential minima $\phi_{\pm}$ [Eq. (9)]:

$$|R_n\rangle \equiv \frac{1}{\sqrt{2}}(|S_n\rangle + |A_n\rangle), \quad |L_n\rangle \equiv \frac{1}{\sqrt{2}}(|S_n\rangle - |A_n\rangle). \quad (18)$$

Equation (17) becomes

$$\begin{aligned} G(\phi, \phi'; \delta\tau) &= \sum_n e^{-\bar{\omega}_n \delta\tau} \left[\langle \phi' | R_n \rangle \langle R_n | \phi \rangle \right. \\ &\quad + \langle \phi' | L_n \rangle \langle L_n | \phi \rangle \cosh \left(\frac{\Delta\omega_n \delta\tau}{2} \right) \\ &\quad \left. + (\langle \phi' | R_n \rangle \langle L_n | \phi \rangle + \langle \phi' | L_n \rangle \langle R_n | \phi \rangle) \sinh \left(\frac{\Delta\omega_n \delta\tau}{2} \right) \right]. \end{aligned} \quad (19)$$

We next define the wave functions $\Psi_{n,\zeta}(\phi) \equiv \langle \phi | \zeta_n \rangle$, where $\zeta = +(-)$ denotes the isospin $R(L)$. Since these wave functions are not known exactly, we implement a variational approach and assume the trial function

$$\Psi_{n,\zeta}(\phi) = f_n(\phi) \exp \left\{ -\frac{(\phi - \zeta \phi_0)^2}{2l_n^2} \right\}, \quad (20)$$

where $f_n(\phi)$ for $n \geq 1$ is an oscillatory, symmetric function of ϕ with a number of nodes increasing with n ; for the lowest energy states $n = 0$ we assume $f_0(\phi) = 1/(\sqrt{\pi}l)^{1/2}$, so that $l \equiv l_0$ is a single variational parameter. The dependence of

$\Psi_{n,\zeta}(\phi)$ on the magnitude and sign of ϕ can be made explicit using the substitution $\phi = |\phi|\sigma$, which yields

$$\begin{aligned} \Psi_{n,\zeta}(\phi) &= f_n(|\phi|) \exp \left\{ -\frac{(|\phi| - \phi_0)^2}{2l_n^2} \right\} \\ &\quad \times \left(\delta_{\sigma\zeta} + \exp \left\{ \frac{-2|\phi|\phi_0}{l_n^2} \right\} \delta_{\sigma,-\zeta} \right). \end{aligned} \quad (21)$$

The first term in Eq. (21) dominates as long as $\phi_0 > l_n$.

To complete the derivation of an effective field theory in terms of the discrete fields $\sigma_j(\tau)$, one needs to perform the path integral [Eq. (11)] over the magnitude field $|\phi_j(\tau)|$. Due to the Gaussian factor in Eq. (21), the integration over $\phi_j \equiv \phi_j(\tau)$ (for each n) can be written schematically as

$$\int d\phi_j \exp \left\{ -\frac{(\phi_j - \sigma_j \phi_0)^2}{2l_n^2} \right\} \exp \{ F(\phi_j) \delta\tau \}, \quad (22)$$

where $F(\phi_j)$ encodes the remaining ϕ_j dependence, including in particular the interparticle coupling terms $(K/2)(\phi_j - \phi_{j\pm 1})^2$ [the last term in Eq. (12)]. If we now consider the case where $\phi_0 \gg l_n$ (which is valid deep in the zigzag phase), a saddle-point approximation of the integral yields (up to a multiplicative constant factor) $e^{F(\phi_0 \sigma_j) \delta\tau}$. This implies that the partition function [Eq. (13)] can be recast as

$$Z = \text{Tr} \{ \hat{T}_{\text{eff}}^M \}, \quad (23)$$

with $\text{Tr} = \sum_{\{\sigma_j\}}$ and $\hat{T}_{\text{eff}}$ a $2^N \times 2^N$ matrix related to the original transfer matrix $\hat{T}$ by

$$T_{\text{eff}}[\{\sigma_j\}, \{\sigma'_j\}] = T[\{\phi_0 \sigma_j\}, \{\phi_0 \sigma'_j\}]. \quad (24)$$

Recalling Eq. (14), we find that $T_{\text{eff}}[\{\sigma_j\}, \{\sigma'_j\}]$ can be expressed as

$$\begin{aligned} T_{\text{eff}}[\{\sigma_j\}, \{\sigma'_j\}] &= \prod_{j=1}^N T_{\text{loc}}[\sigma_j, \sigma'_j] \exp \\ &\quad \times \left\{ \frac{K \phi_0^2 \delta\tau}{2\hbar} (\sigma_j \sigma_{j+1} + \sigma'_j \sigma'_{j+1}) \right\}, \end{aligned} \quad (25)$$

where $T_{\text{loc}}[\sigma, \sigma'] = \text{const} \times G(\phi_0 \sigma, \phi_0 \sigma'; \delta\tau)$, and the propagator $G(\phi_0 \sigma, \phi_0 \sigma'; \delta\tau)$ can be obtained by inserting Eq. (21) into Eq. (19).

The final stage in the mapping to the quantum Ising chain involves a derivation of an explicit expression for the 2×2 matrix $\hat{T}_{\text{loc}}$, which encodes the single-particle dynamics. By inspection of Eqs. (21) and (19) it is evident that $\hat{T}_{\text{loc}}$ obeys

the symmetry $T_{\text{loc}}[\sigma, \sigma'] = T_{\text{loc}}[-\sigma, -\sigma']$. It can therefore be written in the form

$$\hat{T}_{\text{loc}} = \text{const} \times (A_0 \sigma^0 + A_X \sigma^x), \quad (26)$$

where σ^α are Pauli matrices in the basis where $\{\sigma = \pm 1\}$ denote the eigenvalues of σ^z , and σ^0 is the 2×2 unit matrix. This is the crucial point where we formulate the symmetry of the problem, which stems from the symmetry relations leading to Eqs. (16)–(18). The general expressions for A_0 and A_X are

$$\begin{aligned} A_0 &= \sum_n e^{-\bar{\omega}_n \delta \tau} f_n^2(\phi_0) \left(\cosh \left\{ \frac{\Delta \omega_n \delta \tau}{2} \right\} \right. \\ &\quad \left. + \Gamma^2 \sinh \left\{ \frac{\Delta \omega_n \delta \tau}{2} \right\} \right), \\ A_X &= \sum_n e^{-\bar{\omega}_n \delta \tau} f_n^2(\phi_0) \left(\sinh \left\{ \frac{\Delta \omega_n \delta \tau}{2} \right\} \right. \\ &\quad \left. + \Gamma^2 \cosh \left\{ \frac{\Delta \omega_n \delta \tau}{2} \right\} \right), \end{aligned} \quad (27)$$

where

$$\Gamma \equiv e^{-\phi_0^2 / l_n^2}. \quad (28)$$

Equation (27) implies that in general A_0 and A_X are nontrivial functions of the time interval $\delta \tau$. Restrictions on the parameters must therefore be set in order to establish a well-defined effective model for arbitrarily small $\delta \tau$. A simplification can be achieved in view of the fact that the sum over n is rapidly converging: A semiclassical calculation indicates that $\omega_n \sim n^{4/3}$ for large n (see Appendix for details); that is, the level spacing increases with n . In the regime where the tunnel splitting obeys $\Delta \omega_n \ll \bar{\omega}_n$ (realized far enough from the quantum transition so that the wells of V_0 are well separated), the sum is dominated by the first term $n = 0$ up to exponentially small corrections. Even closer to the phase transition, where the tunnel splitting becomes comparable to the barrier between the wells, the sum in Eq. (27) is dominated by the first few terms. As we show in the next section, provided the quartic term in V_0 (i.e., the parameter g) is sufficiently large, all the energy levels $\hbar(\bar{\omega}_n \pm \Delta \omega_n)$ are given (up to a numerical factor) by the same energy scale $(\hbar^4 g / m^2)^{1/3}$. Since the differences $(\Delta \omega_n - \Delta \omega_{n-1}) \sim n^{-2/3}$ are typically smaller than $\Delta \omega_n$, the dependence on n of all terms in the brackets in Eq. (27) may be neglected. One can therefore approximate $\Delta \omega_n$ for all n by $\Delta \omega \sim (\hbar g / m^2)^{1/3}$. This yields

$$\begin{aligned} T_{\text{loc}} &\approx \text{const} \times \left[\left(\cosh \left\{ \frac{\Delta \omega \delta \tau}{2} \right\} + \Gamma^2 \sinh \left\{ \frac{\Delta \omega \delta \tau}{2} \right\} \right) \sigma^0 \right. \\ &\quad \left. + \left(\sinh \left\{ \frac{\Delta \omega \delta \tau}{2} \right\} + \Gamma^2 \cosh \left\{ \frac{\Delta \omega \delta \tau}{2} \right\} \right) \sigma^x \right]. \end{aligned} \quad (29)$$

Assuming in addition that the overlap factor Γ [Eq. (28)] obeys

$$\Gamma \ll \tanh\{\Delta \omega \delta \tau / 2\} \ll 1, \quad (30)$$

Eq. (29) reduces to

$$T_{\text{loc}}[\sigma, \sigma'] \approx T_0 \left(\cosh \left\{ \frac{\Delta \omega \delta \tau}{2} \right\} \delta_{\sigma \sigma'} + \sinh \left\{ \frac{\Delta \omega \delta \tau}{2} \right\} \delta_{\sigma, -\sigma'} \right), \quad (31)$$

where T_0 is a constant prefactor. In terms of Pauli's matrices, this becomes

$$\begin{aligned} \hat{T}_{\text{loc}} &\approx T_0 \left(\cosh \left\{ \frac{\Delta \omega \delta \tau}{2} \right\} \sigma^0 + \sinh \left\{ \frac{\Delta \omega \delta \tau}{2} \right\} \sigma^x \right) \\ &= T_0 \exp \left\{ \frac{\Delta \omega \sigma^x \delta \tau}{2} \right\}. \end{aligned} \quad (32)$$

As a result, the expression for Z [Eqs. (23) and (25)] effectively reduces to

$$Z \approx Z_0 \int \mathcal{D}\sigma e^{-S_I[\sigma]/\hbar}, \quad (33)$$

in which Z_0 is a constant and S_I is the action of an Ising chain in a transverse field [17,26] subject to the Hamiltonian

$$H_I = - \sum_{j=1}^N (J \sigma_j^z \sigma_{j+1}^z + h \sigma_j^x). \quad (34)$$

Here the fictitious exchange coupling J and transverse field h are given by

$$J = K \phi_0^2 = \frac{K m \omega^2}{a^2 g}, \quad h = \frac{\hbar \Delta \omega}{2}, \quad (35)$$

where we have used Eq. (9) for ϕ_0 . The model described by Hamiltonian (34) is known to exhibit a quantum phase transition at $h/J = 1$ and $T = 0$, separating an ordered phase at $J > h$ (in our case, the stable zigzag configuration) from a disordered phase at $J < h$ (the linear chain). In both phases the spectrum of excitations is characterized by a gap with energy $\Delta = 2|J - h|$. The corresponding phase diagram, showing the critical behavior as a function of ϵ (and hence ν_t) and T is sketched in Fig. 1. The critical regime ($k_B T > \Delta$) is characterized by universal power-law T dependence of correlation functions with the critical exponents of the quantum transition [17]. In the next section we evaluate the gap in terms of the atom chain system parameters and in particular relate it to the parameter ϵ [Eq. (8)]. This will enable an estimate of the critical value ϵ_c satisfying $\Delta(\epsilon_c) = 0$.

It should be noted that the condition (30) was required to obtain the form (32) for the local transfer matrix, and thus the final stage in the derivation of Eqs. (33) and (34). Namely, the mapping to the Ising model Eq. (34) is valid only as long as the lowest energy levels are below the barrier in the potential V_0 . In this regime, the tunneling between the wells is small and hence necessarily $h \ll J$. This is satisfied deep in the ordered (zigzag) phase, in which case all our approximations are justified. It does *not* hold near the critical point, which we estimate in the next section. However, we note that conformal symmetry strongly restricts the number of universality classes in $1 + 1$ dimensions [27]. Moreover, it was argued that the number of relevant operators in two dimensions is the same as in $4 - \epsilon$ dimension [27]; therefore, the resulting ϕ^4 field theory describing our model is expected to be in the same universality class as the two-dimensional Ising model. Based on the symmetry properties of the present system [as manifested by Eq. (26) and the following derivation] it is reasonable to assume that a quantum Ising model is the appropriate field theory, which correctly describes its critical behavior at $h \sim J$. This hypothesis is further supported by numerical studies, for example, by Barma and Fisher [28] and a later work by Kim,

Lin, and Rieger [29]. Under these assumptions we estimate the quantum critical point in the regime of parameters where classically zigzag order is suppressed by quantum tunneling and find that it belongs to a universality class [17,27] that differs from the one of the classical Landau model.

IV. ESTIMATE OF THE QUANTUM CRITICAL PARAMETERS

As we show below, the effective coupling parameter h/J of the Ising model [Eq. (35)] can be expressed in terms of two dimensionless parameters characterizing the system: The first is the ratio of energy scales U_K/U_P , where

$$U_K \equiv \frac{\hbar^2}{ma^2} \quad (36)$$

is a typical kinetic energy scale of atoms in the chain, and

$$U_P \equiv \frac{A^2}{a^\alpha} \quad (37)$$

is an energy scale associated with the interaction. In atomic systems, this ratio can be tuned most effectively by controlling the density of atoms $1/a$, for example, by means of the lateral confinement. The second dimensionless parameter ϵ [Eq. (8)] can in principle be tuned independently by controlling the transverse confining potential frequency ν_t .

The expression for the fictitious exchange coupling J in terms of the above definitions can be obtained directly from Eq. (35). Employing Eqs. (7), (10), and (37), we rewrite the parameters as

$$K = C_1[\alpha] \alpha U_P, \quad m\omega^2 = \frac{4C_2[\alpha + 2] \alpha U_P \epsilon}{a^2}, \quad (38)$$

$$g = \frac{8C_2[\alpha + 4] \alpha (\alpha + 2) U_P}{a^4}.$$

This yields

$$J = C_J U_P \epsilon, \quad \text{where} \quad C_J \equiv \frac{C_1[\alpha] C_2[\alpha + 2] \alpha}{2C_2[\alpha + 4] (\alpha + 2)}. \quad (39)$$

Note that since we focus on the regime $\epsilon \geq 0$, and by definition $\epsilon \leq 1$, the energy scale J can be tuned continuously from 0 to $\sim U_P$. A quantum phase transition is expected to occur at ϵ_c , dictated by the ratio U_K/U_P at which J is equal to the “transverse field” energy scale h .

To get a concrete estimate of h in terms of U_K and U_P , we perform a variational calculation of the splitting energy $\hbar\Delta\omega$. To this end, we consider the trial wave functions

$$\Psi_{\pm}(\phi) = \frac{1}{(2\sqrt{\pi}l)^{1/2}} \times \left(\exp \left\{ -\frac{(\phi - \phi_0)^2}{2l^2} \right\} \pm \exp \left\{ -\frac{(\phi + \phi_0)^2}{2l^2} \right\} \right) \quad (40)$$

for the lowest energy states [i.e., the symmetric and antisymmetric combinations of Eq. (20) with $n = 0$], and search for a minimum of the energies

$$E_{\pm} = \frac{\langle \pm | H_0 | \pm \rangle}{\langle \pm | \pm \rangle}, \quad (41)$$

with respect to the variational parameter l . Here H_0 is the Hamiltonian of a particle of mass m subject to the double-well potential V_0 , and $\Psi_{\pm}(\phi) = \langle \phi | \pm \rangle$. It is convenient to eliminate the parameters of the quadratic part of H_0 by introducing the length scale $\lambda = \sqrt{\hbar/m\omega}$ and the energy scale $\hbar\omega/2$. Using the normalized coordinate $\bar{\phi} = (a/\lambda)\phi$ we write the Hamiltonian as

$$H_0 = \frac{1}{2} \hbar\omega \bar{H}_0, \quad \bar{H}_0 = -\frac{d^2}{d\bar{\phi}^2} - \bar{\phi}^2 + B\bar{\phi}^4, \quad (42)$$

depending on a single dimensionless parameter

$$B \equiv \frac{\hbar g}{2m^2\omega^3}. \quad (43)$$

The nature of the eigenstates and eigenvalues of H_0 crucially depends on B being small or large.

The exact minimum condition for $E_+[l]$ yields a cumbersome, transcendental equation for the variational parameter l . In particular, it includes the exponential factors $e^{-\bar{\phi}_0^2/\bar{l}^2}$, with $\bar{\phi}_0 = (a/\lambda)\phi_0$, $\bar{l} = (a/\lambda)l$. These factors are associated with the overlap of the right and left-centered wave functions. However, since we are interested in a regime of parameters close to the critical point [see discussion between Eqs. (46) and (47)], we focus on the approximation of a “quasiflat” potential, corresponding to $B \gg 1$ and $\bar{\phi}_0^2/\bar{l}^2 \ll 1$. Essentially, this regime amounts to a dominance of the quartic term in the potential, while the barrier separating the two wells is relatively small. In fact, the parameter B can be written as $B = \hbar\omega/(2\Delta V)$, where ΔV is the difference between the energy of the minima of V_0 and the top of the bump separating them. Therefore, B is the ratio between the zero-point energy $\hbar\omega/2$ and the potential energy of the barrier. As becomes clear from the following discussion, the regime $B > 1$ is relevant for the critical point. In this regime also the two Gaussian functions of Eq. (40) are expected to mix; therefore, $\bar{\phi}_0^2/\bar{l}^2 < 1$. To find an analytic expression we take these inequalities to the extreme. We find from Eq. (9) $\bar{\phi}_0^2 = \frac{1}{2B}$. To leading order in $1/B$, this yields a minimum of $E_+[l]$ at

$$l_{\min} = \frac{\lambda}{a} \bar{l}_{\min}, \quad \bar{l}_{\min}^2 \approx \left(\frac{1}{3B} \right)^{1/3}. \quad (44)$$

Both $E_+[l]$ and $E_-[l]$ are computed using Eq. (41) within the above approximations, with the value of $\bar{l}_{\min}^2$ which was found to minimize $E_+[l]$. We checked that if we extremize $E_-[l]$, a value with the same dependence on parameters that differs only by 3% would be obtained.

The resulting energy eigenvalues $E_{\pm} = E_{\pm}[l_{\min}]$ are separated by a splitting energy $\Delta E = E_-[l] - E_+[l]$, where

$$h \approx \frac{\Delta E}{2} = \frac{1}{2} \hbar\omega (3B)^{1/3}. \quad (45)$$

This sets the scale of the transverse field.

Recalling Eq. (43) for B , we note that the dependence on ω (and hence on ϵ) cancels out. We thus get

$$h \approx \frac{1}{2} \left(\frac{3\hbar^4 g}{2m^2} \right)^{1/3} = C_h (U_K^2 U_P)^{1/3}, \quad (46)$$

$$C_h \equiv \left(\frac{3C_2[\alpha + 4] \alpha (\alpha + 2)}{2} \right)^{1/3},$$

where we have used Eq. (38) to relate g to U_P . It should be pointed out that (up to a numerical factor close to unity) the above estimate for h coincides with the energy scale dictating the higher energy eigenvalues of H_0 in the semiclassical approximation (formally valid for $n \gg 1$): $E_n \sim n^{4/3}h$ [see Appendix, Eq. (A5)]. We hence conclude that in this regime of parameters, all energy levels are determined by the same energy scale.

We finally employ Eqs. (39) and (46) to evaluate the critical value of ϵ for a given U_K/U_P : The condition

$$h = J$$

dictates

$$\epsilon_c \approx C_c \left(\frac{U_K}{U_P} \right)^{2/3}, \quad C_c \equiv \frac{C_h}{C_J} \approx \left(\frac{12(\alpha + 2)^4}{\alpha^2} \right)^{1/3}, \quad (47)$$

where we have used the approximation $C_1[\alpha] \sim C_2[\alpha] \sim 1$ for arbitrary α . For $\alpha = 1$, $\alpha = 3$ the numerical prefactor is $C_c \sim 10$. This implies that for given $U_K/U_P \ll 1$, a quantum critical point is typically expected at $\epsilon_c \gg U_K/U_P$.

V. EXPERIMENTAL REALIZATION

A. Ion Coulomb crystals

An interesting system to study the above-predicted quantum phase transition would be an ion crystal in a quasi-one-dimensional trap [9,10,21,30,31]. For singly ionized alkali-earth-metal atoms, the generalized charge A is the electron charge ($A = e$), and the mass of the ions can be written as $m = n_A m_p$, where m_p is the proton mass and n_A the atomic number. In these systems it is possible to tune through the critical point by controlling either the transverse confinement frequency ν_t (which is typically in the MHz regime) or the spacing between neighboring ions a , which is conveniently measured in units of micrometers: $a = a_0 \times 1 \mu\text{m}$.

To be able to distinguish between the quantum disordered phase and the ordered (zigzag) phase, one must first make sure that the frequency difference $\delta\nu = \nu_c - \nu_t$ implied by our estimated ϵ_c [via Eq. (8)] is not limited by the experimentally accessible resolution. To this end, it is useful to write ϵ_c in terms of n_A and a_0 defined above. Inserting Eqs. (36) and (37) and the numerical values of $\hbar$, e , and m_p in Eq. (47), we obtain

$$\epsilon_c \approx 10^{-4} \frac{1}{(n_A a_0)^{2/3}}. \quad (48)$$

From Eq. (8), we therefore obtain an upper bound to the frequency resolution

$$\delta\nu \approx 10^{-4} \frac{1}{2(n_A a_0)^{2/3}} \nu_c, \quad (49)$$

which ranges from 100 Hz (for protons with $a_0 \sim 1$) to 1 Hz for heavier ions. This bound has to be compared with the time scale of heating in ion traps. In order to be able to measure the quantum phase transition, the heating and decoherence time scale of the trap, T_{decoh} should be such that $\delta\nu T_{\text{decoh}} \ll 1$, which leads to demanding conditions for the existing trapping setups (see, for instance, the discussion in Refs. [31,32]).

Another requirement on the experimental setup is the possibility to reduce the temperature T below the energy

scale characteristic of the gap $\Delta \sim h$. Using Eq. (46), the estimated restriction on T (defined for convenience in units of millikelvin) is therefore given by

$$T [\text{mK}] \ll \frac{10^3 C_h (U_K^2 U_P)^{1/3}}{k_B}. \quad (50)$$

To derive a numerical estimate, we again employ Eqs. (36) and (37) and rewrite the mass and inter-ion spacing in terms of n_A and a_0 . This yields

$$T [\text{mK}] \ll 0.25 \left(\frac{1}{n_A^2 a_0^5} \right)^{1/3}, \quad (51)$$

implying an upper bound of order ~ 0.1 mK for protons to μK for magnesium ions. These values are challenging for large crystals, but could be accessed when, for instance, only the transverse motion is cooled. (Methods for cooling ion Coulomb crystals to ultralow temperatures are discussed in Refs. [33,34]).

We note that the condition on $\delta\nu$ can be relaxed in the presence of screening with permittivity $\epsilon > \epsilon_0$, with ϵ_0 the vacuum permittivity: In this case the potential energy U_P decreases as ϵ_0/ϵ , and the upper bound on $\delta\nu$ increases with $\epsilon^{2/3}$. It is interesting to note that, correspondingly, the condition of the temperature becomes more restrictive, as the upper bound decreases with $\epsilon^{-1/3}$. This situation could possibly be realized, for instance, in the case of an ion chain embedded in a crystal, as in the experiment reported in Ref. [21].

B. Dipolar gases

Another physical system, where the quantum phase transition can be experimentally observed, consists of ultracold dipolar gases, such as polar molecules [23]. Here, the interaction is repulsive provided the dipoles are aligned perpendicularly to the plane where their motion is studied, for instance, in a very steep trap which freezes out the motion in the perpendicular direction. In Ref. [2] a zigzag ordering across tubes, containing gases of ultracold polar molecules, has been predicted when the distance between the tubes was below a certain value. Long-range order is found in the presence of an additional external periodic potential which localizes the dipoles in an equidistant array in one dimension and could be realized by means of an optical lattice. The regime here studied would then correspond to the realization of a Mott-insulator state of the polar molecules in a one-dimensional optical lattice, where the transverse direction must be confined by a dipole trap, whose steepness is changed in order to reach several points of the phase diagram [23]. An estimate of the parameters, which make it possible to access the low-dimensional, quasicrystalline region, has been presented in Ref. [16].

C. Measurement: Structure form factor

In atomic and molecular systems, the measurement of the disordered phase, where quantum fluctuations dominate in the transverse direction, can be performed by means of the structure form factor, here defined by the expression

$$S(\mathbf{k}) = \frac{1}{N} \int d\mathbf{x} \int d\mathbf{x}' e^{i\mathbf{k} \cdot (\mathbf{x} - \mathbf{x}')} \langle n(\mathbf{x}) n(\mathbf{x}') \rangle, \quad (52)$$

where $n(\mathbf{x}) = n(x, y)$ is the density of atoms in the two-dimensional plane. For wave vectors in the limit $k_x \rightarrow k_0$, where $k_0 = \pi/a$ is the wave number of the zigzag, $S(\mathbf{k}) = S_f + S_0 \delta(k_x - k_0)$ in which S_0 is proportional to the squared order parameter, $S_0 \propto \phi_0^2$, while S_f is the contribution of the fluctuations and is proportional to the isothermal susceptibility χ of the corresponding Ising system [17,35]. Approaching the quantum critical point for $T \ll \Delta$ (i.e., for $\epsilon \rightarrow \epsilon_c$ below the dashed lines in Fig. 1), $\chi \sim |\epsilon_c - \epsilon|^{-\gamma}$ and $\phi_0^2 \sim |\epsilon_c - \epsilon|^{2\beta}$ in the ordered, zigzag phase ($\epsilon > \epsilon_c$), where $\beta = 1/8$ and $\gamma = 7/4$ are the exponents of the classical two-dimensional Ising model. In the critical region $T \gg \Delta$ (shaded area in Fig. 1), these behave as $\chi \sim T^{-7/4}$, $\phi_0^2 \sim T^{1/4}$, respectively, where we have used the critical scaling of the correlation length $\xi \sim 1/\Delta \sim |\epsilon_c - \epsilon|^{-\nu}$ with $\nu = 1$ [17]. Note that the predicted critical behavior is strictly valid for an infinite system and assumes a uniform density of particles. However, in practice it is expected to be approximately valid, for example, in the center of a linear Paul trap of ions, when the variation of the density in a large region is negligible within a correlation length.

The distinct regions in the phase diagram (Fig. 1) can be identified experimentally also away from criticality (i.e., for $\mathbf{k}$ that is sufficiently different from $\mathbf{k}_0$) with the help of light scattering at the appropriate wave vector. The structure factor will take a different form in each of three cases: (i) the linear (string) chain ($\epsilon < 0$), (ii) the quantum disordered phase ($0 < \epsilon < \epsilon_c$), and (iii) the zigzag configuration ($\epsilon > \epsilon_c$) for $N \gg 1$ atoms.

In regime (i), where the ion string is assumed, the atomic density can be written as $n(x, y) = n_x(x)n_y(y)$ such that $n_x(x)$ is the sum of well spatially separated Gaussians, centered in ja and with width $l_x \ll a$, while $n_y(y)$ is a Gaussian with width $l_y = la$ such that $l \ll 1$. The structure form factor is then given by

$$S_{\text{lin}}(k_x, k_y) \simeq N \sum_n \delta_{k_x, G_n} \tilde{S}(k_x, k_y), \quad (53)$$

with

$$\tilde{S}(k_x, k_y) = e^{-k_x^2 l_x^2 / 2} e^{-(k_y a)^2 l^2 / 2} \quad (54)$$

and corresponds to δ peaks along the x axis at the location of the vectors of the reciprocal lattice, $G_n = 2\pi n/a$, where the height of the peaks is embedded in a Gaussian function of width $\sqrt{2}/l_x$, while the dependence on k_y has the form of a Gaussian function of width $\sqrt{2}/(la)$ [see Fig. 2(a)].

We next consider the zigzag ordered phase regime (ii). Denoting by $y_0 = \phi_0 a$ the transverse displacement from the x axis, for $\phi_0 \gg l$ we obtain

$$S_{\text{zz}}(k_x, k_y) \simeq 4N \sum_n \delta_{k_x, \frac{\pi n}{a}} \tilde{S}(k_x, k_y) \cos^2 \left(\frac{\pi n}{2} - k_y a \phi_0 \right), \quad (55)$$

which provides an interference pattern in the y direction, with a maximum or a zero at $k_y = 0$ depending on whether the corresponding x component is even or odd, as displayed in Fig. 2(b). We note that the appearance of an interference pattern for n odd (i.e., the doubling of the unit cell) is a

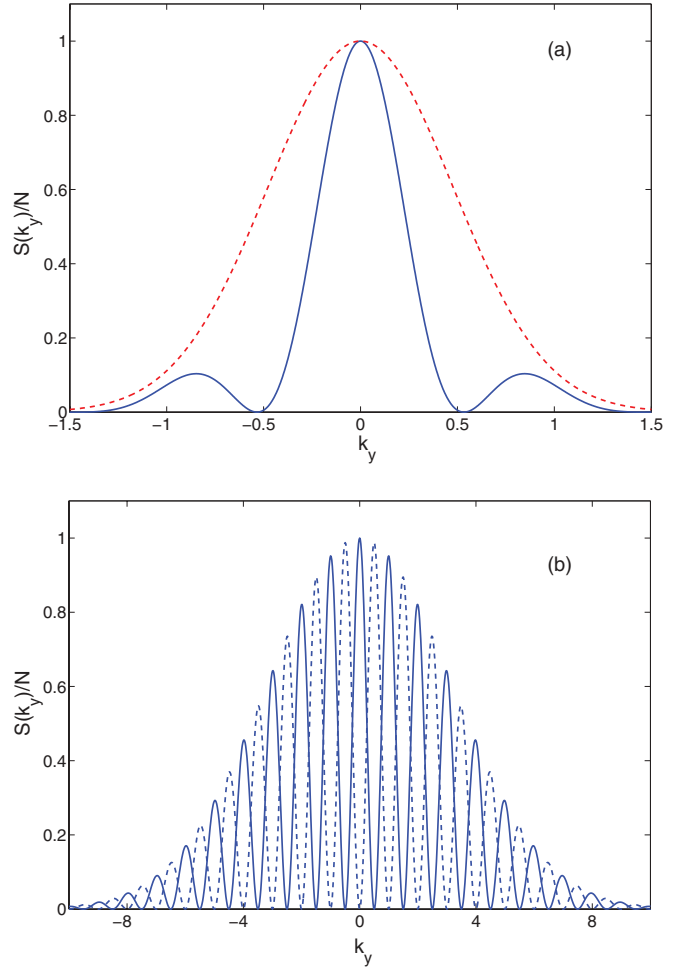


FIG. 2. (Color online) Structure form factor $S(k_y)/N$ as a function of k_y (in units of the transverse length $\phi_0 a/\pi$). (a) For an ion string ($\epsilon < \epsilon_c$). The red dashed curve corresponds to the classically stable regime (i), where $S(k_y)$ is given by S_{lin} [Eq. (53)]; the blue solid curve corresponds to the ion string in the quantum disordered phase regime (ii) [S_{dis} in Eq. (56) with $\phi_0/l = 1.5$]. (b) For a zigzag structure, regime (iii) (with $\phi_0 = 10l$). The dashed and solid lines correspond to $S_{\text{zz}}(k_y)$ [Eq. (55)] when $k_x = \pi n/a$ with n even and odd, respectively.

primary signature of this ordered phase. In both cases, the pattern is characterized by peaks separated by $\pi/a\phi_0$. These expressions are in agreement with the results found numerically for the linear and zigzag configuration in ultracold dipolar gases [36].

Finally, we focus on regime (ii), namely, the phase where the zigzag order found in the framework of the classical theory is destroyed as a result of quantum fluctuations, and the disordered linear chain is found. This regime is characterized by a wave function whose width in the transverse direction is of the order of the distance between the two minima of the potential V_0 of Eq. (6) (see, for instance, the numerical result reported in Ref. [16]). For this purpose, we assume that the density along $y = a\phi$ is given by $n_y(y) = \mathcal{N}|\Psi_+(\phi)|^2/a$ with $\Psi_+(\phi)$ given in Eq. (40) and $\mathcal{N} = 1/(2 + 2\Gamma)$ giving the right normalization, where $\Gamma = \exp(-\phi_0^2/l^2)$ is the overlap

factor [Eq. (28)]. The corresponding structure form factor reads

$$S_{\text{dis}}(k_x, k_y) \simeq N \sum_n \delta_{k_x, \frac{2\pi n}{a}} \tilde{S}(k_x, k_y) \left(\frac{\Gamma + \cos(k_y a \phi_0)}{\Gamma + 1} \right)^2, \quad (56)$$

where nonlocality is here in the dependence on the parameter Γ , giving the overlap between the two wave functions in the two wells. This result was already obtained for the case of a single atom in a double-well potential [37] and can be understood as an interference pattern arising from a photon, which is elastically scattered by one of the atoms. In the disordered phase the scattered photon will follow two possible pathways, associated with the coherent superposition of the two positions where the atom can be found with largest probability. Figure 2(a) displays the function S_{dis} as a function of k_y . The existence of sidebands [Fig. 2(a)] is the signature of the regime (ii). This demonstrates how one can distinguish the various regimes and measure the shift of the critical point resulting from quantum tunneling.

We also remark that autocorrelation functions of the crystal can be measured by means of Ramsey interferometry, by driving the internal transition of one ion in the chain, as proposed in Ref. [38]. This method would allow one to extract the critical exponents characterizing the critical behavior. Methods for revealing quantum tunneling between zigzag configurations of few ions have been proposed in Ref. [39].

VI. CONCLUSIONS

In this paper, it has been argued that the structural phase transition between a chain and a zigzag for ions or atoms interacting via a power-law interaction falling off as $1/r^\alpha$ (where r is the distance and $\alpha \geq 1$) can be mapped on an Ising model in a transverse field. In this way the classical theory for the phase transition can be extended to account for quantum fluctuations. Such correspondence was proposed in the past for electronic systems [1]. Here the mapping is explicitly justified deep in the ordered zigzag phase [see Eq. (30)]. Based on symmetry arguments [see Eq. (26)] we postulate that this mapping can be extended to the critical regime. The number of universality classes in two dimensions is restricted by conformal field theory [27]. Therefore, we argue that identifying the symmetry (Z_2 in our case) determines the universality class and implies that it is the same as of the one-dimensional Ising model in a transverse field. In other words, we assume that all operators obtained in our theory that differ from the ones of the conformal field theory of the one-dimensional Ising model in a transverse field are irrelevant in the sense of the renormalization group. To the best of our knowledge, there are no existing theoretical tools to verify such statements. However, this hypothesis is further supported by numerical studies [28,29].

Under these assumptions, we have estimated the quantum critical point as well as the regime of parameters where classically zigzag order would be found, but quantum tunneling and fluctuations suppress it and the linear chain is recovered. In this calculation it was assumed that the effective potential V_0

[Eq. (6)], obtained in the vicinity of the critical point according to the classical theory, still holds.

Our analysis allows us to consider possible realizations of a suitable system in which the predicted quantum phase transition would be observable. In particular for trapped-ion systems, we identify the physical parameters determining the critical point, as well as the experimental parameters which are required in order to access this regime. Schemes for measuring the transition are proposed, which are based on photon scattering.

We remark that this work addresses the two-dimensional case, in which the transition to a zigzag may only happen in a predetermined plane, and give also the full phase diagram including the thermal fluctuations. In three dimensions, where a Goldstone mode is predicted corresponding to rotations of the plane, in which the zigzag is formed around the axis of the chain, one could consider an extension of this mapping. On this basis we conjecture that the system at the quantum phase transition can be mapped to the XY model, and the phase transition is of Kosterlitz-Thouless type.

We finally note that our theory provides a general framework which allows one to study further effects, such as dynamics at the quantum critical point. It is worth mentioning that here one expects the creation of topological defects, that is, domain walls. It would be interesting to apply this theory to defect formation, extending the work done on the classical system in Ref. [13], and to explore whether these systems allow for the creation of special kind of entangled states of the ions.

To conclude, using a quantum-field theoretical description we argue that the linear-zigzag instability in two-dimensional systems of trapped ions or polar molecules can be mapped to the one-dimensional Ising model in a transverse field. This result demonstrates once more the potentialities offered by these systems as quantum simulators [23,31,40,41] and more generally for quantum technological applications.

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APPENDIX: SEMICLASSICAL ENERGY EIGENVALUES FOR THE DOUBLE-WELL POTENTIAL

In this appendix the eigenvalues of the Hamiltonian H_0 [Eq. (42)] are calculated in the semiclassical limit. In this limit the term proportional to ϕ^2 in the potential can be ignored.

The energy levels can be found by the Bohr-Sommerfeld rule where the action I is quantized:

$$I_n = n + \text{const} \approx n \quad (\text{A1})$$

for large n . Here, similarly to Eq. (42), we have used units where length scales are normalized by $\lambda = \sqrt{\hbar/m\omega}$ and energy scales by $\hbar\omega/2$. For large energy [$\bar{E} = E/(\hbar\omega/2)$] where the semiclassical approximation is relevant,

$$I = \oint \bar{p} d\bar{\phi} = \frac{1}{2\pi} \oint \sqrt{\bar{E} - B\bar{\phi}^4} d\bar{\phi}, \quad (\text{A2})$$

where $\bar{p}$ is the conjugate momentum of the normalized coordinate $\bar{\phi}$, and $B = \hbar g/2m^2\omega^3$ [see Eq. (43)]. The integral

is over a closed trajectory of the particle. By elementary rescaling one finds

$$I = \left(\frac{\bar{E}}{B^{1/3}} \right)^{3/4} C, \quad C \equiv \frac{1}{2\pi} \oint \sqrt{1 - y^4} dy. \quad (\text{A3})$$

Note that the normalized energies scale as $B^{1/3}$, as we found also for low energies within the approximation $B \gg 1$ [see Eq. (45)]. The semiclassical energies are therefore

$$\bar{E}_n = B^{1/3} \left(\frac{n}{C} \right)^{4/3}. \quad (\text{A4})$$

The energy spacings increase with energy. In the physical units the eigenenergies are given by

$$E_n = \frac{\hbar\omega}{2} \bar{E}_n = \left(\frac{\hbar n}{C} \right)^{4/3} \left(\frac{g}{16m^2} \right)^{1/3}. \quad (\text{A5})$$

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