

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

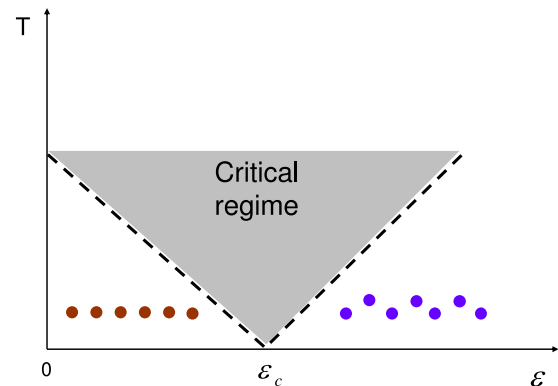


FIG. 1 (color online). Phase diagram for a linear-zigzag transition, according to the mapping to the quantum Ising transition in 1D, where T is the sample temperature and the dimensionless parameter ε is tuned by the confining potential or the interparticle distance. The classical instability of the 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 $g = 24C_5Q^2/a^5$, with $C_\alpha \equiv \sum_{j \geq 1} 1/(2j+1)^\alpha$. 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}_{loc} encodes the single particle dynamics within the double-well potential. The propagator \hat{T}_{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 ($4 - \varepsilon$). 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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