

Universality in dynamical phase transitions of diffusive systems

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Universality, where microscopic details become irrelevant, takes place in thermodynamic phase transitions. The universality is captured by a singular scaling function of the thermodynamic variables, where the scaling exponents are determined by symmetries and dimensionality only. Universality can persist even for nonequilibrium phase transitions. It implies that a hydrodynamic approach can capture the singular universal scaling function, even far from equilibrium. In particular, we show these results for phase transitions in the large deviation function of the current in diffusive systems with particle-hole symmetry. For such systems, we find the scaling exponents of the universal function and show they are independent of microscopic details as well as boundary conditions.

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I. INTRODUCTION

A longstanding goal in the study of nonequilibrium is to generalize and implement the vast knowledge accumulated in the study of thermodynamic phase transitions [1–3]. In equilibrium, the relevant thermodynamic potential, e.g., the free energy, becomes nonanalytic at the transition point. For a continuous phase transition, the thermodynamic potential is composed of a regular part and a singular universal part—a scaling function of the relevant thermodynamic variables. The scaling function is characterized by critical exponents, which in turn classify the physics into universality classes that depend only on the symmetry and dimensionality of the model.

Nonequilibrium systems are generally sensitive to microscopic details, boundary conditions, and initial conditions. Therefore, it is appealing to find where universality can take over in nonequilibrium systems, from both a theoretical and a practical viewpoint. If universality takes over, it is tempting to assume that a coarse-grained (hydrodynamic) theory can capture the singular universal behavior. The purpose of this paper is to show that this is indeed the case for an analytically tractable setup.

It was suggested long ago to build a thermodynamic formalism for nonequilibrium systems by looking at probabilities over time realizations rather than looking at the instantaneous energy states [4]. To illustrate this idea, let us consider two particle reservoirs, coupled through a 1D transport channel of size L —a common nonequilibrium setup. The hallmark of nonequilibrium in such systems is a nonvanishing current. For this reason, a natural quantity of interest is $P_t(Q)$, the

probability to observe a transfer of Q particles in the system during the time interval $[0, t]$. For $t \gg 1$, the probability to observe an atypical particle transfer, i.e., different than the steady state, is usually exponentially unlikely. Thus, the large deviation function (LDF) is defined by the function $I(J) = -\frac{1}{t} \log P_t(Q)$ for $J = Q/t$ —the atypical mean current. Starting from the discovery of fluctuation theorems in the 1990s [5,6], LDFs have played an important role in the modern development of nonequilibrium theories [7]. Since the LDF constrains the system to exhibit a mean atypical current J , we can define an associated mean spatiotemporal particle occupancy in the system, where the mean is over all spatiotemporal evolutions that support the particle transfer Q [8].

Similarly to thermodynamic phase transitions, dynamical phase transitions (DPTs) are defined as nonanalytic points in the LDF. A variety of DPTs are identified in a broad range of nonequilibrium systems, such as in high-dimensional chaotic chains [9–11], kinetically constrained glass models [12–18] or active self-propelled particles [19–21]. The transition is manifest in, e.g., a dramatic change in the mean spatiotemporal particle occupancy [22–27]. In this paper, we especially consider 1D diffusive processes that are symmetric to the exchange of particles and vacancies. In this case, it is known that the observed particle occupancy becomes independent of both space and time in a range determined by the critical value J_c [23–27]. We show that the singular part of the LDF is universal, irrespective of microscopic details and boundary conditions. Namely $I(J) = I_{\text{reg}} + I_{\text{sing}}$, where

$$I_{\text{sing}} = \frac{1}{L^{2+\alpha}} \phi(\delta u L^\beta), \quad (1)$$

such that δu is a universal parameter that vanishes as $J \rightarrow J_c$.

To exhibit the universality and find the scaling exponents α, β , we employ analytical tools as well as corroborating results using numerical analysis. First, we use the macroscopic

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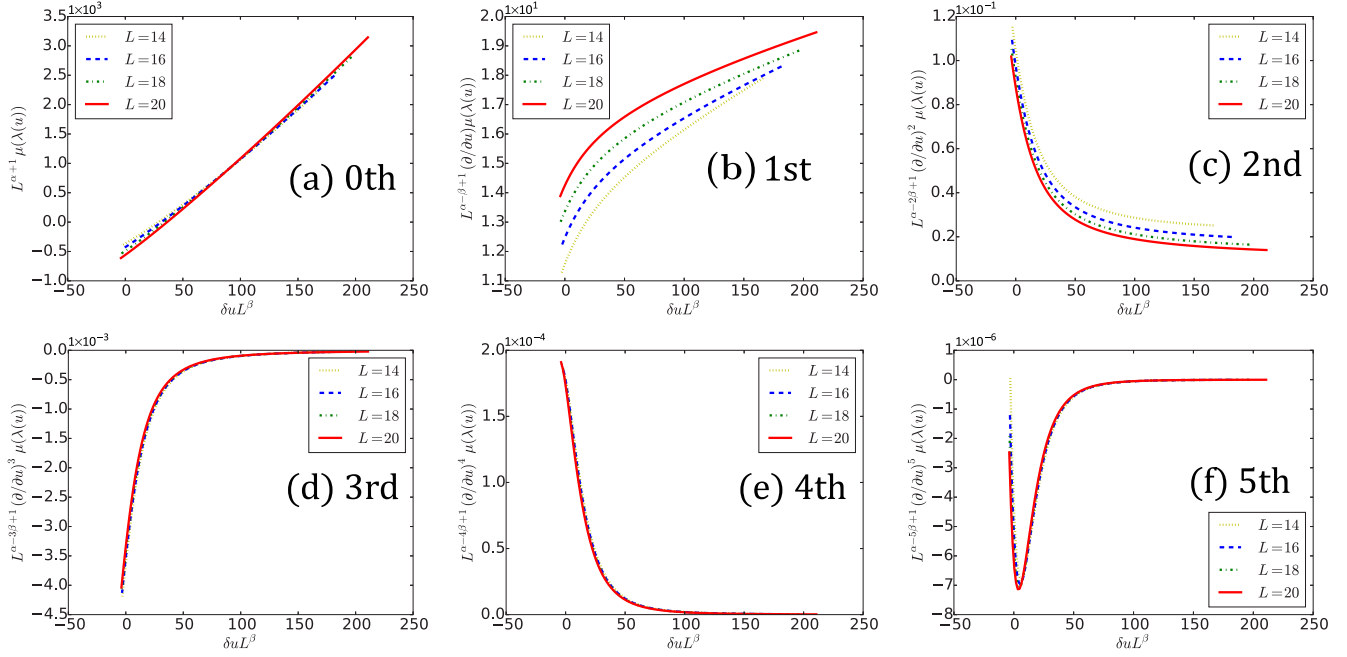


FIG. 1. The d th derivative with respect to the universal parameter u of the cumulant generating function $\mu(\lambda)$ and a proper rescaling with $L^{\alpha-d\beta}$ as a function of $\delta u L^\beta$ is plotted for the weakly asymmetric exclusion process (WASEP) on a ring [41–43]. The cumulant generating function $\mu(\lambda)$, as defined in the text, is a Legendre-Fenchel transform of the LDF and carries the same scaling behavior for the singular term. For the third derivative, the universal function becomes dominant over the nonuniversal part even for a relatively small system size L . The convergence to a scaling function $\tilde{\phi}(r)$ is convincing already for small systems $L = 14, 16, 18, 20$ with $\alpha = 1/3$, $\beta = 2/3$ for the $d = 3$ derivative. As mentioned in Sec. VII, the singular point $r = 0$ may be shifted, especially for small systems. In the WASEP, as detailed in Appendix A, each site is occupied by at most one particle. Particles hop to a left or right empty neighbor with a $\exp(1 \pm E/L)$ rate, where we take here $E = 10$. To get this figure, we diagonalize the corresponding biased matrix [50,51] numerically. See Sec. VII for more details.

fluctuation theory (MFT). The MFT is a hydrodynamic theory of diffusive systems. It was used to obtain various results, e.g., current fluctuations, nonequilibrium fluctuation induced forces, escape times of interacting particles, statistics of tagged particles in single-file diffusion [28–35], and many more [36–40]. The predictions are exact, up to $1/L$ corrections. The second approach relies on an exact solution of a microscopic model—the simple symmetric exclusion process (SSEP) [41–43] via the Bethe ansatz. The Bethe ansatz allows to determine the energy eigenstates of many-body integrable quantum systems [44] as well as evaluating current statistics of nonequilibrium systems [45–47]. The SSEP is an important model in the study of classical and quantum nonequilibrium systems [32,46,48,49]. By using both methods, we evaluate $1/L^2$ corrections. Close to the transition, the leading singular behavior allows to obtain the scaling exponents α, β . The singular term in the LDF is subleading. However, it becomes more dominant for higher and higher derivatives of the LDF with respect to $J_C - J$ (equivalently δu). Then, as shown in Fig. 1, the third derivative is sufficient to capture the universal behavior.

II. THE MACROSCOPIC FLUCTUATION THEORY

To unveil the universal structure of DPTs in nonequilibrium diffusive systems, we introduce the MFT. Taking the limit $t, L \rightarrow \infty$ with the fixed diffusive scaling t/L^2 , we define rescaled coordinates: $\tau = t/L^2$ and $x \in [0, 1]$. At these

scales, the coarse-grained density $\rho(x, \tau)$ is assumed to be a smoothly varying function. Here, we focus only on processes that conserve particles at the bulk. The current density $j(x, \tau)$ allows us to write the continuity equation,

$$\partial_\tau \rho = -\partial_x j. \quad (2)$$

At the steady state, diffusive processes satisfy Fick’s law $j = \mathfrak{J}(\rho)$, where $\mathfrak{J}(\rho) = -D(\rho)\partial_x \rho + \sigma(\rho)E$. For a vanishing field E , Fick’s law in Eq. (2) gives the steady-state diffusion equation with D the diffusion. The conductivity σ is a measure of the response to an external field E . Generally, D, σ are density-dependent.

The fluctuating hydrodynamics approach posits that Fick’s law can be extended to a dynamical Langevin equation,

$$j(x, \tau) = \mathfrak{J}[\rho(x, \tau)] + \sqrt{\frac{\sigma[\rho(x, \tau)]}{L}} \xi(x, \tau), \quad (3)$$

where $\xi(x, \tau)$ is a Gaussian white noise. The strength of the noise in diffusive systems $\sqrt{\sigma/L}$ is tuned to be consistent with the Einstein relation [43]. The dynamics of diffusive systems is thus expressed through D and σ only.

From the Langevin Eq. (3) and by using the Martin-Siggia-Rose formalism [52], the fundamental result of the MFT is derived. Namely, we find that the probability to observe a history $\{\rho, j\}$ of the system during time $[0, T = t/L^2]$ is

given by

$$\mathcal{P}(\{\rho, j\}) \sim \exp[-L \mathcal{I}_{[0,T]}(\rho, j)],$$

$$\mathcal{I}_{[0,T]}(\rho, j) = \int_0^1 dx \int_0^T d\tau \frac{(j + D\partial_x \rho - \sigma E)^2}{2\sigma}, \quad (4)$$

where the continuity equation is implicitly assumed. The MFT becomes exact for $L \rightarrow \infty$. Indeed, trying to extract microscopic details from a hydrodynamic theory is usually an ill fated attempt. Notice that any observable obtained through Eq. (4) will be dominated by the saddle-point since L is large.

It is convenient to define the rescaled LDF $\Phi(J) = LI(J)$, so that Φ is L independent to leading order. Then, using the MFT to calculate the LDF of diffusive systems boils down to solving the minimization problem,

$$\Phi(J) = \frac{1}{T} \min_{j, \rho} \mathcal{I}_{[0,T]}(\rho, j), \quad (5)$$

where $\{\rho, j\}$ satisfy the continuity Eq. (2) and the macroscopic particle transfer $Q = L^2 \int dx d\tau j$ for a large diffusive time $T \gg 1$ [53]. Since we consider nonequilibrium processes, boundary conditions usually strongly impact the results. Here, we consider periodic boundary conditions and boundary driven processes—where the system is coupled to two particle reservoirs with densities $\rho_{l,r}$, respectively. The reservoirs' state is assumed to be unaffected by the interaction with the system. For a periodic system, the integrated number of particles is conserved. Therefore, one requires that $\int dx \rho(x, \tau)$ is fixed for any τ . Moreover, $\rho(x=0, \tau) = \rho(x=1, \tau)$. For boundary driven processes, $\rho(x = \{0, 1\}, \tau)$ is fixed to the boundary values $\rho_{l,r}$.

III. DYNAMICAL PHASE TRANSITIONS

Finding a solution to Eq. (5) is hard even for simple models. It requires solving a partial differential nonlinear problem with constraints. In Ref. [33], it was conjectured that the optimal density profile in current fluctuations is time-independent, which is the so-called additivity principle. For 1D systems, it implies $j(x, \tau) = J$, $\rho(x, \tau) = \rho(x)$. The particle transfer and continuity constraints are relaxed and the variational principle Eq. (4) is simplified to

$$\Phi_{\text{AP}}(J) = \min_{\rho(x)} \int dx \frac{(J + D\partial_x \rho - \sigma E)^2}{2\sigma}. \quad (6)$$

This is clearly a significant improvement, as the solution of Eq. (6) requires solving a nonlinear ordinary differential equation [22,33,54]. See Refs. [22,55,56] for discussions on the validity of the additivity principle. However, even for a time-independent density profile, the solution need not be unique which will usually give rise to a DPT. For periodic systems, translational symmetry suggests a spatial invariant density profile so that $\rho(x) \rightarrow \rho$, which fixes the solution. This constant solution can be overtaken by a traveling wave solution as was shown in Refs. [23,24,57], amounting again to a DPT.

IV. FINITE-SIZE CORRECTIONS

From now on, we focus only on models with dynamics that satisfy particle-hole symmetry. This implies that odd

derivatives of D, σ with respect to ρ vanish at $\rho = 1/2$. The solution of the LDF to Eq. (6) of periodic boundary conditions with mean density $\rho = 1/2$ as well as a boundary driven process with $\rho_{l,r} = 1/2$ clearly bears a special symmetry. Assuming the additivity principle, the constant density solution $\rho(x) = 1/2$ is a solution for any J which results in $\Phi_{\text{AP}}(J) = J^2/2\sigma$. From here on out, D, σ and their derivatives are always evaluated at $\rho = 1/2$. Taking small fluctuations around this solution, namely $\rho(x, t) \rightarrow 1/2 + \delta\rho$ and $j(x, t) \rightarrow J + \delta j$, allows us to explore the finite-size corrections and whether the solution is indeed optimal. Note that $\delta\rho, \delta j$ have to satisfy the continuity equation and the integrated current constraint. For a boundary driven case the fluctuations can be recast using the Fourier representation,

$$\delta\rho = \frac{1}{2} \sum_{k, \omega} k \sin(kx) (a_{k, \omega} e^{i\omega\tau} + a_{k, \omega}^* e^{-i\omega\tau}),$$

$$\delta j = \frac{1}{2} \sum_{k, \omega} i\omega \cos(kx) (a_{k, \omega} e^{i\omega\tau} - a_{k, \omega}^* e^{-i\omega\tau}), \quad (7)$$

where $k = \pi n$ and $\omega = \frac{2\pi}{T} m$ for $n, m \in \mathbb{Z}$. Moreover, $a_{k, \omega}^* = a_{k, -\omega}$ and $a_{-k, \omega} = a_{k, \omega}$. We remark that the k, ω values have a finite cutoff of the order $|k| \sim L$ and $|\omega| \sim L^2$ for the hydrodynamic theory to be valid. Let us keep that in mind, and set these cutoffs by $k_{\text{max}}, \omega_{\text{max}}$ (for periodic boundary condition a slightly different representation is required, see Ref. [23]).

To find $\Delta\Phi \equiv \Phi - \Phi_{\text{AP}}$, we rescale $a_{k, \omega} \rightarrow a_{k, \omega}/\sqrt{L}$ and obtain a perturbative Landau-like theory as

$$\Delta\Phi = -\frac{1}{TL} \log \prod_{k \geq 0, \omega \geq 0} \int d^2 a_{k, \omega} e^{-\int dx d\tau \sum_{j \geq 2} \frac{S_j}{L^{1-j/2}}}, \quad (8)$$

with the Gaussian term $S_2 = \sum_{k, \omega} f(k, \omega) |a_{k, \omega}|^2$ such that $f = \frac{\omega^2}{2\sigma} + \frac{D^2}{2\sigma} k^2 (k^2 - 2u)$ with $u = \epsilon \frac{J^2 - E^2 \sigma^2}{16D^2 \sigma} \sigma''$ and $\epsilon = 4(1)$ for boundary driven (periodic) systems. The higher-order terms S_i , explicitly detailed in Appendix D, were considered here only for the boundary driven case.

Evaluating $\Delta\Phi$ boils down to performing a perturbation theory for Gaussian integrals. Let us define $\Delta\Phi = \sum_{j=1,2,\dots} L^{-j} \Phi_j$. We then find

$$\Phi_1 = dD\mathcal{F}(u) + cJ^2, \quad (9)$$

where c is a constant that depends on the cutoffs and cannot be evaluated from a hydrodynamic theory, $d = \frac{1}{8}(1)$ for boundary driven (periodic) systems and \mathcal{F} is

$$\mathcal{F}(u) = -4 \sum_{n=1,2,\dots} n\pi \sqrt{n^2 \pi^2 - 2u} - n^2 \pi^2 + u, \quad (10)$$

already recovered in this context [23,54,58] as well as others [59,60]. For $u = u^* = \pi^2/2$, $\mathcal{F}(u)$ is nonanalytic and its derivatives diverge. This singularity has been discussed as the onset of a DPT [23,54,58]. It also implies the break down of the perturbation theory close to the transition point (see Appendices B and C), i.e., all the higher-order perturbation coefficients Φ_j diverge at this point. The singular part of the $1/L$ correction is universal—independent of microscopic details and fully captured by the macroscopic D, σ . Therefore,

it is natural to assume that a singular universal function, just like in Eq. (1), emerges from the sum of all the singular corrections. To obtain the scaling exponents α, β , it is sufficient to find the dominant singular behavior of Φ_2 , as shown below.

The $1/L^2$ correction is cumbersome and littered with nonuniversal terms, depending on microscopic details (see Appendix D). Focusing on the leading singular term and defining $\delta u = u^* - u$, we find that

$$\Phi_2 = \frac{15\pi^4(D\sigma'' - 2\sigma D'')}{16D\delta u} + O\left(\frac{1}{\sqrt{\delta u}}\right) \quad (11)$$

as $\delta u \rightarrow 0$. We expect periodic systems to yield a similar leading term. Let us now evaluate the critical exponents.

V. THE SCALING FUNCTION

We have shown that the finite-size corrections diverge at the critical point u^* . For a continuous phase transition, we expect (to leading order)

$$L\Delta\Phi(J) = \frac{1}{L^\alpha}\phi(\delta u L^\beta) + \text{nonuniversal terms}. \quad (12)$$

Here, $\phi(r)$ is the scaling function and the nonuniversal terms are of order 1. From Eqs. (9), (10), and (11), we find that the leading singular term is of the form $\phi_0\sqrt{\delta u} + \frac{\phi_1}{L\delta u} + O(\frac{1}{L^2})$ where $\phi_{0,1}$ are constants. To keep the scaling Eq. (12), we find that $\alpha = \beta/2 = 1 - \beta$. This leads to the exponents $\alpha = 1/3, \beta = 2/3$.

VI. BETHE ANSATZ FOR THE SSEP

To test whether the critical exponents are indeed universal, we corroborate our result by analyzing the finite-size corrections of an integrable microscopic model—the SSEP. The SSEP is defined by setting $E = 0$ in the WASEP (see the caption of Fig. 1 or Appendix A). Macroscopically, it corresponds to $D = 1, \sigma = 2\rho(1 - \rho)$. Note that, since u is always negative in this case, the singularity of $\mathcal{F}(u)$ is not attained for real values of J . Yet it can still teach us about the formal structure of the universality by investigating the poles appearing in the perturbation coefficients.

For a technical reason, instead of trying to find the LDF $I(J)$, we consider equivalently the cumulant generating function (CGF) $G(s) = \sum_Q e^{-sQ} P_t(Q)$. Note that the CGF is a Legendre-Fenchel transform of the LDF. For diffusive processes, it is natural to define the rescaled CGF $\mu(\lambda) = LG(s)$, where $\lambda = sL$, similarly to the rescaled LDF structure $\Phi(J)$. For a Markov process, the CGF is the ground state energy (lowest eigenvalue) of an operator H associated to the Markov matrix [46] (see Appendix A). This property makes the CGF appealing from both a numerical and theoretical perspectives as we shall see in the following.

For the SSEP, the CGF $G(s)$ corresponds to the ground state energy of a quantum spin chain operator [46],

$$H = \frac{L}{2} - \frac{1}{2} \sum_{i=1}^L \left[\cosh s(\sigma_i^x \sigma_{i+1}^x + \sigma_i^y \sigma_{i+1}^y) + \sigma_i^z \sigma_{i+1}^z - i \sinh s(\sigma_i^x \sigma_{i+1}^y + \sigma_i^y \sigma_{i+1}^x) \right]. \quad (13)$$

Its eigensystem can be exactly determined via Bethe ansatz [44]. In the coordinate formulation of the Bethe ansatz, each particle is described by a plane-wave with their interactions embodied in a pairwise factorizable scattering matrix [61]. Considering N particles on a ring of size L , such that mean density $\rho = N/L \in (0, 1)$, the corresponding wave-function is parametrized by the complex parameters $\{\xi_i\}_{i=1}^N$ which are quantized according to the so-called Bethe equations,

$$\xi_i^L = \prod_{\substack{j=1 \\ j \neq i}}^N \left[-\frac{e^s - 2\xi_i + e^{-s}\xi_i\xi_j}{e^s - 2\xi_j + e^{-s}\xi_i\xi_j} \right]. \quad (14)$$

The eigenvalues are expressed in terms of the solutions of these equations through

$$G(s) = -2N + e^{-s} \sum_{j=1}^N \xi_j + e^s \sum_{j=1}^N \frac{1}{\xi_j}. \quad (15)$$

Note that the ground state is shifted here by $2N$ to obtain $G(s)$. Based on Bethe ansatz, the CGF was already calculated to order $1/L$ [23]. Using an alternative method based on the Baxter equation [60], we compute the $1/L^2$ corrections and numerically validate our results.

Generally, solving Eq. (14) analytically is unfeasible for arbitrary finite N and L but in the thermodynamic limit where $N, L \rightarrow \infty$, they become tractable. The key observation is that under the change of variables $\xi_i = e^s(z_i + i/2)/(z_i - i/2)$, the Bethe Eq. (14) becomes

$$\left(\frac{z_i + i/2}{z_i - i/2} \right)^L = e^{-\lambda} \prod_{\substack{j=1 \\ j \neq i}}^N \frac{z_i - z_j + i}{z_i - z_j - i}, \quad i = 1, \dots, N. \quad (16)$$

Equations (16) are precisely the Bethe equations for the twisted XXX $_{1/2}$ spin-chain with λ playing the role of the twist [62]. Finite-size corrections to the spectrum of spin chains of this type are well studied. In particular, a powerful method based on the so-called Baxter equation was developed in Ref. [60] and applied for the closely related $sl(2)$ spin chain. Based on the results of Ref. [60], we determine the finite-size corrections of the SSEP to order $1/L^2$. Namely, we determine μ_0, μ_1 , and μ_2 , where we have defined $\mu(\lambda) = \sum_{i=0}^{\infty} \mu_i L^{-i}$. The expressions μ_0, μ_1 (see Appendix C) agree with the previously obtained results [23]. The full expression of μ_2 , which is one of our main results, has a long expression given in the Appendix. These theoretical predictions of $\mu_{0,1,2}$ are confirmed in the appendix by comparing to a population dynamics algorithm [9,63–70].

The interesting part of the μ_2 arises at its strongest singularity. For illustration we consider the lowest mode in the Appendix, Eq. (C19), namely $k = 1$, and we find the following singular behavior,

$$\mu_2 \sim \frac{2\pi^4(\theta^2 - 1)}{\delta u \theta^2} + O\left(\frac{1}{\sqrt{\delta u}}\right), \quad (17)$$

where we have introduced $\delta u \equiv \frac{1}{8}\theta^2\lambda^2 + \frac{\pi^2}{2}$ and $\theta = 2\sqrt{\rho(1 - \rho)}$. Under the continuation to complex values of λ , we find simple poles at the positions $\lambda = \pm \frac{2i\pi}{\theta}$. We then get

the same type of singularity in δu as in the hydrodynamics analysis, i.e., $[\mu_2 = O(1/\delta u)]$. Combined with the results of the MFT, we deduce that the $1/L^2$ correction diverges with $1/\delta u$.

VII. NUMERICAL VERIFICATION

It is numerically hard to single-out the singular universal function ϕ from the (unknown) nonuniversal terms. However, differentiation accentuates the singular term as detailed below.

In terms of CGF $\mu(\lambda)$, the scaling form Eq. (12) is written as

$$L[\mu(\lambda) - \mu_{\text{AP}}(\lambda)] = \frac{1}{L^\alpha} \tilde{\phi}(\delta u L^\beta) + \text{nonuniversal terms}, \quad (18)$$

where $\delta u = \pi^2/2 - u$ and

$$u(\lambda) = \mu_{\text{AP}}(\lambda) \frac{\sigma''}{8D^2}, \quad (19)$$

$$\mu_{\text{AP}}(\lambda) = \lim_{L \rightarrow \infty} \mu(\lambda). \quad (20)$$

To derive these expressions, we have used $J = -\mu'_{\text{AP}}(\lambda)$ [71]. This scaling form indicates that the higher order derivatives of $\mu(\lambda)$ with respect to δu is dominated by the universal function $\tilde{\phi}$. More precisely,

$$L^{\alpha-d\beta+1} \mu^{(d)}(\lambda) \Big|_{r=\delta u L^\beta} = \tilde{\phi}^{(d)}(r) + O(L^{\alpha-d\beta+1}), \quad (21)$$

where $\mu^{(d)}$ is the d th derivative of μ with respect to δu and r is the scaling variable given as $r = \delta u L^\beta$. We thus can see that sufficiently large derivatives d (more precisely, $d = 3$ given $\alpha = 1/3$, $\beta = 2/3$) allows us to neglect $O(L^{\alpha-d\beta+1})$. Using the method detailed in the next paragraph, we have numerically probed $\mu(\lambda)$ for the WASEP to search for the universal scaling function. We present the plot, showing the left-hand side of Eq. (21) in Fig. 1. One can clearly see that the function starts to overlap from the third order derivative, supporting the prediction of the scaling exponents.

To obtain $\mu(\lambda)$ and its derivatives, we numerically diagonalize the s -biased operator $L_{\mathcal{C},\mathcal{C}'}^s$, whose explicit expression is detailed as Eq. (A2) in Appendix A. To obtain the derivatives of the CGF in a stable manner, we use the following method: We denote the eigenvalue equation of L^s by

$$L^s \zeta = G(s) \zeta, \quad (22)$$

where ζ is the right eigenvector associated with the principal eigenvalue $G(s)$. To get the first-order derivative, we numerically solve the following equation:

$$(L^s)' \zeta + L^s \zeta' = G'(s) \zeta + G(s) \zeta', \quad (23)$$

together with the eigenvalue equation. Similarly, to get the second-order derivatives, we add another equation $(L^s \zeta)'' = (G(s) \zeta)''$ to these equations. Higher-order derivatives can be also calculated in the same strategy. Thanks to this method, we do not have to rely on the difference method, which increases the error of the estimation of the higher-order derivatives.

VIII. DISCUSSION

We have probed the LDF (CGF) of the current in diffusive systems using a hydrodynamical theory, a Bethe ansatz approach and numerical simulations. For dynamics with particle-hole symmetry, a singular scaling function with universal exponents is observed. This implies that near the transition, macroscopic fluctuations dominate and hydrodynamic theories are sufficient to observe the critical behavior [58,72]. Thus, it is understood that nonequilibrium systems are prone to universality, where not only microscopic bulk dynamics, but also boundary condition details may be washed away.

Our observation leads us to conjecture a similar scaling exponents for current fluctuations in an infinite chain, starting from a step initial conditions [73–75]. Consider an infinite 1D chain, where at time $t = 0$ the sites $i \leq 0$ have mean density ρ_l and the sites $i > 0$ have mean density ρ_r with Bernoulli distribution (no correlations between the sites). For the SSEP, the CGF was completely determined (see Eq. (2) in Ref. [74]). One can notice that for $\rho_{l,r} = \frac{1}{2}$, the CGF becomes singular for the unphysical value $\lambda = \pm i\pi$, similarly to the value obtained for the boundary driven setup. From the similar structure, it is indeed appealing to conjecture that the universal structure shown here is carried through also in the infinite chain setup as well.

While the universality class here involves diffusive processes with particle-hole symmetry, it is tempting to check whether the exponents are valid even outside the range of validity currently considered, e.g., in models of ballistic or anomalous transport. The nonlinear fluctuating hydrodynamics theory [76] may allow to detect the universality class in these regimes.

Two more remarks are in order for the scaling function. Notice that for the SSEP on a ring, with the mean density $\rho = 1/2$, the singular terms vanish in Eq. (17) as well as the subleading diverging terms (see Appendix C). This does not imply that the singular behavior changes as the density is changed by an infinitesimal amount. We expect that a similar scaling will be recovered in the next leading order expansion. Secondly, as is verified for the SSEP on a ring, the diverging term is a simple pole in Eq. (17) even without the particle-hole symmetry in the density. Therefore, the critical exponents do not change for periodic boundary conditions, irrespective of the symmetry. It would be interesting to find whether the scaling exponents remain the same even when the particle-hole symmetry is broken for boundary driven processes. To verify that, it is necessary to find continuous DPTs in boundary driven processes, which are analytically tractable. Unfortunately, such transitions are not expected to support a constant density profile that enable the direct perturbation theory performed here [77].

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APPENDIX A: THE WASEP AND THE S -BIASED MATRIX

For completeness, we detail here the definition of the WASEP and the SSEP. We also discuss the s -biased ensemble that allows to recast finding the CGF as a ground state of an operator. Denoting the configuration of the particles by $\mathcal{C} = (n_i)_{i=1}^L$, where $n_i = 1(0)$ means the site i is occupied (empty), the transition rates of the WASEP $w(\mathcal{C} \rightarrow \mathcal{C}')$ are given by

$$w(\mathcal{C} \rightarrow \mathcal{C}') = \sum_{i=1}^L [n_i(1 - n_{i+1})e^{E/L} + (1 - n_i)n_{i+1}e^{-E/L}], \quad (\text{A1})$$

where we use the periodic boundary conditions $n_0 = n_L$ and $n_{L+1} = n_1$. Note that when $E = 0$, the model is reduced to the SSEP.

The CGF of the current $G(s)$ in this model [see the main text for the definition of $G(s)$] is the largest eigenvalue of the following s -biased matrix [51]:

$$L_{\mathcal{C},\mathcal{C}'}^s = w(\mathcal{C} \rightarrow \mathcal{C}')e^{-s\hat{j}(\mathcal{C} \rightarrow \mathcal{C}')} - \sum_{\mathcal{C}''} w(\mathcal{C} \rightarrow \mathcal{C}''), \quad (\text{A2})$$

where $\hat{j}(\mathcal{C} \rightarrow \mathcal{C}')$ is a microscopic current, which takes 1(0) when a particle moves to the right (left) direction in the transition $\mathcal{C} \rightarrow \mathcal{C}'$.

To bridge to the macroscopic description, as discussed in the main text, we define $\lambda = sL$ and $\mu(\lambda) = LG(\lambda/L)$. Then, the Legendre-Fenchel transform of $\mu(\lambda)$ corresponds to $\Phi(J)$ given as Eq. (5) in the main text. Note also that $D = 1$, $\sigma = 2\rho(1 - \rho)$ in WASEP. When the additivity principle is satisfied, $\lim_{L \rightarrow \infty} \mu(\lambda)$ becomes simply a quadratic function

$$\lim_{L \rightarrow \infty} \mu(\lambda) = \mu_{\text{AP}}(\lambda) \equiv -E\sigma\lambda + \frac{\sigma\lambda^2}{2} \quad (\text{A3})$$

in this case.

APPENDIX B: NONCONVEXITY CLOSE TO THE TRANSITION

For the WASEP, we show numerical examples of $L(\partial/\partial u)[\mu(\lambda) - \mu_{\text{AP}}(\lambda(u))(1 + 1/L)]$ in Fig. 2, which converges to $\mathcal{F}'(u)$ away from the transition point $u^* = \pi^2/2$ [23]. Close to the transition point, although $\mathcal{F}'(u)$ diverges at u^* , there is no sign of the precursor of the corresponding divergence in numerics up to $L = 100$ in the figure. This corroborates that $\mathcal{F}(u)$ does not describe the CGF (LDF) close to the transition u^* .

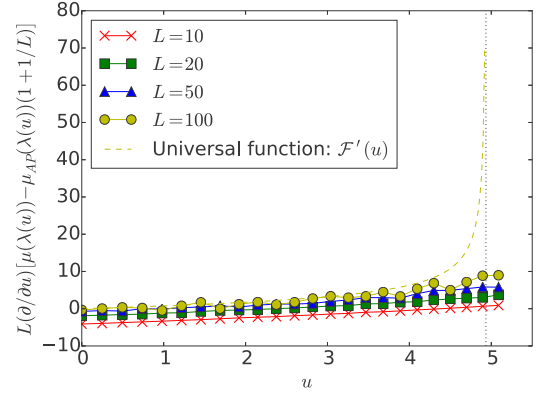


FIG. 2. $L(\partial/\partial u)[\mu(\lambda) - \mu_{\text{AP}}(\lambda(u))(1 + 1/L)]$ for the WASEP close to u^* , where $\mu(\lambda)$ is estimated using the cloning algorithm [63]. Different markers represent different values of L . Away from the transition point u^* , the $1/L$ correction \mathcal{F}' correctly captures the first derivative of the cumulant generating function, as predicted [23]. As $u \rightarrow u^*$, the derivative of $\mathcal{F}(u)$ diverges. It is clear that $\mathcal{F}(u)$ does not capture the finite-size corrections near the transition.

Aside from the divergence of the higher-order corrections, let us argue that $\mathcal{F}(u)$ cannot describe the LDF close to the transition point. It is safe to assume the existence and the differentiability of μ in the domain around u^* for finite, but large, system size L . Indeed, this is what we observe numerically as seen in Fig. 2 for example. From the Gartner-Ellis theorem (see, e.g., Ref. [7] and references therein), we find that the corresponding LDF exists and the LDF needs to be convex function. However, to order $1/L$, the LDF becomes nonconvex for $u \rightarrow u^*$ for any finite L . This can be seen from the negative divergence of the second derivative of \mathcal{F} close to the transition point. Therefore, the first order perturbation Eq. (9) in the main text cannot describe the correct behavior of the LDF close to the transition.

This violation of the first order perturbation implies that higher order corrections also need to diverge as a compensation. Resumming all the corrections restores the convexity below the transition.

APPENDIX C: FINITE-SIZE CORRECTIONS FOR THE SSEP ON A RING

A powerful method to study finite-size corrections in integrable spin chain models is based on the so-called Baxter equation [60],

$$\mathcal{T}(z) = e^{\frac{z}{2}} \left(z + \frac{i}{2} \right)^L \frac{\mathcal{Q}(z-i)}{\mathcal{Q}(z)} + e^{-\frac{z}{2}} \left(z - \frac{i}{2} \right)^L \frac{\mathcal{Q}(z+i)}{\mathcal{Q}(z)}, \quad (\text{C1})$$

where $\mathcal{Q}(z) = \prod_{j=1}^N (z - z_j)$ is the Baxter polynomial. $\mathcal{T}(z)$ is the transfer matrix which is a polynomial of degree L whose explicit form will not be important here but it can be fixed by self-consistency of the equation. The Bethe Eqs. (16) follow from Eq. (C1) by requiring that the residues in the right-hand side at the location of the zeros of $\mathcal{Q}(z)$ vanish.

We will now consider the thermodynamic limit of the Baxter equation as $N, L \rightarrow \infty$ with $z_j \sim O(L)$ following

the method introduced in Ref. [60]. In this limit, it is useful to introduce the rescaled rapidity w as $w \equiv z/L$ and use the notations $\varphi(w) \equiv \frac{1}{L} \sum_{j=1}^N \log(w - w_j)$, the potential $V(w) \equiv \log(w)$ and the rescaled transfer matrix $t(w) \equiv \mathcal{T}(Lw)/[2(Lw)^L]$, where all these functions are now of $O(1)$. In this notation, the Baxter equation looks like

$$t(w) = \frac{1}{2} \left[\exp \left(L \Lambda^+(w) + \frac{\lambda}{2} \right) + \exp \left(L \Lambda^-(w) - \frac{\lambda}{2} \right) \right] \quad (\text{C2})$$

with

$$\Lambda^\pm(w) \equiv \varphi \left(w \mp \frac{i}{L} \right) - \varphi(w) + V \left(w \pm \frac{i}{2L} \right) - V(w). \quad (\text{C3})$$

In addition, we introduce the *quasimomentum* $p(w)$, which will play a major role in the subsequent analysis as

$$p(w) \equiv \varphi'(w) - \frac{V'(w)}{2} + \frac{i\lambda}{2}. \quad (\text{C4})$$

By definition, the expansion of $p'(w)$ around $w = 0$ is given by

$$p'(w) - \frac{1}{2w^2} \underset{w \rightarrow 0}{\simeq} -\frac{1}{L} \sum_{j=1}^N \frac{1}{w_j} = G. \quad (\text{C5})$$

The idea is now to expand the Baxter equation in $1/L$ and solve it for $p(w)$, order by order in this parameter. The first few orders look as follows:

$$t(w) = \cos[p(w)] \left[1 - \frac{4p'(w) + 3V''(w)}{8L} \right] + O(1/L^2). \quad (\text{C6})$$

We aim at finding the first corrections to $p(w)$ and hence, we will expand both $p(w)$ and $t(w)$ in powers of $1/L$ as

$$\begin{aligned} p(w) &= p_0(w) + \frac{1}{L} p_1(w) + O(1/L^2), \\ t(w) &= t_0(w) + \frac{1}{L} t_1(w) + O(1/L^2). \end{aligned} \quad (\text{C7})$$

The polynomiality condition on the transfer matrix $\mathcal{T}(z)$ lead us to assume that the coefficients t_i contain only one singularity at $w = 0$ (by construction) but apart from that they are analytic everywhere in w .

At each order, we will have a Riemann-Hilbert problem defining the quasi-momentum whose asymptotic conditions are imposed directly from its definition Eq. (C4) and the analytic properties follow from the properties of the functions involved in Eq. (C2).

1. Leading-order correction

Let us gain some intuition of what happens to the Bethe roots when we consider the thermodynamic limit at the level of the Bethe Eq. (C8). Taking the logarithm of these equations we get that

$$L \log \left(\frac{z_j + \frac{i}{2}}{z_j - \frac{i}{2}} \right) = \sum_{j=1}^N \log \left(\frac{z_i - z_j + i}{z_i - z_j - i} \right) + 2\pi i \left(n_j + \frac{i\lambda}{2\pi} \right), \quad (\text{C8})$$

where n_j is an integer called mode number that parametrizes the branches of the logarithms and the twist λ corresponds to a shift of such mode number. As we go to the thermodynamic limit it is well known that the Bethe roots condense into cuts in the complex plane whose position depends on the choice of the mode number n_j . The presence of the twist will merely change the shape of the cuts as well as their positions. To specify for the ground state, we use the observation made in Ref. [23] that the distribution of Bethe roots is along a single contour (often called a one-cut solution) where $n_j = n$ for all j and as we will see we further need to set n to zero.

In terms of the quasimomentum, the thermodynamic limit of Eq. (C8) reads [60]

$$p_0(z + i0) + p_0(z - i0) = 2\pi n_j \text{ for } z \in C_j, \quad (\text{C9})$$

where C_j denotes the cut in the complex plane formed by the Bethe roots. Considering the derivative of the quasimomentum $p'(z)$, we see that it satisfies

$$p'_0(z + i0) = -p'_0(z - i0), \quad (\text{C10})$$

which means that $\pm p'_0(z)$ defines a two-sheeted Riemann surface with square-root type branch points.

To see this from the point of view of the Eq. (C2), we have that at leading order

$$t_0(z) = \cos[p_0(z)], \quad (\text{C11})$$

which implies that the derivative of the quasimomentum at this order will be given by

$$p'_0(z) = \frac{t'_0(z)}{\sqrt{1 - t_0^2(z)}}. \quad (\text{C12})$$

Given the analyticity of t_0 we see explicitly the square-root branch points emerging from the denominator of the expression above. Using the definition of the quasimomentum Eq. (C4), we can supplement the previous equation with the asymptotic condition

$$p'_0(z) \sim \frac{1}{2z^2} + O(1) \text{ as } z \rightarrow 0 \quad (\text{C13})$$

and

$$p'_0(z) \sim \frac{1}{z^2} \left(\frac{1}{2} - \rho \right) \text{ as } z \rightarrow \infty, \quad (\text{C14})$$

with $\rho = N/L$ being the density of particles. This fixes $p'_0(z)$ to be

$$p'_0(z) = \frac{2\theta_1\theta_2 - z(\theta_1 + \theta_2)}{4z^2 \sqrt{\theta_1\theta_2} \sqrt{(z - \theta_1)(z - \theta_2)}}, \quad (\text{C15})$$

where θ_1 and θ_2 are the branch points where the distribution of the Bethe roots ends. We can relate them back to the rapidity variables ξ of the original Bethe equations and replace the location of the branch points found in Ref. [23], namely, $\xi = e^{-is(\pm\theta + 2i\rho)}$ with $\theta = 2\sqrt{\rho(1 - \rho)}$. Using Eq. (C5), we then obtain the leading term for the energy to be

$$\mu_0 = \frac{\theta^2 \lambda^2}{4}, \quad (\text{C16})$$

which matches the result found in Ref. [23].

2. Subleading corrections

We could proceed in expanding one order further the Eq. (C2) and solve the corresponding Riemann-Hilbert problem. Instead, we will use the results already available in literature derived by this method in Ref. [60] to recover the already known next-to-leading order correction and make a new prediction for the next-to-next-to-leading order. The result of Ref. [60] was derived for a closely related spin chain model, namely, the (untwisted) $sl(2)$ spin chain, whose Bethe equations are related to those in Eq. (14) simply by replacing $L \rightarrow -L$. Additionally we have seen that the twist shifts the mode numbers. The one-cut solution of the leading and next-to-leading correction to the energy in Refs. [59,60] for the $sl(2)$ spin chain reads

$$\begin{aligned} \mu_0 &= -4\pi^2 n^2 \rho(\rho + 1), \\ \mu_1 &= -4\pi^2 \left\{ \sum_{k=1}^{\infty} [k\sqrt{k^2 + 4n^2\rho(\rho + 1)} - k^2 \right. \\ &\quad \left. - 2n^2\rho(\rho + 1)] - n^2\rho(\rho + 1) \right\}. \end{aligned} \quad (\text{C17})$$

Upon the transforming $L \rightarrow -L$ (and thus $\rho \rightarrow -\rho$) as well as $n \rightarrow n + \frac{i\lambda}{2\pi}$ we obtain the complete result of Ref. [23] when we finally set $n = 0$ (which corresponds to selecting the ground state). This encourages us to proceed to the next-to-next-to-leading order and apply the same heuristic rule to the result written in Appendix B of Ref. [60] to obtain the model under study. Let us first define the following auxiliary sums:

$$\begin{aligned} \mathcal{S}_1 &= \sum_{l=1}^{\infty} \frac{\sqrt{\theta^2 \lambda^2 + 4\pi^2 l^2}}{2\pi l} - 1, \\ \mathcal{S}_2 &= \sum_{l=1}^{\infty} \left(-\frac{\theta^2 \lambda^2}{8\pi^2} + \frac{l}{2\pi} \sqrt{\theta^2 \lambda^2 + 4\pi^2 l^2} - l^2 \right), \\ \mathcal{S}_3(k) &= \sum_{l=1}^{\infty} \frac{k\sqrt{\theta^2 \lambda^2 + 4\pi^2 k^2} - l\sqrt{\theta^2 \lambda^2 + 4\pi^2 l^2}}{2\pi k^2 - 2\pi l^2} - 1, \end{aligned} \quad (\text{C18})$$

we have that the correction reads

$$\begin{aligned} \mu_2 &= \frac{\lambda^2}{96} \left\{ \theta^2 [(19\theta^2 - 14)\lambda^2 + 24] \right. \\ &\quad \left. + 96(4\theta^2 - 3)(\mathcal{S}_1^2 - \mathcal{S}_1) \right\} + 8\pi^2 \mathcal{S}_2 \\ &\quad - \sum_{k=1}^{\infty} \left\{ 2(3\theta^2 - 2)\lambda^2 + \frac{\theta^2(4\theta^2 - 3)\lambda^4}{4\pi^2 k^2} \right. \\ &\quad \left. + 8\pi^2(k^2 + 2\mathcal{S}_2) \right. \\ &\quad \left. + \frac{(2\mathcal{S}_3(k) - 1)[\theta^2(4\theta^2 - 3)\lambda^4 + 32\pi^4 k^4]}{2\pi k\sqrt{\theta^2 \lambda^2 + 4\pi^2 k^2}} \right. \\ &\quad \left. + \frac{(2\mathcal{S}_3(k) - 1)[4\pi^2(7\theta^2 - 4)\lambda^2 k^2]}{2\pi k\sqrt{\theta^2 \lambda^2 + 4\pi^2 k^2}} \right\}. \end{aligned} \quad (\text{C19})$$

The sums above mimic the sums over Fourier modes of the wave fluctuations in the MFT. We verified this result numerically via the cloning algorithm; see Fig. 3.

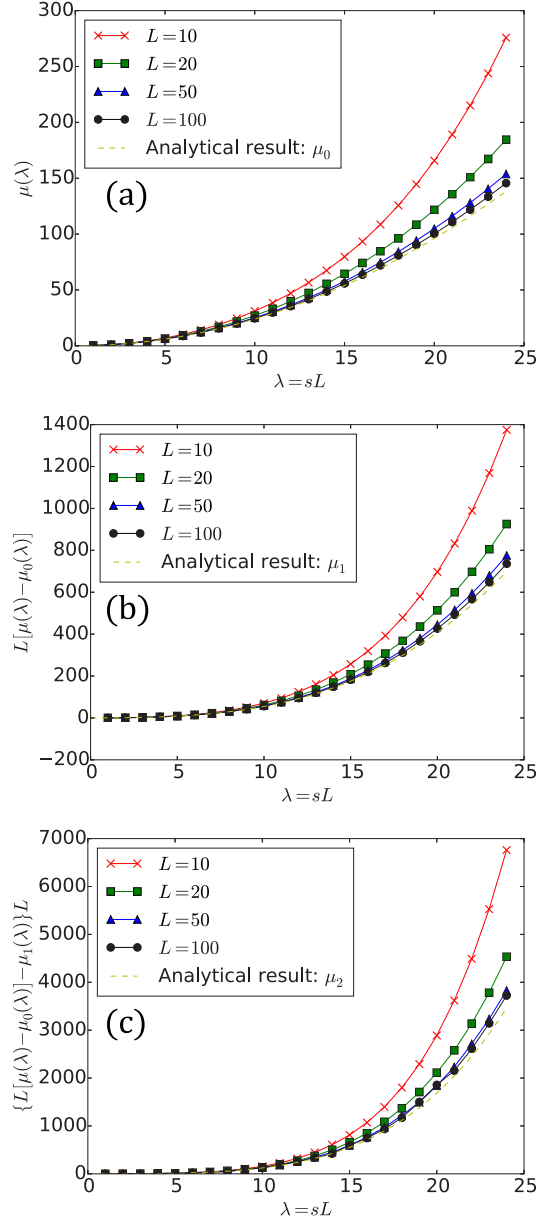


FIG. 3. Analytical results of μ_0 , μ_1 Eq. (C17) and μ_2 Eq. (C19) for $\rho = 0.4$ are shown as yellow dashed lines in (a), (b), and (c), respectively. We also plot the corresponding numerical results obtained from the cloning algorithm [63] for several values of L . We can see the convergence of numerical results to the corresponding analytical predictions as $L \rightarrow \infty$.

APPENDIX D: FINITE-SIZE CORRECTIONS USING THE MFT FOR BOUNDARY DRIVEN SYSTEM

Let us bring in full details the finite-size corrections to the LDF $\Phi(J)$ to order $1/L^2$.

First, the \mathcal{S}_3 , \mathcal{S}_4 terms are given by

$$\mathcal{S}_3 = \sum_{\vec{k}, \vec{\omega}} \chi_0 h_0 V_3, \quad \mathcal{S}_4 = \sum_{\vec{k}, \vec{\omega}} \sum_{l=1,2,3} \chi_l g_l V_4, \quad (\text{D1})$$

where $V_m = \prod_{j=1,\dots,m} a_{k_j, \omega_j} \delta(\sum k_i) \delta(\sum \omega_i)$ and

$$\begin{aligned} \chi_0 &= -\frac{J\sigma''}{2\sigma^2}, & \chi_1 &= \frac{DD''}{2\sigma}, \\ \chi_2 &= \frac{J^2(\sigma'')^2}{8\sigma^3} + \frac{\sigma^{(4)}}{48}(E^2 - J^2/\sigma^2), \\ \chi_3 &= -\frac{\sigma''}{4\sigma^2}, & h_0 &= -i\omega_3 k_1 k_2, \\ g_1 &= -k_1 k_2 k_3^2 k_4^2, & g_2 &= k_1 k_2 k_3 k_4, \\ g_3 &= k_1 k_2 \omega_3 \omega_4. \end{aligned} \quad (\text{D2})$$

Performing the perturbative expansion to order $1/L^2$, we find

$$\begin{aligned} \Phi_2 &= \frac{15\sigma^2}{4D^2} \left(\chi_1 u + \frac{3}{2} \chi_2 \right) (1 - \sqrt{2u} \cot \sqrt{2u}) \\ &\times \frac{15\sigma^2}{4D^2} (\chi_1 \mathcal{G}_1 \mathcal{G}_3 - 2\chi_1 \mathcal{G}_2^2 + 3\chi_2 \mathcal{G}_1^2) \\ &+ \frac{2\sigma^3}{D^2} \chi_0^2 \mathcal{G}_2 + \frac{2\chi_0^2}{\pi^2} [F_a(u) + F_b(u)] \\ &- \frac{15\sigma^2}{2\pi^2} \chi_3 (\mathcal{H}_1 + \mathcal{H}_2) \\ &+ (Au + Bu^2) \left(1 + \frac{C}{\sqrt{\delta u}} \right), \end{aligned} \quad (\text{D3})$$

where A , B , and C are nonuniversal terms that depend on the cutoffs and with the functions

$$\begin{aligned} F_a(u) &= \sum_{k_1, k_2} \int d\omega_1 d\omega_2 \frac{k_1 k_2^3 \omega_1 (\omega_1 + \omega_2)^2}{f(k_1, \omega_1) f(k_2, \omega_2) f(k_1 + k_2, \omega_1 + \omega_2)}, \\ F_b(u) &= \sum_{k_1, k_2} \int d\omega_1 d\omega_2 \frac{k_1^2 k_2^2 (\omega_1 + \omega_2)^2}{f(k_1, \omega_1) f(k_2, \omega_2) f(k_1 + k_2, \omega_1 + \omega_2)}, \\ \mathcal{G}_1 &= \sum_k \frac{k}{\sqrt{k^2 - 2u}} - 1, \\ \mathcal{G}_2 &= \sum_k \frac{k^2}{\sqrt{k^2 - 2u}} - k - \frac{u}{k}, \\ \mathcal{G}_3 &= \sum_k \frac{k^3}{\sqrt{k^2 - 2u}} - k^2 - u, \\ \mathcal{H}_1 &= 8 \sum_k k^2 \log Dk \log(k^2 - 2u) \\ &\quad - k^2 \log Dk \log k^2 + 2u \log Dk, \\ \mathcal{H}_2 &= \sum_k k^2 \log^2(k^2 - 2u) - 4k^2 \log^2 k + 8u \log k. \end{aligned} \quad (\text{D4})$$

One can show that as $\delta u \rightarrow 0$, only the first two lines of Eq. (D3) contribute to the leading $1/\delta u$ divergence.

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