

Interacting Langevin equation and a microscopic mechanism for kinks in trapped ionsWei Wen,¹ Yue-Xin Huang,² Wei Wu,³ Baoquan Ou,³ Yi Xie,³ and Pingxing Chen^{3,4,*}¹*College of Science, Hunan University of Technology, Zhuzhou 412007, China*²*CAS Key Laboratory of Quantum Information, University of Science and Technology of China, Hefei 230026, China*³*College of Science, National University of Defense Technology, Changsha 410072, China*⁴*Synergetic Innovation Center for Quantum Effects and Applications, Hunan Normal University, Changsha 410081, China*

(Received 25 November 2018; published 9 May 2019)

The transition between the linear phase and zigzag phase in an ion trap is widely used to study the mechanism of the second-order continuous phase transition. For a linear ion chain, during the quenching across the critical point, kinks are formed. The relation between the density of kinks and quenching rate can be described by the Kibble-Zurek mechanism. In this work, we consider a one-dimensional trapped-ion chain with the motion on the phase-transition plane. Using the interacting Langevin equation, we show that when one ion is kicked out from the chain, the off-axis action caused by this ion will propagate to others one by one with a defined velocity. This velocity will be the same as the sound velocity in some extreme cases but has obviously different meaning. In the presence of finite temperature, which is modeled using a many-body stochastic Langevin equation to unveil a microscopic mechanism for kink formations in this model, we find that the kink can be formed when the diffusion radius is larger than the mean displacement of the ions along the radial direction. This criterion provides an alternative mode for the formation of kinks in realistic experiments. The predictions based on this mechanism can be qualitatively consistent with those from the Kibble-Zurek mechanism in homogeneous structures; however, the microscopic details, such as kink formation and kink disappearance can be seen much clearer in our simplified model.

DOI: [10.1103/PhysRevA.99.053409](https://doi.org/10.1103/PhysRevA.99.053409)**I. INTRODUCTION**

Defects, such as kinks and vortices, can be formed during quench dynamics, when their physical parameters are quenched below the second-order critical points. The formation of these defects can be generally described by the Kibble-Zurek (KZ) mechanism, that is, the density of defects is proportional to $\tau_Q^{-\alpha}$, where τ_Q is the quenching rate, and α is the corresponding exponent [1–5]. This scaling law is valid in various systems from cosmology to condensed matter physics. Recently, it has been carefully examined in a lot of physical models, including Bose-Einstein condensates [6,7], trapped ions [8,9], and liquid Helium [10,11]. Some authors have even drawn a connection between the KZ mechanism and the Landau-Zener transition in a transverse Ising model [12–15], in which after some nonlocal transformation the many-body system is reduced to a series of single-particle models labeled by momentum. With the efforts of some researchers, the mechanism that was originally used for the linear quenching is generalized to the quenching regime with the nonlinear power form, in which the defect density also exhibits similar scaling laws [16–19]. In order to verify the universality of this mechanism, the KZ mechanism was examined using a single qubit with the aid of tomography, in which the magnetic field serves as momentum degree of freedom and the wave functions in each momentum are measured in experiments to reconstruct the whole dynamics [20–22]. These researches

show that although the microscopic mechanisms of the formation of these defects are totally different, there is still a common theory that can be used to describe the variation of these defects with the quenching rate.

Although the KZ mechanism within the Ginzberg-Landau equation provides an important tool for us to understand various physical phenomena [11,23,24], it is still hard for us to derive some equations and relations used by the KZ mechanism from a more fundamental theory. In the KZ mechanism, the defect density is inversely proportional to the correlation length ξ at freeze-out time \hat{t} [25,26]. This relation yields scaling that agrees with the experimental observations [4,11,20], but it is not enough for us basing on a more fundamental theory to answer these questions that why the freeze-out time is determined by the equation $\tau(\hat{t}) = \hat{t}$ under the linear quenching [4,22,25,27] and how to get the freeze-out time under the nonlinear quenching in theory. This leads to a problem that the KZ mechanism can only provide in most cases the trend of defects varying with quenching rate, but cannot provide the exact value of the density of defects. Another problem is that KZ mechanism cannot explain the anomalous exponents in quantum systems with edge states [5,28–31]. Moreover, the KZ mechanism cannot support the experimental results of the defects density in the nonlinear quenching process with the nonpower function driving rate. In this work, we focus on the defect formulations in trapped ions carried out in several experiments [8,9], and try to find out an interpretation for the KZ mechanism from the view of a microscopic mechanism. To account for this mechanism, we consider a one-dimensional trapped ion chain with

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long-range Coulomb interaction [32–37]. The temperature effect is modeled using a many-body stochastic Langevin equation. We show that at extremely low temperature, the off-axis action of the kicked ion propagates across the whole chain with velocity slightly different from the sound velocity that defined in previous work. This mechanism gives rise to zigzag phase [38–40]. At relatively higher temperature, the atoms move stochastically along the radial direction. When its diffusion radius is larger than the mean displacement, kinks are formed. We have also verified this picture by solving the many-body stochastic equation. This picture provides an alternative mechanism for the formation of kinks in this system and will be helpful for us to investigate other systems.

This article is organized in such a way that we will first introduce a special model, the ion-kicking model, which is a transition status of an ion system from the linear phase to the zigzag phase. It can also be argued that the zigzag structure is excited by this status. In this section, we will show the ions' motion in the ion-kicking model. According to the movement of ions, we will derive the propagation velocity, with which the off-axis action of some ions will propagate to the entire ion chain. In the next section, we will introduce the correlation function of the ion system that has been crossed at the second-order critical point. This correlation function shows us the relaxation time and correlation length, which are different from those of the previous literature. Next we will talk about the calculation of the diffusion radius in Brownian motion. Finally, we will exhibit our important conclusion that the kinks formation of ions is due to a competition between the ordered propagation motion with finite propagation velocity and the disordered Brownian motion. We will present a criterion that has been tested by many simulations in our work for the formulation of kinks. It is shown that the assumption about the freeze-out time is unnecessary and a more general formula that is used to determine the defect density will be given in the last part of this article. This work will provide us with another way to further understand the KZ mechanism.

II. THE ION-KICKING MODEL AND ITS SOLUTION

A. Langevin equation and the ion-kicking model

We consider the physical model depicted in Fig. 1 for a one-dimensional trapped ion chain. The distance between neighboring ions of this homogeneous ion chain is typically of the order of $a \sim 1-10 \mu\text{m}$ [9,36,41,42]. At finite temperature, as used in experiments with $T \sim 10^{-3}-10$ K, the ions have random subtle thermal motions, which can be modeled as the Brownian motion in the ion trap. In experiments, the secular motion frequency ω_t along the plane of zigzag configuration is set to be a less than that in its vertical direction on the transverse plane. The difference between them is about 10%–30% of ω_t depending on the demands of experiments. That is enough to make the zigzag phase formed on a plane along the r direction as shown in Fig. 1. Thus, by neglecting the contribution from other unimportant directions, we have the following model:

$$H = \sum_i \frac{p_i^2}{2m} + \frac{1}{2} m \omega_t^2 r_i^2 - \sum_{j \neq i} \frac{Q}{|(i-j)a\hat{e}_z + r_{ij}\hat{e}_r|}, \quad (1)$$

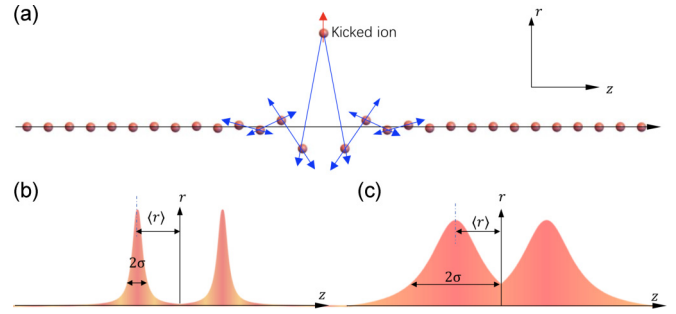


FIG. 1. (a) One-dimensional trapped ions considered in this work. When one of the atoms at $l = 0$ is kicked out from the chain, its influence will spread across the whole system, giving rise to zigzag phase. (b) With variance much smaller than the mean displacement and (c) with variance larger than the displacement showing the basic picture for kink formation at relatively high temperature regime.

where $r_i = r_i(t)$ is the position in the one-dimensional chain at time t , $r_{ij} = r_i - r_j$, $\omega_t = \omega(t)$, and $Q = e^2/(4\pi\epsilon_0)$. The three terms on the right are kinetic energy, trapping potential, and Coulomb repulsive potential along the transverse direction respectively. This model is related to the experiments about trapped ions in the sense that (1) the axial direction and the radial direction with the minimum trapping frequency determine the phase transition plane; and (2) the trapping frequency of one of the directions ω_t is set to be a little less than critical frequency $\omega_{t,c}$, wherefore the displacement of ion radial motions is much less than the distance between neighboring ions, so that the motion along the axial direction has no effect on kink formation. For these reasons, we only restrict to the dynamics along the phase transition plane.

A simple picture of the dynamics is presented in Fig. 1. In the short-time case, the atoms will oscillate periodically around their equilibrium positions. When one atom is kicked out from the one-dimensional chain, it will lead to a repulsive interaction to the two neighboring sites. After the neighboring sites are off axis, the new off-axis repulsive interactions are produced and act on their next neighboring sites. The influence of the kicked ion spreads throughout the ion chain through this off-axis action. Next, we will aim to mathematically depict this kind of dynamics with the ion-kicking model. In the regime $|r_{ij}| \ll a$ [see simulated data in Figs. 3(b), 4(a), and 4(b)], then using perturbation theory to the leading term by ignoring the constant term, one has

$$H = \sum_i \frac{p_i^2}{2m} + \frac{1}{2} m \omega_t^2 r_i^2 - \frac{Q}{2a^3} \sum_{j \neq i} \frac{r_{ij}^2}{(i-j)^2}. \quad (2)$$

Next, we consider the dynamics of the above model at finite temperature, in which the contribution of temperature is introduced into the dynamics using a stochastic force $\varepsilon_i(t)$, as used in the Langevin equation for Brownian motion [43,44],

$$\langle \varepsilon_i(t) \varepsilon_j(t) \rangle = 2k_b T m \eta \delta_{i,j} \delta(t_1 - t_2), \quad (3)$$

where η is the damping coefficient caused by the environment. $\delta_{i,j}$ and $\delta(t_1 - t_2)$ here are the Kronecker delta and Dirac delta function, respectively. The stochastic force can be produced by the trapped potential noise or cooling laser fluctuation. In

this way, the Newtonian motion can be written as

$$m\ddot{r}_i = -m\eta\dot{r}_i + m\omega_a^2 \sum_{j \neq i} \frac{r_j - r_i}{|i - j|^3} - m\omega_i^2 r_i + \varepsilon_i, \quad (4)$$

where ω_a is the character frequency of homogeneous linear ion chain with the expression $\omega_a^2 = Q/a^3$ [45]. Due to the presence of translational symmetry, one can solve the above equation in momentum space using

$$R(q, t) = \sum_{l=1}^N r_l(t) e^{iql}, \quad (5)$$

where $qN = 2n\pi + \nu\pi$, with ν determined by $r(l, t) = (-1)^\nu r(l + N, t)$. N here is the total number of trapped ions. The ignoring of the motion in the other direction can be seen clearly now, that is, to the leading approximation, their dynamics are generally decoupled. We can compute the dynamics in momentum space by showing that

$$m\ddot{R}(q, t) = -m\eta\dot{R}(q, t) + m\mathcal{G}(q)R(q, t) + \varepsilon_q(t), \quad (6)$$

where $\mathcal{G}(q) = \omega_a^2 [g(e^{iq}) - \frac{7}{2}\zeta_3]$, $\zeta_3 \simeq 1.202$ is the Euler-Riemann zeta function, and the function g is defined as

$$g(q) = 2\zeta_3 - \sum_{n=1}^{\infty} \frac{q^n + q^{-n}}{n^3} + \frac{\delta^2}{\omega_a^2}. \quad (7)$$

δ here is the detuning between critical frequency and trapped frequency, defined as $\delta^2 = \omega_{t,c}^2 - \omega_t^2$. In this article, we focus on the ions' motion when ω_t is a little less than $\omega_{t,c}$, thus δ^2 is a positive. Critical $\omega_{t,c}$ here is the critical frequency of the zigzag phase transition and $\omega_{t,c} = (7\zeta_3/2)^{1/2}\omega_a \simeq 2.05\omega_a$ [27,45]. The solution to the above inhomogeneous equation can be written as

$$R(q, t) = R_0(e^{iq}, t) + R_1(e^{iq}, t), \quad (8)$$

where R_0 accounts for the homogeneous solution and R_1 for the inhomogeneous solution by including the contribution of the noise term. The homogeneous solution can be easily calculated according to the homogeneous part of the second-order ordinary differential equation in Eq. (6),

$$R_0(q, t) = e^{-(1/2)\eta t} [c_1 \sinh(\Omega_{1,q} t) + c_2 \cosh(\Omega_{1,q} t)], \quad (9)$$

where $\Omega_{\lambda,q} = [\eta^2/4 + \lambda\mathcal{G}(q)]^{1/2}$. In the ion-kicking model, one site of a linear ion chain has obviously much more axial displacement than the others. The obvious axial displacement of this site might be caused by the kicking effect of stochastic force and therefore it is called an ion-kicking model. Without losing generality, in this article, the kicked site is assumed to be the central ion with axial displacement c_0 when $t = 0$. Based on this, we have the constant $c_1 = c_0\eta/(2\Omega_{1,q})$, and $c_2 = c_0$ from our solution in Eq. (9).

B. The inhomogeneous solution to Langevin equation

We see that the contribution of Eq. (6) is made up of two terms: a regular term, which can be well described by the Newtonian equation, and a stochastic term due to random force $\varepsilon_q(t)$. The second term can only be understood from the statistic sense. These two terms can also be found in the single-particle Langevin equation, in which the first

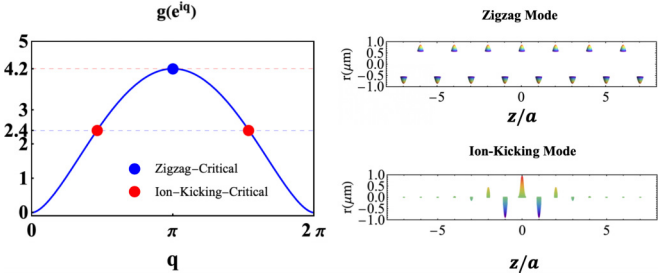


FIG. 2. $g(e^{iq})$ is the quantity that is used to measure the Coulomb repulsive force between ions of the homogeneous ion chain. The left graph denotes the value of $g(e^{iq})$ varying with q when $\delta = 0$. $q = \pi$ is the critical point of the phase transition between linear chain and zigzag; $q = 1.45$ and $q = 4.83$, corresponding to $g(e^{iq}) = 2\zeta_3$, are all the critical points of phase between the linear chain and the ion-kicking model. The zigzag mode and ion-kicking mode are shown on the right side. The ion-kicking mode with a lesser value of $g(e^{iq})$, namely, with less Coulomb repulsive force, can excite the zigzag mode. According to the left graph, $g(e^{iq})$ is always greater than zero when $\delta^2 \geq 0$.

term contributes to the mean position and the second term, after ensemble averaging, gives rise to the diffusion radius. The formation of kinks depends strongly on the competition between these two terms.

The inhomogeneous solution to Eq. (6) can be obtained from a Green's function,

$$m\ddot{G}(t, t_0) = -m\eta\dot{G}(t, t_0) + m\mathcal{G}(q)G(t, t_0) + \delta(t - t_0). \quad (10)$$

$G(t, t_0)$ is called the Green's function of Eq. (6) and its Fourier transform $G_\omega = (2\pi)^{-1} \int_{-\infty}^{\infty} G(t, t_0) e^{-i\omega(t-t_0)} dt$ can be obtained as

$$G_\omega = \frac{1}{(i\omega - \omega_+)(i\omega - \omega_-)}, \quad (11)$$

where $\omega_\pm(e^{iq}) = -\eta/2 \pm \Omega_{1,q}$. Via the reverse Fourier transformation, we get the inhomogeneous solution $R_1(q)$ with integral formula

$$\begin{aligned} R_1(q, t) &= \int_{-\infty}^{\infty} \varepsilon(q, t_0) G(t, t_0) dt \\ &= \frac{1}{2\pi} \int_{-\infty}^{\infty} \varepsilon(q, t_0) dt_0 \int_{-\infty}^{\infty} G_\omega e^{i\omega(t-t_0)} d\omega \\ &= i \int_{-\infty}^t \text{Res}(G_\omega e^{i\omega(t-t_0)}, -i\omega_-) \varepsilon(q, t_0) dt_0 \\ &\quad - i \int_t^{\infty} \text{Res}(G_\omega e^{i\omega(t-t_0)}, -i\omega_+) \varepsilon(q, t_0) dt_0. \end{aligned} \quad (12)$$

Res denotes the residue here. These two residues above come from the contour integrals on the complex plane. We should notice $\omega_+ > 0$ and $\omega_- < 0$ when $g(e^{iq})$ is positive (seen in Fig. 2). For this reason, the contour integral should adopt the upper half-plane of the complex plane when $t_0 < t$ and the lower half-plane when $t_0 > t$ to make $e^{i\omega(t-t_0)}$ convergent at the boundary of infinity. Subsequently, the final expression of R_1 is derived as the following with the Eq. (11) and Eq. (12),

$$R_1(q, t) = \int_0^t e^{-(1/2)\eta t} \text{sinc}(-i\Omega_{1,q} s) \varepsilon_q(t - s) ds. \quad (13)$$

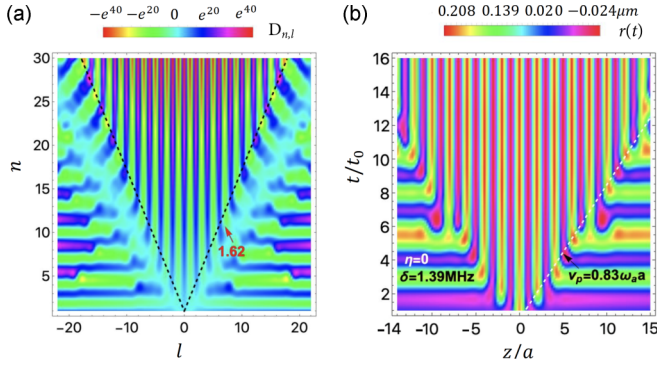


FIG. 3. (a) Properties of the function D_{nl} . (b) Formation of perfect zigzag phase without disorder after one trapped ion is kicked off from the chain. v_p denotes the propagation velocity that agrees well with the rate of sequentially varying ion motion (the white dashed line). a here is the neighboring distance, $8.92 \mu\text{m}$, and $t_0 = 0.25\pi \mu\text{s}$.

This formula satisfies the causality relation, in which the influence from $t \rightarrow -\infty$ to $t \rightarrow 0$ exactly equals zero.

C. The position of the trapped ions in ion-kicking model

The position of the trapped ions can be obtained via the inversion Fourier transformation for $R(q, t)$ shown in Eq. (5). We first consider the mean value of $r_l(t)$, which is determined by the first term R_0 under the consideration $N \rightarrow \infty$,

$$\langle r_l(t) \rangle = \frac{1}{2\pi} \int_0^{2\pi} R_0(q, t) e^{-iq_l} dq. \quad (14)$$

One may treat the above integral over a closed circuit by defining $z = e^{iq}$, thus $q = -i \ln z$. In this way, the above integral can be written as

$$\langle r_l(t) \rangle = \oint_c \frac{R_0(-i \ln z, t)}{2\pi i z^{l+1}} dz = \text{Res} \left(\frac{\tilde{R}_0(z, t)}{z^{l+1}}, 0 \right). \quad (15)$$

The contour of the above contour integral is the unit circle $|z| = 1$. Although there are two singular points in this unit circle, only the residue at points $z = 0$ should be noted because the other singular $z = \exp\{i\pi - \delta/[\ln(2)\omega_a]\}$ has no contribution to this contour integral. In our model, the cosine functions can be expanded with the series of spherical Bessel functions using the identities $\cos(\sqrt{b^2 - 2bx})/b = \sum_{n=0}^{\infty} x^n/n! j_{n-1}(b)$, where j_n is spherical Bessel functions [46], and $b = \omega_{c,\eta} t$ and $x = g\omega_a^2 t/(\omega_{c,\eta})$ by setting $\omega_{c,\eta} = (\omega_{l,c}^2 - \eta^2/4)^{1/2}$. This expansion has very good properties for fast convergence, which enables us to model the dynamics even in the long time evolution. With the aid of this expansion, we find

$$\langle r_l(t) \rangle = c_0 \sum_{n=0}^{\infty} e^{-n/2} [2d_n(t) + \eta d'_n(t)] D_{n,l}, \quad (16)$$

where $D_{n,l} = \text{Res} \left(\frac{g^n}{z^{l+1}}, 0 \right)$ and

$$d_n(t) = \frac{\omega_a^{2n}}{2\omega_{c,\eta}^{n-1}} \int_0^t s^{n+1} j_{n-1}(s) ds. \quad (17)$$

The numerical result of D_{nl} is presented in Fig. 3. Although this expansion is complex, $\langle r_l(t) \rangle$ still has a simple expression

when $t \gg \omega_{l,c}^{-1}$ or $t \ll \omega_{l,c}^{-1}$. We find that when $n > |l|/1.62$,

$$D_{nl} \simeq (-1)^l e^{s(l)} \left(\frac{7\zeta_{3,l}}{2} \right)^n, \quad (18)$$

where $\zeta_{3,l} \simeq \zeta_3 + \delta^2/(7\omega_a^2)$ and $s(l) \simeq -1.2|\delta|l/\omega_a$ when $l \gg 1$. The term $(-1)^l$ will directly influence the properties of the position from term $\langle r_l(t) \rangle$,

$$\langle r_l(t) \rangle = (-1)^l c_0 \chi_\eta e^{(t/\tau)+s(l)} = (-1)^l A_\eta e^{(v_p t - l a t)/\xi}, \quad (19)$$

where $\chi_\eta = \delta^2 \tau / \Omega_{2,\pi} \in (1.0, 2.0)$ and $A_\eta = c_0 \chi_\eta$. We therefore see that the sign of D_{nl} can influence the motion direction of the atoms, after one of them is kicked off from the chain. Without stochastic forces in the ion trap, the ion chain will form a perfect zigzag structure through the ion-kinking model. The τ and ξ in Eq. (19) with a new quantity v_p are defined as

$$\tau^{-1} = -\frac{\eta}{2} + \sqrt{\frac{\eta^2}{4} + 2\delta^2}, \quad \xi = \frac{\omega_a a}{1.2|\delta|}, \quad v_p = \frac{\xi}{\tau}. \quad (20)$$

It is important to note that the τ here differs from that described in Refs. [39,47]. In these references, $\tau \propto \delta^2$ under the overdamping and $\tau \propto \delta$ under the underdamping (δ here is the squared value of that in these two references). The τ here can be seen as a unified form of expression in these two extreme cases. The v_p has the definite physical meaning if we notice Eq. (19) can be written as $|\langle r_l(t) \rangle| = |\langle r_0(t - z_l/v_p) \rangle|$, that is, the influence of the action ‘‘ion be kicked off’’ spreads to the l th site in the time z_l/v_p , where v_p we called is propagation velocity.

The evidence of the speed of propagation can be found in Figs. 3 and 4. These two figures evidence that under the action of the kicked ion, which is the central ion here, other ions move away from the axis equilibrium position one by one. This can be seen as the action of kicked ions gradually propagating to all parts of the ion chain like wave propagation, no matter whether or not the damping force exists in the ion trap. From simulation experiments, the off-axis velocity of the ions is in good agreement with the propagation velocity we define. The propagation velocity depends on the degree of the system deviating from the critical point and the arrangement structure of the ion chain. It can be used to measure the response speed of the ion chain to the kicked ion.

It is worth noting that in previous literature, Adolfo del Campo *et al.* defined similar velocities: the front velocity v_F and sound velocity (or characteristic velocity) v_x [47,48]. However, these velocities are all different from the propagation velocity we get in this article. If the difference in the expressions of relaxation time and correlation length in these works is not taken into account, the sound velocity v_x can be treated as a special case of propagation velocity at the freeze-out time \hat{t} . As for the front velocity v_F , which is defined as the ratio between the characteristic length of the control parameter and the characteristic timescale at which it changes [47], it is even more different from the propagation velocity v_p .

One might think that $\langle r_l(t) \rangle$ shown in Eq. (19) is an approximate expression. However, it is one of the exact solutions to Eq. (4). In fact, when we plug the expression of $\langle r_l(t) \rangle$ into

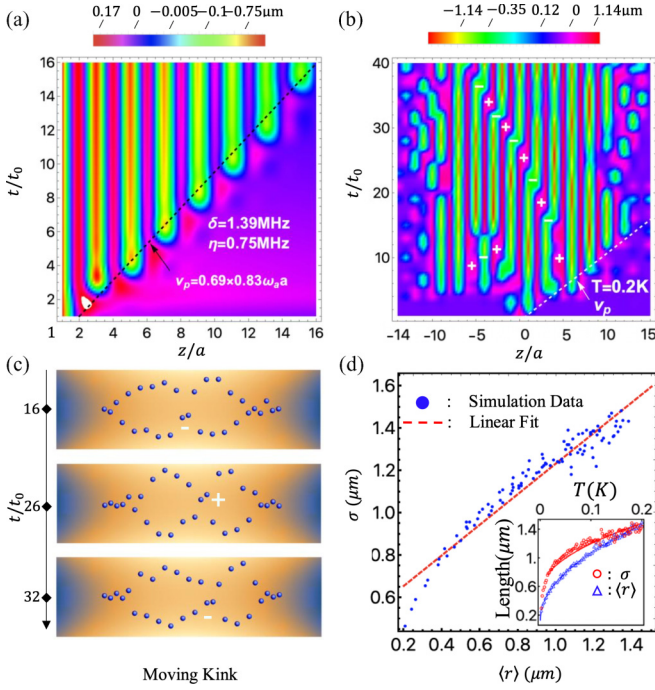


FIG. 4. Formation of kinks. t_0 here is $0.25\pi \mu\text{s}$, and $a = 8.92 \mu\text{m}$. (a) Zigzag phase with weak dispersion and detuning. Sequentially varying ion motion presents a steady propagation velocity that agrees well with the v_p defined in Eq. (20). (b) Formation of kinks at high temperature ($T = 0.2 \text{ K}$). The positive and negative signs correspond to the position of kinks. The obvious movement of one kink is observed in our work. (c) A snapshot of the configuration of the trapped ions at three typical times ($t/t_0 = 16, 26, 36$), which indicates the evolution and motion of kinks. (d) The variance σ and mean displacement $\langle r \rangle$ as a function of temperature $T \in (0, 0.2) \text{ K}$. These two quantities keep a good linear relation when $T > 0.4 \text{ K}$.

Eq. (4), the second term on the right of it will become

$$\begin{aligned}
 & m\omega_a^2 \sum_{m \neq l} \frac{\langle r_m \rangle - \langle r_l \rangle}{|m - l|^3} \\
 &= m\omega_a^2 A_\eta e^{t/\tau} \sum_{m \neq l} \frac{(-1)^l e^{-l(1.2\delta/\omega_a)} - (-1)^m e^{-m(1.2\delta/\omega_a)}}{|l - m|^3} \\
 &= m\omega_a^2 \langle r_l \rangle [2\zeta_3 - P_3(-e^{1.2\delta/\omega_a}) - P_3(-e^{-1.2\delta/\omega_a})] \\
 &= m\omega_a^2 \langle r_l \rangle \left[\frac{7}{2}\zeta_3 + \ln(2)1.2^2 \frac{\delta^2}{\omega_a^2} + O\left(\frac{\delta^4}{\omega_a^4}\right) \right] \\
 &\approx m\omega_a^2 \langle r_l \rangle \left(\frac{7}{2}\zeta_3 + \frac{\delta^2}{\omega_a^2} \right). \quad (21)
 \end{aligned}$$

Hence, Eq. (4) can be simplified into

$$\begin{aligned}
 m\langle \ddot{r}_l \rangle &= -m\eta \langle \dot{r}_l \rangle + m\omega_a^2 \langle r_l \rangle \left(\frac{7}{2}\zeta_3 + \frac{\delta^2}{\omega_a^2} \right) - m\omega_l^2 \langle r_l \rangle \\
 &= -m\eta \langle \dot{r}_l \rangle + \frac{7}{2}m\omega_a^2 \langle r_l \rangle - m\omega_l^2 \langle r_l \rangle + m\delta^2 \langle r_l \rangle \\
 &= -m\eta \langle \dot{r}_l \rangle + 2m\delta^2 \langle r_l \rangle. \quad (22)
 \end{aligned}$$

We used $\delta^2 = \omega_{l,c}^2 - \omega_l^2$ here. A solution to this unary second-order ordinary differential equation is $\langle r_l(t) \rangle =$

$(-1)^l A_\eta e^{(v_p t - l a \tau)/\xi}$. Therefore, Eq. (19) is a rational solution to the ion-kicking model.

$\langle r_l(t) \rangle$ is the average value of an ion's radial displacement. This displacement is caused by the kicked ion, acting as the crystal nucleus. Under the effect of the kicked ion, the structure of zigzag will be formed gradually.

D. The propagation length under quenching

What we discuss above is the variation of the average off-axis position of the ion over time under the condition when the trapping frequency is constant. Next, we will discuss the variation of the average radial displacement of ions over time under general quenching conditions (including linear quenching and nonlinear quenching).

For general quenching conditions, we find the general formula of $\langle r_l(t) \rangle$ can be expressed as the following if $t\delta(t)' \sim \Delta\delta \ll \eta$:

$$\langle r_l(t) \rangle = (-1)^l A_\eta e^{\beta(t)} e^{\gamma(t)} \exp\left(\frac{1}{\xi} [x_l - x_p(t)]\right), \quad (23)$$

where

$$\beta(t) = \int_0^t \frac{\xi(s)'}{\xi(s)^2} ds \int_0^s v(\sigma) d\sigma; \quad (24)$$

$$\gamma(t) = \int_0^t \frac{ds}{\tau(s)} - \frac{t}{\tau}; \quad (25)$$

$$x_p(t) = \int_0^t v_p(s) ds. \quad (26)$$

The functions $\beta(t)$ and $\gamma(t)$ are called the correlation-length-deformation exponent and the relaxation-time exponent, respectively. They are caused by the changing of ξ and τ under quenching and lead to the change in the amplitude of motion. x_p is called the propagation length, which represents the distance that the off-axis action of the kicked ion propagates in the interval time t .

III. THE CORRELATION FUNCTION AND CORRELATION LENGTH, RELAXATION TIME

To understand how the kicked ion affects the far-distance ion, let us define the correlation,

$$F_c(l, t) = \frac{\langle r_0(0)r_l(t) \rangle_T - \langle r_0(0) \rangle_T \langle r_l(t) \rangle_T}{\langle r_0(t)^2 \rangle_T}. \quad (27)$$

The subscript is used for thermal average. This correlation function has an obvious physical meaning. The term $\langle r_0(0)r_l(t) \rangle_T - \langle r_0(0) \rangle_T \langle r_l(t) \rangle_T$ describes the dependence of the l th ion motion at t on the ‘‘initial kicking.’’ $\langle r_0(t)^2 \rangle_T$ here is used to eliminate the divergence of motion.

Using the property of Eq. (19), and $\langle r_0(0) \rangle_T \langle r_l(t) \rangle_T = 0$, we can find

$$\begin{aligned}
 \langle r_0(0)r_l(t) \rangle_T &= \langle A_\eta (-1)^l A_\eta e^{t/\tau} e^{z_l/\xi} \rangle_T; \\
 &= (-1)^l e^{t/\tau} e^{z_l/\xi} \langle A_\eta^2 \rangle_T; \quad (28)
 \end{aligned}$$

$$\begin{aligned} \langle r_0(0) \rangle_T \langle r_l(t) \rangle_T &= \langle A_\eta \rangle_T \langle (-1)^l A_\eta e^{t/\tau} e^{z_l/\xi} \rangle_T \\ &= 0; \end{aligned} \quad (29)$$

$$\langle r_0(t) r_0(t) \rangle_T = e^{2t/\tau} e^{2z_l/\xi} \langle A_\eta^2 \rangle_T. \quad (30)$$

Based on these three equations, we obtain the final expression of the correlation function:

$$F_c(l, t) = (-1)^l e^{-(z_l/\xi) - (t/\tau)}. \quad (31)$$

Therefore, ξ and τ here have the definite physical meaning, that is, they are correlation length and relaxation time respectively. This result also naturally yields the density of kinks, $N_k \propto 1/\xi \propto |\delta|^{-1}$, as used in Refs. [4,5,49]. The above result is consistent with the solution in Refs. [47,48] from several different aspects. This correlation gives rise to the zigzag structure spontaneously in experiments with weak transverse confinement or strong longitudinal trap.

$\langle A_\eta \rangle_T$ does not appear in the final expression of $F_c(l, t)$ because $\langle A_\eta \rangle_T$ is roughly reduced in Eq. (27), however, its concrete value is still very important for us in estimating the density of kinks in the following. So, we will spend some time to figure out how to get its value.

For an ion in plane motion, its average kinetic energy in thermodynamic motion is $k_b T$, where k_b is the Boltzmann constant. One kicked ion will reach the maximum radial displacement c_0 under the action of the random force when its kinetic energy of the kicked ion is totally converted into the confinement potential energy U_e and the work W_e that is used to overcome the damping forces. Hence, the thermal averages of initial radial displacement are the same as for c_0 . The confinement potential energy U_e is determined by the Coulomb repulsive forces among the ions and the secular motion frequency ω_l :

$$\begin{aligned} U_e &\approx -\frac{Q^2}{8\pi\epsilon_0 a^3} \sum_n \frac{\langle [r_0(t) - r_n(t)]^2 \rangle_T}{n^3} \\ &+ \frac{3Q^2}{64\pi\epsilon_0 a^5} \sum_n \frac{\langle [r_0(t) - r_n(t)]^4 \rangle_T}{n^5} + \frac{1}{2} \omega_l^2 \langle r_0^2 \rangle_T. \end{aligned} \quad (32)$$

Moreover, the thermal disturbances of different ions are independent of each other. Therefore, we have the following relations:

$$\langle r_l \rangle_T = 0; \quad \langle r_l(0) r_m(0) \rangle_T = \langle c_0^2 \rangle_T \delta_{l,m}. \quad (33)$$

Based on Eq. (33), U_e leads to

$$\begin{aligned} U_e &= -2\zeta_3 m \omega_a^2 \langle c_0^2 \rangle_T + \frac{3m}{a^2} \omega_a^2 \zeta_5 \langle c_0^2 \rangle_T^2 + \frac{7}{4} m \omega_a^2 \langle c_0^2 \rangle_T \\ &= -\frac{1}{4} m \omega_a^2 \langle c_0^2 \rangle_T + 3m \omega_a^2 \zeta_5 \langle c_0^2 \rangle_T^2 a^{-2}. \end{aligned} \quad (34)$$

We made the approximations $\langle r_l^3 \rangle_T = \langle r_l \rangle_T \langle r_l^2 \rangle_T$ and $\langle r_l^4 \rangle_T = \langle r_l^2 \rangle_T^2$ here to get the above equation. In addition, we adopt the relation $\omega_l \approx \omega_{l,c} = \sqrt{7/2} \omega_a$ because in this article, only the process of phase transition near the critical point is considered here.

When the maximum radial displacement is reached, the kinetic energy of the ion is zero. A part of the kinetic energy

is converted into the work W_e to overcome the damping force. We can also regard this process in such a way that the impulse of the damping force consumes a portion of the momentum of the ion, thereby reducing the kinetic energy of the ion. Therefore, in this case, the reduced kinetic energy should correspond to the momentum that is consumed by the damping force, namely,

$$W_e = \Delta E_k \approx \frac{\langle \Delta p^2 \rangle_T}{2m} = \frac{\langle (m\eta c_0)^2 \rangle_T}{2m}. \quad (35)$$

Finally, according to the relation $k_b T = U_e + W_e$, we can solve c_0^2 as

$$\langle c_0^2 \rangle_T = -\lambda_0^2 + \sqrt{\lambda_0^4 \left(\frac{T}{T_0} + 1 \right)}, \quad (36)$$

where

$$\lambda_0 = a \sqrt{\frac{2\eta^2 - \zeta_3 \omega_a^2}{24\zeta_5 \omega_a^2}}, \quad T_0 = \frac{3m\lambda_0^4 \omega_a^2 \zeta_5}{k_B a^2}. \quad (37)$$

Therefore, using the relations $A_\eta = c_0 \chi_\eta$ and $\chi_\eta = \delta^2 \tau / \Omega_{2,\pi}$, we get

$$\langle A_\eta^2 \rangle_T = \frac{\delta^4 \tau^2}{\Omega_{2,\pi}^2} \left[-\lambda_0^2 + \sqrt{\lambda_0^4 \left(\frac{T}{T_0} + 1 \right)} \right]. \quad (38)$$

IV. THE VARIANCE AND THE DIFFUSION RADIUS

From the above analysis we have known the motion of ions in the ion-kicking model. Without the participation of stochastic forces $\varepsilon_i(t)$, the ions in the linear ion chain will exponentially accelerate away from the axis of the equilibrium position one by one with time, forming an ordered zigzag structure. The above expression of correlation function shows that the ion system still has a descriptive correlation length and relaxation time although it has crossed the critical point of phase transition. The stochastic forces make the role of correlation length in controlling the length of crystal domain appear. This effect will make the ion chains form crystallization regions with the different ion motion orientations, and therefore lead to the formation of kinks on the crystal interfaces.

From our research, although the correlation length is an important physical variable to determine the length of the crystallization region, the two lengths are not exactly equal even from a statistical point of view. To understand the origin of kinks, one needs to calculate the mean value $\langle r_l(t)^2 \rangle_T$, denoted as r_T^2 , under temperature as well as the corresponding variance $\langle \sigma_l^2(t) \rangle_T = \langle (r_l(t)^2) - \langle r_l(t)^2 \rangle_T^2 \rangle_T$, denoted as σ_T^2 . σ_T here is the thermal average value of the diffusion radius of ions under Brownian movement. To some extent, it also represents the degree of disorder in the movement of ions. The larger the value is, the greater the influence of random force on the ion motion will be, and subsequently, it is more likely for the ion to break the ordered phase transition.

The variance $\sigma_l(t)$ is defined as the deviation between the true value and the average value of the position of the ion in motion. $\sigma_l(t)$ also represents the diffusion radius of the l th ion

under Brownian motion:

$$\begin{aligned}\sigma_l^2 &= \langle [r_l(t) - \langle r_l(t) \rangle]^2 \rangle \\ &= \left\langle \left(\int_0^{2\pi} R_1(q, t) e^{-iql} dq \right)^2 \right\rangle \\ &= \frac{k_B T \eta}{m} \int_0^t \text{Res} \left(\frac{\cosh(2\Omega_{1,q(z)} s) - 1}{e^{\eta s} z^{l+1} \Omega_{1,q(z)}^2}, 0 \right) ds. \quad (39)\end{aligned}$$

Here, we used the relation

$$\langle \varepsilon_{q_1}(t_1) \varepsilon_{q_2}(t_2) \rangle = 4\pi k_b T m \eta \delta(q_1 - q_2) \delta(t_1 - t_2). \quad (40)$$

For a thermodynamic process, in an ion chain with homogeneous structure, the kicking site mentioned above may occur at any site rather than just at the central ion site. Therefore the thermal average of σ satisfies

$$\sigma_T^2 = \frac{1}{N} \sum_{m=-N/2}^{N/2} \langle \sigma_{l-m}^2 \rangle_T. \quad (41)$$

Similarly, the thermal average of $r_l(t)$ is

$$r_T^2 = \frac{1}{N} \sum_{m=-N/2}^{N/2} \langle r_{l-m}(t)^2 \rangle_T. \quad (42)$$

The σ_T and r_T^2 of different ions are proved to be the same and therefore we omit the subscript l in these two terms. In the following, for simplification, we will make no distinction below, using them to represent both the thermal average of the ion chain and the thermal average of an individual ion.

V. THE CRITERION OF THE FORMATION OF KINKS

In this section, we aim to provide the following criterion for the formation of kinks. As mentioned above, the diffusion radius σ_T and ion average motion radius r_T are important factors to understand the formation of kinks. The former is a measure of disordered motion caused by random forces, while the latter is that of ordered motion under the influence of one crystal nucleus which is caused by some kicked ion. If the ordered motion of one ion dominates, this ion will participate in the formation of the ordered zigzag structure under the influence of the crystal nucleus. On the contrary, if the disordered motion of it dominates, it will leave the ordered motion sequence, choosing its own direction of motion, and thus forming a new crystal nucleus.

Based on a large number of experimental and simulated data about the occurrence of kinks in ionic chains, we suggest that the boundary between the region dominated by disordered motion and that by ordered motion be determined by this relation:

$$\sigma_T \sim r_T. \quad (43)$$

This relation is the criterion of the formation of kinks. It determines a transition time τ_c between the ordered motion of ions and the disordered motion. The transition time τ_c in fact is the freeze-off time \hat{t} defined in the KZ mechanism because in an ion trap, the ordered motion caused by the crystal nucleus can be regarded as an adiabatic evolution process, and the disordered motion caused by the random force can be seen

as an impulse evolution process. The physical picture for this criteria is rather clear. The kinks are formed because the random fluctuation is comparable with the mean value, causing two neighboring sites to move in the same direction simultaneously; in the case when $\sigma_T \ll r_T$, the zigzag structure may be deformed, but will never be altered. One may try to understand this picture from Fig. 1, in which when $\sigma_T \geq r_T$, it will have small chance that the two neighboring sites have the same motion.

Using the solution to Brownian motion, Eq. (39), and the expression of σ_T in Eq. (41), we can find the thermal average of the diffusion radius σ_T to be

$$\sigma_T^2 = \frac{1}{N} \sum_{m=-\infty}^{\infty} \sigma_{l-m}^2 = \frac{2k_B T \eta t^3}{3mN} + O(t^4), \quad (44)$$

and the average motion radius r_T is

$$\begin{aligned}r_T^2 &= \frac{1}{N} \sum_{l=-\infty}^{\infty} \langle A_{\eta}^2 \rangle_T \frac{\omega_a^4}{l^6 \delta^2} t^2 \sin(\delta t)^2 + O(t^6) \\ &= 2 \frac{\delta^4 \tau^2}{N \Omega_{2,\pi}^2} \frac{\omega_a^4}{\delta^2} t^2 \sin(\delta t)^2 \zeta_6 + O(t^6).\end{aligned} \quad (45)$$

This result is obtained by using Eqs. (16) and (17). Only the first few terms after the spherical Bessel function expanding for the numerator are left for making approximation when t is small.

From the analysis above, we think that ions are generally involved in both disordered and ordered motion. However, when the diffusion radius σ_T is larger than average motion radius r_T , ions will enter the disordered motion-dominated region irresistibly. This moment can be used to determine the boundary between the stable time and unstable time. The transition time τ_c is this boundary time.

According to the expression of r_T^2 , because

$$1 \leq \frac{\delta^2 \tau}{\Omega_{2,\pi}} \leq 2; \quad \Omega_{2,\pi} = \sqrt{\frac{\eta^2}{4} + 2\delta^2} \geq \frac{\eta}{2}. \quad (46)$$

Therefore, $r_T^2 \leq \frac{8\tau}{\eta} \langle c_0^2 \rangle_T \omega_a^4 t^2 \zeta_6$. If we want $\sigma_T^2 > r_T^2$ to be always tenable, then

$$\frac{2k_B T \eta t^3}{3m} \geq \frac{8\tau}{\eta} \langle c_0^2 \rangle_T \omega_a^4 t^2 \zeta_6. \quad (47)$$

The transition time τ_c is determined by the equal sign, namely,

$$\frac{2k_B T \eta \tau_c^3}{3m} = \frac{8\tau}{\eta} \langle c_0^2 \rangle_T \omega_a^4 \tau_c^2 \zeta_6. \quad (48)$$

The required time τ_c to reach this point is roughly

$$\tau_c = \frac{12\zeta_6 m \omega_a^4 \langle c_0^2 \rangle}{k_B T \eta^2} \tau. \quad (49)$$

Using the expression of $\langle c_0^2 \rangle = -\lambda_0^2 + \sqrt{\lambda_0^4 (T/T_0 + 1)}$, we find that in the low-temperature limit, $\langle c_0^2 \rangle_T \simeq \lambda_0^2 T / (2T_0)$, and

in the high-temperature limit, $\langle c_0^2 \rangle_T \simeq \lambda_0^2 \sqrt{T/T_0}$. λ_0 and T_0 are shown in Eq. (37). With a rough estimation, $\lambda_0 \sim 0.5a$ and $T_0 \sim 0.5$ K when $\eta \sim \omega_{l,c} = 4.6$ MHz and $a = 8.9$ μm .

The transition time τ_c is the criterion that is used to distinguish the stable area and unstable area. An ion in the stable area will become a part of zigzag that is led by one kicked ion when the off-axis action caused by this kicked ion arrives. Hence, statistically speaking, the ions in the region that the off-axis action can propagate to in the interval time τ_c will all become the parts of the zigzag structure led by this kicked ion, and other ions out of this region will produce new kicked ions and might lead to a new structure with opposite orientation. The boundaries among the zigzag structures with different orientations form defects. The number of defects therefore can be determined by the reciprocal of the propagation length ξ_c in the interval time τ_c ,

$$N_d = \frac{L}{\xi_c} = L \left(\int_0^{\tau_c} v_p dt \right)^{-1}. \quad (50)$$

L is the length of the ion chain. In this way, the density of kinks ρ_d can be defined as the linear density of the number of kinks

$$\rho_d = \frac{N_d}{L} = \frac{1}{\xi_c} = \left(\int_0^{\tau_c} v_p dt \right)^{-1}. \quad (51)$$

This equation holds not only under linear quenching but also under nonlinear quenching in the homogeneous ion chain. For the linear quenching or the nonlinear quenching with power exponent driving rate,

$$v_p = \frac{\xi}{\tau} = \begin{cases} \frac{\omega_d a \delta}{0.6\eta} \propto t^\alpha & \text{if } \eta \gg \delta \\ \frac{\sqrt{2}\omega_d a}{1.2} \propto t^0 & \text{if } \eta \ll \delta \end{cases} \Rightarrow \rho_d \propto \xi (\tau_c)^{-1}. \quad (52)$$

It is the definition that was used in the KZ mechanism [2,11,23,47,48], in which the defect density is defined as the quantity that is inversely proportional to the healing length $\xi(\hat{t})$. This also explains why a system can exhibit the scaling law described by the KZ mechanism under the nonlinear quenching with power exponent driving rate, but not under other nonlinear quenching conditions.

For the inhomogeneous structure, the definition of ρ_d should be revised as

$$\rho_d = \frac{1}{\bar{\xi}}, \quad (53)$$

where

$$\bar{\xi} = \frac{1}{N_d} \sum_{i=1}^{N_d} \xi_{c_i} = \frac{1}{N_d} \sum_{i=1}^{N_d} \int_0^{\tau_{c_i}} v_{p_i}(x(t), t) dt. \quad (54)$$

v_{p_i} denotes the velocity of the i th domain. In the inhomogeneous structure, the velocity is no longer constant with the change of ion site, and moreover, the critical frequency of the different region is also no longer the same. These make it difficult for us to determine the transition time τ_{c_i} and propagation region ξ_{c_i} . We may need to use partial differential equations to compute these two values.

At last, to ensure the validity of the criteria in Eq. (43), we numerically determine the ratio between σ_l and $\langle r_l \rangle$ for the formation of kinks as shown in Fig 4(d). Each point in this figure is obtained through 15 000 phase transition cycles, and the final values $\sigma_l, \langle r_l \rangle$ are the average of these cycles in which the kink appears on the l th site [the l in Fig. 4(d) is 6]. Using linear quench, we find that the ratio between them is 1.38, nearing $\sqrt{2}$, which is consistent with the criteria shown in Eq. (43).

VI. CONCLUSION

To conclude, in this work, we present a microscopic model to understand the density of defects in the trapped ions after quenching. We find that without stochastic force, after one atom is kicked out from the one-dimensional chain, its influence will propagate away from this atom, affecting the other ions one by one, gradually forming a perfect zigzag chain. This kicked-off ion, which is formed by the competition between these ions with thermal motion, acts as a ‘‘nucleation’’ that triggers the structure phase. Stochastic force plays an important role that forms the nucleation but at the same time is also a chief culprit that brings the defects in. The motion of one ion will become unpredictable if its diffusion radius $\langle \sigma_l \rangle_T$ is far more than its absolute transverse displacement $|\langle r_l(t) \rangle_T|$, causing the disorder kink stochastically. The transition time τ_c deduced by the relation between $\langle \sigma_l \rangle_T$ and $\langle r_l \rangle_T$ is an important quantity to understand the dynamics of the quenching ion chain. After crossing the critical point, ions can keep stable around the axis line in the time interval τ_c and then are far away from the axis line with exponential growing velocity.

In this article, we get the correlation length and relaxation time using a correlation function from our model and show an important criteria to determine the transition time. This criteria is tested to be effective through simulations in this work. The propagation velocity which is different from sound velocity is found in this work. Based on these, we find the method to calculate the density of defects in ion trap. This definition agrees well with the formula that is used in Kibble-Zurek mechanism for homogeneous structures, but is more selective when facing different kinds of structures. This work provides a mechanism for the formation of defects under the zigzag transformation in trapped ions, and explains qualitatively the role of stochastic force, friction, and temperatures on the formation of kinks. It is worth noting that, although the system we discussed in this article is the trapped-ion chain, the main results from our work can be expected to be extended to other condensed matter systems because they are based on the interaction Langevin equation. This work will provide an inspiration and direction for us to generalize the Kibble-Zurek mechanism.

ACKNOWLEDGMENTS

We appreciate Ming Gong for valuable discussion and this work is supported by the fund of science and technology of Hunan Province (Grant No. 2017JJ3062).

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