Structural Defects in Ion Chains by Quenching the External Potential: The Inhomogeneous Kibble-Zurek Mechanism

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The nonequilibrium dynamics of an ion chain in a highly anisotropic trap is studied when the transverse trap frequency is quenched across the value at which the chain undergoes a continuous phase transition from a linear to a zigzag structure. Within Landau theory, an equation for the order parameter, corresponding to the transverse size of the zigzag structure, is determined when the vibrational motion is damped via laser cooling. The number of structural defects produced during a linear quench of the transverse trapping frequency is predicted and verified numerically. It is shown to obey the scaling predicted by the Kibble-Zurek mechanism, when extended to take into account the spatial inhomogeneities of the ion chain in a linear Paul trap.

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The nonequilibrium statistical mechanics of long-range interacting systems is one of the challenging problems in statistical physics [1]. Nevertheless, close to a continuous phase transition it is sometimes possible to use concepts of equilibrium statistical mechanics in order to make some predictions for the system when the value of a control parameter is quenched through the critical value. The Kibble-Zurek mechanism (KZM) has become a useful paradigm in this arena, accounting for a variety of phenomena ranging from the formation of massive particles in the early Universe [2] to the vortex formation in superfluid helium [3]. The model applies to systems with a continuous phase transition, which is well described within Landau theory [4], and allows one to estimate the density of defects which are formed when quenching the control field ν_t across the critical value.

In a nutshell, by comparing the characteristic time τ_Q of change of the control field ν_t with the relaxation time scale $\tau(\nu_t)$ of the system at equilibrium [5], one identifies the corresponding freeze-out time scale, $\hat{t}$, which separates the regime in which the system follows adiabatically the quench from the regime in which the system behaves as if the dynamics was frozen out. The correlation length ξ at the value of the control field $\nu_t(\hat{t})$ then gives the characteristic length over which the system remains correlated, and hence the density of defects. The KZM prediction of the density of defects has been verified in a variety of systems numerically [6,7] and experimentally [8]. Recently, the model has been extended to describe the quench dynamics in a quantum phase transition [9]. The standard model of topological defects formation in homogeneous phase transitions must be revised whenever the quench is local or the critical control parameter (and the resulting transition) become spatially dependent [10,11]. This situation is arguably ubiquitous in nature and the main focus of this Letter.

In this Letter we study the out-of-equilibrium dynamics in an inhomogeneous laser-cooled Wigner crystal, quenched through its critical point. Here, we propose a novel system to test the KZM in a inhomogeneous phase transition which enjoys an unprecedented level of experimental control and amenability for defect detection. The Wigner crystal is composed of single-charged ions, which are confined in Paul or Penning traps and mutually repel via an unscreened Coulomb interaction [12]. In highly anisotropic traps, the ions can form a linear chain, which has a mechanical instability to a degenerate chain, with a zigzag structure, controlled by the density or by the transverse trap frequency [13,14]. The form of the corresponding distribution of charges at equilibrium is shown in Fig. 1(a), for the case in which the ions are confined by a linear Paul trap. At equilibrium, such instability is a

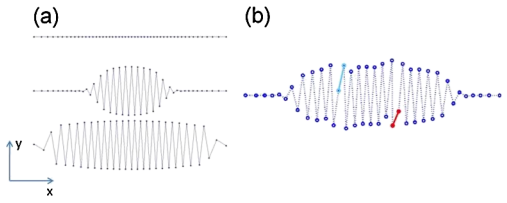

FIG. 1 (color online). (a) Charge distribution at equilibrium of an ion chain in a linear Paul trap for decreasing transverse trapping frequency (from top to bottom). Because of harmonic trapping, the density of ions is larger in the center, where the repulsion is larger and the zigzag instability is first evident. (b) Charge distribution after a quench through the critical transverse frequency exhibiting both types of structural defects (solid lines): kink (light) and antikink (dark).

second-order phase transition [13,15,16]. We determine the scaling of the density of defects after crossing such transition as a function of the cooling rate and of the quenching rate of the transverse trap frequency. In particular, spacelike separated regions may develop zigzag structures with different orientations which are separated by a kink. The classical and quantum properties of these kinks were recently studied in [17], some of which are displayed in Fig. 1(b). These regions are the analogs of magnetic domains in a ferromagnetic material and the interface between domains is a structural defect.

The system we consider is composed of N ions of mass m, charge Q, and coordinates $\boldsymbol{r}_n = (x_n, y_n, z_n)$ that are confined along the x axis by a strongly anisotropic, radial trap. The Lagrangian describing the dynamics of the ions is $L = T - V$ where the kinetic and potential energies take the form, respectively, $T = \frac{1}{2}m\sum_n \dot{\boldsymbol{r}}_n^2$ and $V = \frac{1}{2}m\sum_n[\nu^2 x_n^2 + \nu_t^2(y_n^2 + z_n^2)] + \sum_{n\neq n'} Q^2/(2|\boldsymbol{r}_n - \boldsymbol{r}_n'|)$, with ν and ν_t the frequency of the axial and the transverse confinement. At sufficiently low temperature and sufficiently large values of ν_t the ions form a chain along the x axis. In the local density approximation, the linear density $n(x)$ is approximated by the function $n(x) = \frac{3}{4}\frac{N}{L}(1 - \frac{x^2}{L^2})$ with L the half-length of the chain and x the distance from the center [18]. The interparticle spacing, $a(x) = 1/n(x)$, is a slowly varying function of the position. In the thermodynamic limit, in which $a(0) \to a$ as the number of particles $N \to \infty$, one recovers in the center of the trap the statistical mechanics and dynamical properties of an infinite chain with uniform interparticle distance a [13,19]. The mechanical stability of the ion chain is warranted provided that the transverse trap frequency fulfils the relation $\nu_t > \nu_t^{(c)}$, where $\nu_t^{(c)}$ is a function of the axial trap frequency and the ion density. At $\nu_t^{(c)}$ the chain undergoes a transition to a zigzag configuration, with transverse size b [20]. In the thermodynamic limit, the structural change is a second-order phase transition, with ν_t a control field and b the order parameter [13]. In particular, the critical value of the transverse frequency is given by $\nu_t^{(c)} = \omega_0\sqrt{7\zeta(3)/2} = (2.051\ldots)\omega_0$, ζ being the Riemann-zeta function and $\omega_0 = \sqrt{Q^2/ma^3}$. Inside a linear Paul trap the zigzag instability occurs first at the center of the trap, where the density is larger, and at lower values of ν_t extends towards the edge of the chain, as sketched in Fig. 1(a). In this case the transverse size of the chain is position dependent, $b = b(x)$.

The dynamics around the mechanical instability can be described by a Ginzburg-Landau (GL) equation for the position-dependent transverse size $b(x)$ of the zigzag chain, which is here described by a continuum field $\psi(x)$. The GL equation is based on the assumption of a coarse-grained length scale δx, with $\delta x \gg a(x)$ and $a(x) \gg |\delta x(da(x)/dx)|$, and extends the theory in Ref. [13] to the inhomogeneous case. Within the local density approximation, we identify a local value of the critical transverse frequency $\nu_t^{(c)}(x)^2 = 7\zeta(3)/2Q^2/(ma(x)^3)$ and write the Lagrangian $L = \int dx\mathcal{L}(x)$ with

$$\mathcal{L}(x) = \frac{1}{2}\rho(x)\sum_{\sigma=y,z}\{[\partial_t\psi^\sigma(x)]^2 - h(x)^2[\partial_x\psi^\sigma(x)]^2 - \delta(x)\psi^\sigma(x)^2 - \mathcal{A}(x)\psi^\sigma(x)^4\} \quad (1)$$

where $\psi^\sigma(x)$ gives the zigzag size at $\sigma = y, z$ as a function of the position, $\rho(x) = mn(x)$ is the linear mass density, and $\delta(x) = \nu_t^2 - \nu_t^{(c)}(x)^2$. The parameter $h(x) = \omega_0 a(x) \times \sqrt{\log 2}$ is a velocity, and determines the speed with which a transverse perturbation propagates along the chain. Finally, the parameter $\mathcal{A}(x) = [93\zeta(5)/32]\omega_0^2/a(x)^2$ is positive and determines the value of the order parameter when $\delta(x) < 0$. The Lagrangian density $\mathcal{L}(x)$ has the form of a GL equation.

The minimal energy solution of Eq. (1) fulfills the relation $\psi^\sigma\{\delta(x) + 2\mathcal{A}(x)[(\psi^y)^2 + (\psi^z)^2]\} = 0$. It always admits the solution $\psi^\sigma(x) = 0$ corresponding the ions on the x axis, which is stable only for $\delta(x) > 0$. For $\delta(x) < 0$ there is a continuous manifold of solutions of the form, $\varrho(x) = \sqrt{-\delta(x)/2\mathcal{A}(x)}$, with $\varrho(x) = \sqrt{(\psi^y)^2 + (\psi^z)^2}$, corresponding to the zigzag chain [13]. Within Landau theory [4], the correlation function of the linear chain, evaluated for a static perturbation at a point, decays exponentially with the length scale $\xi \sim a\omega_0/\sqrt{\delta(x)}$.

Within the GL description, we now assume that the transverse trap frequency ν_t undergoes a change in time in the interval $[-\tau_Q, \tau_Q]$, sweeping through the mechanical instability from the linear to the zigzag chain, such that $\nu_t^2 = \nu_t^{(c)}(0)^2 - \delta_0\frac{t}{\tau_Q}$ and $\nu_t^{(c)}(0)^2 \gg \delta_0 > 0$. In this parameter regime, we can use the time-dependent parameter $\delta(x, t) = \nu_t^2(t) - \nu_t^{(c)}(x)^2$ inside the GL equation. We also assume that the chain is in contact with a thermal reservoir at low temperature T, which is warranted by laser cooling the chain motion. More specifically, we assume that some ions of the chain are Doppler cooled such that the energy distribution of the crystal modes obeys a Fokker-Planck equation [21]. The equation of motion for the field can be then written as

$$\partial_t^2\psi - h(x)^2\partial_x^2\psi + \eta\partial_t\psi + \delta(x,t)\psi + 2\mathcal{A}(x)\psi^3 = \varepsilon(t) \quad (2)$$

where the scalar $\epsilon(t)$ is the Langevin force, describing the diffusion due to laser cooling, such that its moments fulfill the relations $\langle\varepsilon(t)\rangle = 0$, $\langle\varepsilon(t)\varepsilon(t')\rangle = 2\eta\kappa_B T\delta(t - t')/m$, where κ_B is Boltzmann constant and T is the temperature of Doppler cooling [22]. In deriving Eq. (2), we have neglected axial distortions of the charge density due to the value of ν_t. We have also taken that the trap frequency in the z axis is much larger than the y axis so that $\psi(x)$ is now along y.

We now estimate defect formation following a quench in the tranverse trapping frequency . The nucleation of defects in such a scenario resembles the formation of solitons in a cigar-shaped Bose-Einstein condensate recently discussed by Zurek in Ref. [11]. The transverse frequency is quenched through the critical point at different times along the chain due to the inhomogeneous charge distribution in the system. This gives rise to a propagating front along the axis from the center to the edges, whose coordinates (x_F, t_F) satisfy $\delta(x_F, t_F) = 0$. The front velocity v_F, at which the mechanical instability propagates, can be estimated by taking the ratio between the characteristic length of the control parameter, $[\partial_x \delta(x,t)/\delta(x,t)]^{-1}$, and the characteristic time scale at which it changes, $[\partial_t \delta(x,t)/\delta(x,t)]^{-1}$, giving $v_F \sim \partial_t \delta(x,t)/\partial_x \delta(x,t)$. For the spatial dependence of the local critical frequency $\nu_c^2(x) = \nu_c^2(0)[a(0)/a(x)]^3$, the front velocity $v_F \propto |d\nu_t^{(c)}(x)^2/dx|_{x_F}^{-1}$ takes the form $v_F \sim \frac{\delta_0}{\tau_Q} |d\nu_c^2(x)/dx|_{x_F}^{-1} \sim [L\delta_0/6\nu_t^{(c)}(0)^2\tau_Q][1/X(1-X^2)^2]$, with $X = |x_F|/L$ (which is valid away from the edges). Whenever the transition is homogeneous, $v_F \to \infty$ and the standard scenario of defect formation of Kibble-Zurek applies: the density of defects in this case is simply determined by the correlation length at the freeze-out time scale $\hat{t}$. Elsewhere, the sound velocity comes into play. We first estimate the time scale $\hat{t}$, at which the dynamics stop being adiabatic, by equating the time scale $\delta/\dot{\delta}$ to the relaxation time τ. Two regimes can be identified, which refer to the relation between the damping ratio and the value of δ at $\hat{t}$. In the so-called overdamped regime [6], when $\eta \gg \sqrt{\delta(0,\hat{t})}$, one finds $\hat{t} = (\eta\tau_Q/\delta_0)^{1/2}$, which sets the freezed-out correlation length $\hat{\xi}_x = a\omega_0/\sqrt{|\delta(x,\hat{t})|} = a\omega_0(\eta\delta_0/\tau_Q)^{-1/4}$. Then, the characteristic velocity of a perturbation becomes $\hat{v} \sim \hat{\xi}_x/\hat{\tau}_x \sim a\omega_0(\delta_0/\eta^3\tau_Q)^{1/2}$. The condition for kinks formation reads $\frac{v_F}{\hat{v}_x} \sim \mathcal{A}_o/[X(1-X^2)^2] > 1$ with $\mathcal{A}_o = L/[6\nu_t^{(c)}(0)^2 a\omega_0\xi_0](\frac{\eta\delta_0}{\tau_Q})^{3/4}$. One can estimate the effective size of the chain $2\hat{X}_*$ where the homogeneous KZM applies, by setting $v_F/\hat{v}_x = 1$, and assuming $\hat{X}_* \ll 1$ whence it follows that $\hat{X}_* \sim \mathcal{A}_o$. The density of kinks obeys then the relation

$$d_o \sim \frac{2\hat{X}_*}{\hat{\xi}} \sim \frac{L}{3\nu_t^{(c)}(0)^2 a^2\omega_0^2}\frac{\eta\delta_0}{\tau_Q}. \tag{3}$$

Note that this leads to a stronger dependence on τ_Q than in the homogeneous case, where defects can nucleate all over the system, and $d_o \sim \hat{\xi}^{-1} = \frac{1}{a}\frac{1}{\omega_0}(\frac{\delta_0\eta}{\tau_Q})^{1/4}$. By contrast, in the underdamped regime $[\eta \ll \sqrt{\delta(0,\hat{t})}]$ [6], the relaxation time diverges as $\tau = 1/\sqrt{|\delta(x,t)|}$, which leads to the freeze-out time scale $\hat{t} = (\tau_Q/\delta_0)^{1/3}$. At this time scale, the correlation length reads $\hat{\xi}_x = a\omega_0(\tau_Q/\delta_0)^{1/3}$ leading to a uniform sound velocity $\hat{v}_x = \hat{\xi}_x/\hat{\tau}_z = a\omega_0$. The causality argument implies that $v_F/\hat{v}_x = \mathcal{A}_u/[X(1-X^2)^2] > 1$, in terms of the parameter $\mathcal{A}_u = \frac{L}{6\nu_t^{(c)}(0)^2 a\omega_0\xi_0}$. For the purpose of deriving a scaling of the density of defects, we assume that formation of kinks arises only in a small central region $2X_* \ll 1$ where $\hat{X}_* \simeq \mathcal{A}_u$, so that

$$d_u \sim \frac{2\hat{X}_*}{\hat{\xi}} = \frac{L}{3\nu_t^{(c)}(0)^2 a^2\omega_0^2}\left(\frac{\delta_0}{\tau_Q}\right)^{4/3}, \tag{4}$$

which should be compared with the density of defects in the homogeneous case $d_u \sim \hat{\xi}^{-1} = \frac{1}{a}\frac{1}{\omega_0}(\frac{\delta_0}{\tau_Q})^{1/3}$. We shall refer to the mechanism above as the inhomogeneous KZM (IKZM), whose main prediction is the scaling found in Eqs. (3) and (4), for the overdamped and the underdamped cases, respectively, and which are in dramatic contrast with their homogeneous counterparts.

To test the IKZM we next consider the dynamics of the structural phase transition for ions in a linear Paul trap, which are continuously Doppler cooled and whose transverse square-frequency is driven through a linear quench as above. The motion dynamics is given by the set of coupled Langevin equations $m\ddot{\mathbf{r}}_i + \partial_{\mathbf{r}_i} V(\{\mathbf{r}_i\}, t) + m\eta\dot{\mathbf{r}}_i + \varepsilon(t) = 0$, $(i = 1, \ldots, N)$ where $\mathbf{r}_i = (x_i, y_i)$, V is the full Coulomb and trap potential, and $\varepsilon(t)$ is Langevin force (whose amplitude we take $\varepsilon = 0.05\ l_0\nu^{3/2}$ with $l_0^3 = Q^2/m\nu^2$), and η is the cooling rate [21]. At $t = 0$ the chain is in the classical ground state, with all the ions at the equilibrium position satisfying $\partial_{\mathbf{r}_i} V(\{\mathbf{r}_i\}) = 0$. The value of $\delta(\hat{t})$ is chosen such that the equilibrium configuration is linear, but close to the critical frequency below which the ground state becomes doubly degenerated. The system is then driven through the transition. Typical defects are shown in Fig. 1(b), and come in two varieties, $\mathbb{Z}_2$ kinks (of topological charge $\sigma = +1$) and antikinks ($\sigma = -1$). These defects resemble the nonmassive kinks of the Frenkel-Kontorova model with a transversal degree of freedom which can be described by an effective ϕ^4 theory for the translational displacement [17,24]. When defects appear near the edges of the chain, they might be lost in the linear part. To minimize defect losses at the edges of the chain (see below), the density of defects d (number of defects over the total number of ions) is computed once the average absolute transverse displacement of the ions $\langle y\rangle = \sum_{i\in\mathcal{C}}|y_i|/N_{\mathcal{C}}$ approaches 90% of that of the ground state in the final trap. $\mathcal{C}$ denotes the set of $N_{\mathcal{C}}$ central ions which would reach the zigzag structure in an adiabatic transition, and where the formation of defects is studied. The average density of defects d over different realizations such as the one in Fig. 1(b) is computed for different values of τ_Q, and a least-squares fit to the list of data is used to extract the exponent governing the scaling. Numerical simulations in Fig. 2 are in good agreement with the IKZM scaling derived in Eqs. (3) and (4). Interactions between the defects lead to a saturation of the density and deviations from IKZM. Further, the applicability of IKZM is restricted by the following effects. (a) Axial and

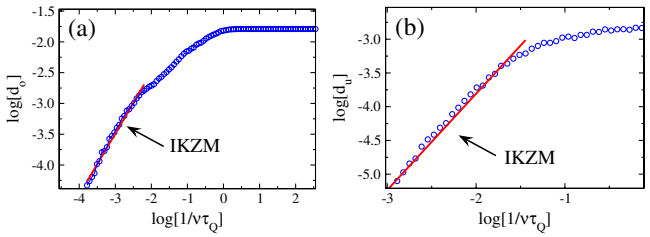

FIG. 2 (color online). Density of defects for a harmonically trapped ion chain as a function of the inverse of the sweeping rate (a) in the overdamped regime ($\eta = 100\nu$), where the slope in the fit is 0.995 with regression coefficient 1, and (b) in the underdamped regime ($\eta = 10\nu$), where the slope in the fit is 1.427 with regression coefficient 0.994. The defects are only considered in the central $N_C = 30$ ions, in order to minimize defect losses ($N = 50$, 2000 realizations).

transverse modes are coupled since the ions shift in the axial direction towards the center of the trap as the structural phase transition takes place. (b) The amplitude of the transverse displacement of the ions increases in the center of the trap, making the amplitude of the effective Peierls-Nabarro potential seen by a kink [24] to decrease towards the edges of the chain, and leading to transport of defects and losses near the edges of the trap. Defect transport remains even if the longitudinal degrees of freedom of the ions are frozen on a lattice due to the transverse motion, and even when the trapping potential makes the inter-ion spacing homogeneous due to a local correction to the transverse critical frequency in the finite system. (c) Scattering between kinks and antikinks can occur leading to their annihilation, a process particularly relevant in the underdamped regime which leads to deviations from the IKZM.

In conclusion, we have proposed an ion crystal as a test bed for the formation of structural defects governed by the KZM. This system is far more amenable to experimental verification and control than other systems with realistic possibilities to enter the quantum regime. Though the paradigmatic result for a homogeneous second-order phase transition can be studied using a ring trap, as in Ref. [20], the inhomogeneities in a linear Paul trap make an ion crystal a natural system to study the IKZM mechanism where the scaling of the number of topological defects as a function of the quenching rates is dramatically altered, as we have shown analytically and confirmed by numerical simulations.

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