

Divergent Stiffness of One-Dimensional Growing Interfaces

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When a spatially localized stress is applied to a growing one-dimensional interface, the interface deforms. This deformation is described by the effective surface tension representing the stiffness of the interface. We present that the stiffness exhibits divergent behavior in the large system size limit for a growing interface with thermal noise, which has never been observed for equilibrium interfaces. Furthermore, by connecting the effective surface tension with a space-time correlation function, we elucidate the mechanism that anomalous dynamical fluctuations lead to divergent stiffness.

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Introduction.—The statistical behavior of many-interacting elements out of equilibrium has attracted attention for a wide range of systems [1–3]. A remarkable feature of such systems is that the standard relations in equilibrium systems no longer hold. For example, phase order in two dimensions is not observed for equilibrium systems at finite temperatures [4,5], while it emerges for active matters [6] or sheared systems [7]. The particular nature of out-of-equilibrium systems is not limited to phase transition problems. The phenomenon we study in this Letter is the singular response against a perturbation.

In studying response properties of equilibrium systems, the fluctuation response relation is useful. That is, the static response against a perturbation is connected to static fluctuation properties in the system without perturbation. As a result of this relation, the response is found to be finite except for phase transition points because static fluctuations are normal in general. In contrast, the static response against a perturbation imposed to a nonequilibrium steady state is not determined by static fluctuation properties. Although several expressions of the static response for out-of-equilibrium systems have been proposed [8–13] and experimentally studied [14–16] for the last two decades, the most primitive method is to consider the time evolution of the perturbation [17–19]. This means that the dynamic properties of fluctuations influence the static response if there is no special property such as a detailed balance condition. Therefore, a singular response behavior can be observed without tuning system conditions.

To demonstrate the singular response of many interacting elements out of equilibrium, we specifically study a one-dimensional interface, whose height is defined in $0 \leq x \leq L$. The interface deforms when a localized stress is applied. For equilibrium interfaces [20], which do not grow but fluctuate in an equilibrium environment, their mean profile in the linear response regime is expressed by a quadratic function of x , where its curvature is determined by the surface tension κ . Now, let us consider growing

interfaces [21]. We can numerically confirm that the deformation against the weak localized stress is still described by a quadratic function of x . In this case, the curvature of the interface is characterized by the effective surface tension κ_{eff} . We then find that κ_{eff} diverges as $L \rightarrow \infty$. In other words, growing interfaces exhibit divergent stiffness.

We attempt to explore the mechanism of the divergent stiffness by formulating a fluctuation-response relation. This problem is reminiscent of the standard linear response theory around an equilibrium state. For example, when considering heat conduction for a Hamiltonian system in contact with two heat baths with temperatures T_1 and T_2 , $T_2 - T_1$ is treated as a perturbation [22]. In this case, the linear response formula is the Green-Kubo formula, which expresses the conductivity in terms of the time integration of the current correlation function at equilibrium [19]. Similarly to heat conduction, we expect that the effective surface tension κ_{eff} can be expressed as the time integration of a certain time correlation function. In this Letter, we derive such a formula using a generalized fluctuation theorem associated with the excess entropy production.

Based on the response formula, we study the divergent stiffness. As is known, some low-dimensional systems exhibit an anomaly in the large-distance and long-time properties of the time correlation function [22]. In such systems, the decay rate of a time correlation function is so small that its time integration is not bounded in the large system size limit [22–24]. By combining this property with the response formula, the mechanism of the divergent stiffness is understood. We emphasize that the method we propose in this Letter can be applied to other spatially extended systems out of equilibrium.

Setup.—The one-dimensional interface defined in $0 \leq x \leq L$ is investigated. The height of the interface at time t is expressed by $h(x, t)$, which is collectively denoted by $\hat{h} = (h(x))_{x=0}^L$. For simplicity, the periodic boundary condition $h(0, t) = h(L, t)$ is assumed. An external stress

$\epsilon p_{\text{ex}}(x)$ is imposed on the interface, where the total force $\epsilon \int p_{\text{ex}}(x) dx$ is set to zero to avoid the additional drift of the interface. We first study an equilibrium interface. The free energy of the interface is assumed to be

$$F^\epsilon(\hat{h}) \equiv \int_0^L dx \left[\frac{\kappa}{2} (\partial_x \hat{h})^2 - \epsilon p_{\text{ex}}(x) \hat{h}(x) \right], \quad (1)$$

where κ represents the surface tension. The fluctuation properties are described by the following stochastic model [20]:

$$\partial_t h = -\frac{1}{\gamma} \frac{\delta F^\epsilon(\hat{h})}{\delta h} + \sqrt{\frac{2T}{\gamma}} \xi, \quad (2)$$

where γ is the dissipation constant; T is the temperature of the bath with the Boltzmann constant set to unity; ξ is the Gaussian white noise satisfying

$$\langle \xi(x, t) \xi(x', t') \rangle = \delta(x - x') \delta(t - t'). \quad (3)$$

Thus, it is immediately confirmed that the expectation of the interface shape under the external stress is given by

$$\kappa \partial_x^2 \langle h(x) \rangle_{\text{eq}}^\epsilon + \epsilon p_{\text{ex}}(x) = 0, \quad (4)$$

where $\langle \cdot \rangle_{\text{eq}}^\epsilon$ denotes the expectation in the equilibrium state of the system with the external stress $\epsilon p_{\text{ex}}(x)$. For simplicity, focus is placed on the case where $p_{\text{ex}}(x) = \delta(x) - 1/L$. By solving (4) [25], we obtain

$$\langle h(x) - h(0) \rangle_{\text{eq}}^\epsilon = \frac{\epsilon}{2L\kappa} \left[\left(x - \frac{L}{2} \right)^2 - \frac{L^2}{4} \right]. \quad (5)$$

Now, let us consider a growing interface described by

$$\partial_t h = v_0 + \frac{v_0}{2} (\partial_x h)^2 - \frac{1}{\gamma} \frac{\delta F^\epsilon(\hat{h})}{\delta h} + \sqrt{\frac{2T}{\gamma}} \xi, \quad (6)$$

as a generalization of (2), where $v_0 \geq 0$ is the propagation velocity of the flat interface. When $\epsilon = 0$, (6) is equivalent to the Kardar-Parisi-Zhang (KPZ) equation [21], which qualitatively reproduces the dynamics of growing interfaces, such as interfaces in liquid-crystal turbulence [29], slow-combustion fronts in paper [30], and fronts of growing bacterial colony [31]. Because interfaces appear at almost all scales of interest in science [2,32], the KPZ equation has been extensively investigated through numerical [33–39], theoretical [40–46], and even mathematical [47–54] approaches. The system given by (6) is interpreted as a perturbed KPZ equation.

Numerical observation.—Let $\langle h(x) - h(0) \rangle_{\text{ss}}^\epsilon$ be the expectation of $h(x) - h(0)$ with respect to the steady state of (6). As an illustration, first, we numerically investigate

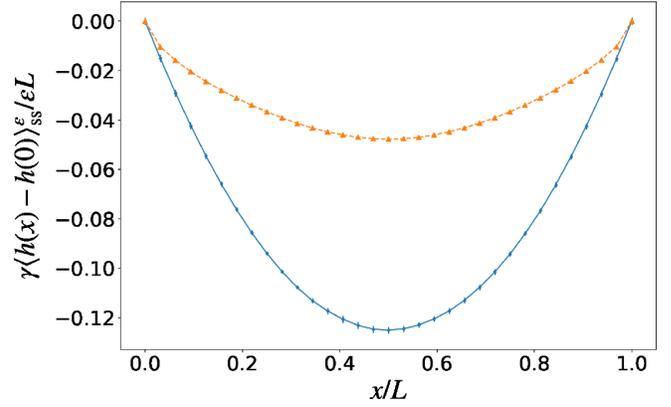


FIG. 1. Time-averaged patterns in steady state under the external stress with $\epsilon/\gamma = 0.01$. The system size is $L = 16$. The curvature of the growing interface ($v_0 = 5$, triangular-orange symbol) is smaller than that of the equilibrium interface ($v_0 = 0$, round-blue symbol). The symbols are joined by lines for visual aid.

$\langle h(x) - h(0) \rangle_{\text{ss}}^\epsilon$ for the specific parameter values $\kappa = T = \gamma = 1$ and $v_0 = 5$. Throughout this Letter, the numerical simulations were conducted using a spatially discretized model with a space interval $\Delta x = 0.5$ [25,35]. More precisely, we define a discrete model and check system size dependence to judge whether it gives a systematic approximation of the KPZ equation. The shapes of the growing interfaces shown in Fig. 2 are fitted to the following form:

$$\langle h(x) - h(0) \rangle_{\text{ss}}^\epsilon = \frac{\epsilon}{2L\kappa_{\text{eff}}} \left[\left(x - \frac{L}{2} \right)^2 - \frac{L^2}{4} \right], \quad (7)$$

which is the generalization of (5) with the replacement of κ by κ_{eff} , where ϵ is assumed to be sufficiently small. The fitting parameter κ_{eff} is interpreted as the effective surface tension characterizing the stiffness of the growing interface. We conjecture that (7) is valid in the limit $\epsilon \rightarrow 0$ because the linear response for the noiseless case is expressed as a quadratic function [25]. Figure 1 shows that κ_{eff} is greater than κ . Furthermore, as shown in Fig. 2, κ_{eff} increases for a larger system size L .

Now, two issues naturally arise. The first issue is quantifying the L dependence of κ_{eff} . From the viewpoint of numerical calculation, however, it becomes harder to accurately observe a slight shift of $\langle h(x) - h(0) \rangle_{\text{ss}}^\epsilon$ caused by the external stress for larger systems. The second issue is to investigate the mechanism of the L dependence. Both issues can be resolved by formulating a fluctuation-response relation for the system under investigation, where κ_{eff} is expressed by dynamical properties of fluctuations in a system without the external stress.

Response formula.—Let $[\hat{h}]$ be a trajectory $(\hat{h}(t))_{t=0}^\tau$. We consider any quantity $A([\hat{h}])$ satisfying $A([\hat{h} + \hat{c}]) = A([\hat{h}])$, where \hat{c} is a constant function in x . For such $A([\hat{h}])$, we

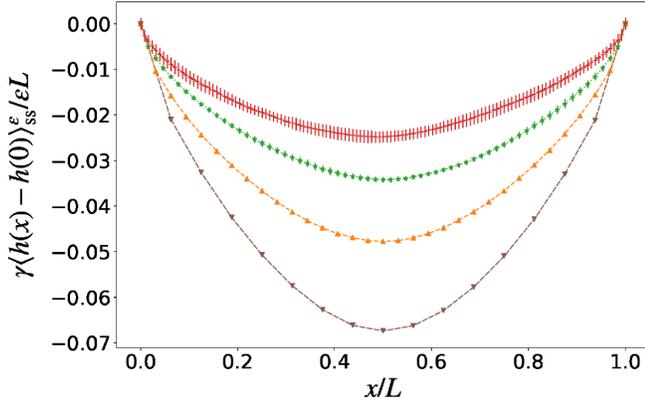


FIG. 2. System size dependence of the curve for $v_0 = 5$ in Fig. 1. The patterns of $L = 8, 16, 32,$ and 64 are shown from bottom to top. The symbols are joined by lines for visual aid. Although the equilibrium ($v_0 = 0$) interface does not depend on L , the growing interface becomes stiffer for larger L .

define A^* as $A^*([\hat{h}]) \equiv A([\hat{h}]^*)$ with $[\hat{h}]^* \equiv (\hat{h}(\tau - t))_{t=0}^\tau$, which represents the time-reversal of $[\hat{h}]$. For equilibrium cases $v_0 = 0$, the detailed balance condition $\langle A \rangle_{\text{eq}}^\epsilon = \langle A^* \rangle_{\text{eq}}^\epsilon$ holds for any ϵ , and the stationary distribution is given by

$$P_{\text{eq}}^\epsilon(h) = \frac{1}{Z} \exp(-\beta F^\epsilon(h)) \quad (8)$$

with $\beta = T^{-1}$. This also leads to (4).

For growing interfaces with $v_0 > 0$, the detailed balance condition does not hold. The extent of the violation is expressed by the entropy production

$$\sigma = \frac{\gamma}{T} \int_0^\tau dt \int_0^L dx (\partial_t h) \left(v_0 + \frac{v_0}{2} (\partial_x h)^2 \right), \quad (9)$$

which is the work done by the nonconservative force divided by the temperature. Using this thermodynamic entropy production, we arrive at the standard fluctuation theorem [25]

$$\langle A \rangle_{\text{tr}}^I = \langle A^* e^{-\sigma} \rangle_{\text{tr}}^I, \quad (10)$$

where $\langle \cdot \rangle_{\text{tr}}^I$ denotes the ensemble average over noise realizations and the initial conditions sampled from the stationary distribution with $v_0 = 0$. This relation holds for a wide range of driven systems in contact with a heat bath [55–58]. However, (10) is not useful to obtain the linear response property around the state with $v_0 \neq 0$ and $\epsilon = 0$.

Here, we notice another time-reversal transformation $[\hat{h}] \rightarrow [\hat{h}]^\dagger \equiv (-\hat{h}(\tau - t))_{t=0}^\tau$ such that $\langle A \rangle_{\text{ss}}^0 = \langle A^\dagger \rangle_{\text{ss}}^0$ holds for $A^\dagger([\hat{h}]) \equiv A([\hat{h}]^\dagger)$ [23,25]. However, this time-reversal symmetry is violated for interfaces under the external stress $\epsilon > 0$. Then, following the standard procedure for the fluctuation theorem [58], we calculate the ratio of path

probabilities of $[\hat{h}]$ and $[\hat{h}]^\dagger$ and take the logarithm of the result to obtain

$$\tilde{\sigma} \equiv -\frac{\epsilon \kappa}{\gamma T} \int_0^\tau dt \int_0^L dx p_{\text{ex}}(x) \frac{\partial^2 h(x, t)}{\partial x^2}, \quad (11)$$

which characterizes the violation of the symmetry associated with the time-reversal transformation $[\hat{h}] \rightarrow [\hat{h}]^\dagger$. Indeed, we can show a generalized fluctuation theorem

$$\langle A \rangle_{\text{tr}}^{II} = \langle A^\dagger e^{-\tilde{\sigma}} \rangle_{\text{tr}}^{II}, \quad (12)$$

where $\langle \cdot \rangle_{\text{tr}}^{II}$ denotes the ensemble average over the noise realizations and initial conditions sampled from the stationary distribution without the external stress. Note that $\tilde{\sigma}$ is not the thermodynamic entropy production, but interpreted as an excess entropy production that appears only when the external stress is imposed [59].

Here, we set $A = h(x, \tau) - h(0, \tau)$, substitute it into (12), take the limit $\tau \rightarrow \infty$, and expand the right-hand side of (12) in ϵ . Noting that $\langle A \rangle_{\text{tr}}^{II}$ goes to $\langle h(x) - h(0) \rangle_{\text{ss}}^\epsilon$, we obtain [25]

$$\lim_{\epsilon \rightarrow 0} \frac{\langle h(x) - h(0) \rangle_{\text{ss}}^\epsilon}{\epsilon} = \frac{\kappa}{\gamma T} \int_0^\infty dt (C(x, t) - C(0, t)) \quad (13)$$

with

$$C(x, t) \equiv \langle \partial_x h(x, 0) \partial_x h(0, t) \rangle_{\text{ss}}^0. \quad (14)$$

This relation is interpreted as the fluctuation-response relation of the system under investigation. Equation (13) is understood from the fluctuation-dissipation theorem for classical stochastic processes [60–62]. However, to our best knowledge, an explicit formula connecting the response to an external perturbation has never been proposed to date. We numerically check the validity of (13) for small systems with $L = 2, 4, 8,$ and 16 . In Fig. 3, the left-hand side of (13) is plotted against the right-hand side of (13) at $x = L/2$ for both cases of $v_0 = 0$ and $v_0 = 5$. The result confirms that (13) holds.

Divergent stiffness.—As explained above, the numerical calculation of κ_{eff} defined by (7) is not easy to carry out for large systems. Thus, using the response formula (13), we study the stiffness of the growing interface. Specifically, from (7) and (13), we obtain

$$\kappa_{\text{eff}} = -\frac{\gamma T L}{8\kappa} \left\{ \int_0^\infty dt \left[C\left(\frac{L}{2}, t\right) - C(0, t) \right] \right\}^{-1}. \quad (15)$$

By dimensional analysis, we find that $\kappa_{\text{eff}}/\kappa$ is expressed as a function of L/L_0 with

$$L_0 = \frac{\ell \kappa^3}{T \gamma^2 v_0^2}, \quad (16)$$

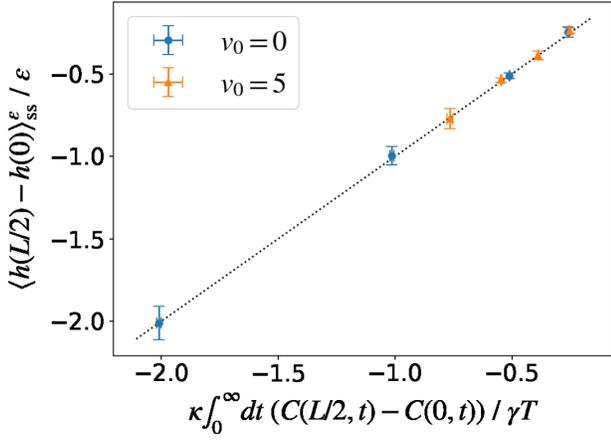


FIG. 3. Comparison of the left-hand side and the right-hand side of (13). The former is estimated by the direct calculation of the response for $\epsilon > 0$, while the latter is calculated in the system with $\epsilon = 0$. The round-blue and triangular-orange symbols represent the data for $v_0 = 0$ ($L = 2, 4, 8, 16$) and $v_0 = 5$ ($L = 2, 4, 8, 16$), respectively. These symbols should be on the dotted line if the left and right-hand sides of (13) are equal.

where ℓ is a numerical constant corresponding to the dimensionless length characterizing the crossover [25]. In other words, the following equation is obtained using a scaling function f whose form has not been determined yet:

$$\kappa_{\text{eff}} = \kappa f\left(\frac{L}{L_0}\right). \quad (17)$$

First, we notice that $\kappa_{\text{eff}} \rightarrow \kappa$ as $L_0 \rightarrow \infty$, because $v_0 \rightarrow 0$ refers to the equilibrium limit. To find the functional form of f , the right-hand side of (15) is numerically calculated for several values of L and v_0 for fixed $\kappa = T = \gamma = 1$. The numerical results are plotted in Fig. 4, such that the following equation holds for $L \gg L_0$:

$$\kappa_{\text{eff}} = \kappa \left(\frac{L}{L_0}\right)^{1/2}, \quad (18)$$

as indicated by the dotted line in Fig. 4. Here, the value of ℓ is numerically estimated as $\ell = 60$. It is found that the data points for $L \geq 16$ are on one curve, which determines the form of the scaling function f . Note that those for $L \leq 8$, which are not shown in Fig. 4, deviate from the curve [25]. This means that the discretized equation used for the numerical calculation is no longer a good approximation of the KPZ equation when $L \leq 8$. From Fig. 4, it is concluded that L_0 with $\ell \simeq 60$ provides the cross-over length from the normal response to the singular response, where the stiffness κ_{eff} shows the divergence as a function of L/L_0 , which is the main result of this Letter.

The divergent stiffness comes from a dynamical singularity of the correlation function $C(x, t)$, as suggested in the

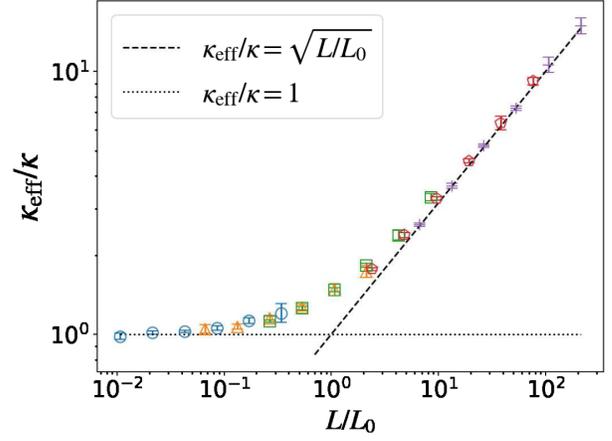


FIG. 4. System size dependence of κ_{eff} . The symbols are the numerical results for $L = 16, 32, 64, 128, 256$, and 512 for $v_0 = 0.2, 0.5, 1, 3$, and 5 from left to right (difference in symbols represents the difference in v_0). κ_{eff} maintains the same value as κ for $L \ll L_0$ and diverges as $(L/L_0)^{1/2}$ for $L \gg L_0$.

formula expressed by (15). The relation is explained in detail. Let $\tilde{C}(k, t)$ be the Fourier transform of $C(x, t)$. By dimensional analysis, we have

$$\int_0^\infty dt \tilde{C}(k, t) = \frac{\gamma T}{\kappa^2 k^2} \Phi\left(\frac{k \kappa^3}{T \gamma^2 v_0^2}\right), \quad (19)$$

where the prefactor is the equilibrium form and the non-equilibrium correction is expressed in terms of a dimensionless scaling function Φ . Now, let us consider the case $L \rightarrow \infty$ with fixed $v_0 \neq 0$. As is known, $\tilde{C}(k, t)$ has the scaling form $g(k^z t)$ in the limit $L \rightarrow \infty$, where the dynamical exponent z is given by $z = 3/2$ [21,23]. Assuming that the scaling part of $\tilde{C}(k, t)$ is dominant for the evaluation of κ_{eff} , we substitute the scaling form into the left-hand side of (19). We then obtain [25]

$$\Phi\left(\frac{k \kappa^3}{T \gamma^2 v_0^2}\right) = c \left(\frac{|k| \kappa^3}{T \gamma^2 v_0^2}\right)^{1/2}, \quad (20)$$

where the numerical constant c is calculated as $c = 2.43$ by the analysis of an exactly solvable stochastic model [44]. For finite but large L cases, it is assumed that (20) holds with the replacement of k by $k_n = 2\pi n/L$, where n is an integer satisfying $-n_c \leq n \leq n_c$. The cutoff integer n_c is given by $n_c = L/(2\Delta x)$. We then calculate [25]

$$\begin{aligned} & \int_0^\infty dt [C(L/2, t) - C(0, t)] \\ &= -\sqrt{L} \left(\frac{16c^2}{8\pi^3}\right)^{1/2} \left(\frac{T}{\kappa v_0^2}\right)^{1/2} \sum_{n=1}^{n_c/2} \frac{1}{(2n-1)^{3/2}}. \end{aligned} \quad (21)$$

By substituting (21) into (15), $\kappa_{\text{eff}} = \kappa(L/L_0^{\text{est}})^{1/2}$ holds with $L_0^{\text{est}} = \ell^{\text{est}}\kappa^3/(T\gamma^2v_0^2)$, where the numerical constant ℓ^{est} is given as

$$\ell^{\text{est}} = \frac{(32c)^2}{(2\pi)^3} \left(\sum_{n=1}^{n_c/2} \frac{1}{(2n-1)^{3/2}} \right)^2. \quad (22)$$

Therefore, the divergent stiffness arises from the singularity expressed by (20). The \sqrt{L} dependence of κ_{eff} corresponds to the $k^{3/2}$ dependence of $\int_0^\infty dt \tilde{C}(k, t)$. The crossover length L_0 observed in the numerical simulations is predictable by considering the asymptotic form of $\int_0^\infty dt \tilde{C}(k, t)$. Indeed, the value $\ell \simeq 60$ obtained by the numerical simulations is consistent with (22). For example, $\ell^{\text{est}} = 62.5$ for $n_c = 128$. When investigating infinitely large systems, the limit $n_c \rightarrow \infty$ should be taken. In this case, ℓ^{est} approaches 69.52 [25].

Concluding remarks.—In this Letter, the response formula (15) expressing the effective surface tension is formulated in terms of the time correlation function $C(x, t)$ of $\partial_x h(x, t)$. Then, it is shown that the divergent stiffness comes from the dynamical singularity expressed by (20).

The stochastic dynamics of the interface can be observed in a much wider context [63]. Keeping the universality in mind, we study the KPZ equation

$$\partial_t h = \frac{\lambda}{2} (\partial_x h)^2 + \nu \partial_x^2 h + \sqrt{2D} \xi \quad (23)$$

defined in $0 \leq x \leq L$, where the standard parameters ν , D , and λ are introduced. By adding a localized force, ν_{eff} instead of κ_{eff} can be operationally defined through (7). Our formula (16) with replacements $\kappa/\gamma \rightarrow \nu$, $v_0 \rightarrow \lambda$, and $T/\gamma \rightarrow D$ can be used to estimate ν , D , and λ when there exists a phenomenon that may be effectively described by the KPZ equation. Specifically, one can estimate $\nu^3/(D\lambda^2)$ by observing crossover length of ν_{eff} . From the fluctuation spectrum of $\partial_x h$, D/ν is determined. The parameter λ is determined from the average propagation velocity. These three data lead to ν , D , and λ . For example, putting oil on boundaries of an interface in combustion of paper [30], we can study a response property. Since the system is described by the model in this Letter, the parameter values of the KPZ equation will be determined by using the method above.

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