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Weak additivity principle for current statistics in d dimensions

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The additivity principle (AP) allows one to compute the current distribution in many one-dimensional nonequilibrium systems. Here we extend this conjecture to general d-dimensional driven diffusive systems, and validate its predictions against both numerical simulations of rare events and microscopic exact calculations of three paradigmatic models of diffusive transport in $d = 2$. Crucially, the existence of a structured current vector field at the fluctuating level, coupled to the local mobility, turns out to be essential to understand current statistics in $d > 1$. We prove that, when compared to the straightforward extension of the AP to high d, the so-called weak AP always yields a better minimizer of the macroscopic fluctuation theory action for current statistics.

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Currents are the hallmark of nonequilibrium behavior. Whenever a system is driven out of equilibrium by a boundary gradient and/or external field, a current of a conjugate observable (mass, energy, momentum, charge, etc.) appears which reflects the associated entropy production [1]. The function controlling current fluctuations seems to play a role akin to the equilibrium free energy in nonequilibrium situations [2,3], and hence the understanding of current statistics in terms of microscopic dynamics has become one of the main goals of nonequilibrium statistical mechanics, a problem which has proven to be very difficult even in the simplest situations. Indeed, up to now only a handful of exactly solvable models are fully understood [3–6] and, despite some exact results in the form of fluctuation theorems [7–21], the overall picture remains puzzling and in need of a general, first-principles approach. This deadlock has changed dramatically with the recent formulation of macroscopic fluctuation theory (MFT) [22–30], a unifying theoretical scheme to study dynamic fluctuations in nonequilibrium systems, based solely on the knowledge of a few transport coefficients easily measurable in experiments, and applicable to a broad class of nonequilibrium problems [31–49].

When applied to current statistics, MFT leads to a well-defined but highly complex variational problem in space and time for the optimal paths responsible for a given current fluctuation, whose solution remains challenging in most cases [24–28]. However, in an effort to explore clarifying hypotheses, Bodineau and Derrida [50] (see also [3,4,28]) have conjectured an additivity principle (AP) which greatly simplifies the MFT variational problem for currents in one dimension (1D), leading to explicit quantitative predictions and thus opening the door to a systematic way of computing the current statistics in general nonequilibrium systems [2]. In other words, the AP amounts to assuming within MFT that the optimal path responsible for a given current fluctuation is time independent. The validity of the AP has been confirmed with high accuracy in rare-event simulations of 1D stochastic lattice gases [51–54], but the question remains, however, as to how to generalize this conjecture to the more interesting case of $d > 1$.

Here we propose such a generalization, which we call weak additivity principle (wAP), and demonstrate its validity and accuracy by comparing our predictions with both numerical simulations of rare events [55–59] and microscopic exact calculations [16,60–63] in three paradigmatic models of diffusive transport, namely, the Kipnis-Marchioro-Presutti (KMP) model of heat conduction [64], the zero-range process (ZRP) [65,66], and the random walk model [28,67], all defined in $d = 2$. A main novelty of our conjecture when compared to the straightforward generalization of the 1D AP to $d > 1$ is the realization of the essential role played by an optimal divergence-free current vector field in the MFT variational problem for current statistics in $d > 1$. This optimal current field turns out to be structured along the gradient direction according to the local mobility, a possibility already suggested in [16]. It is then easy to prove that the wAP always yields a better minimizer of the MFT action for current statistics.

We are interested in a broad class of d-dimensional driven diffusive systems characterized by a conserved density field $\rho(\mathbf{r},t)$ which evolves according to the following fluctuating hydrodynamics equation [3,4,24–28,53]:

$$\partial_t \rho(\mathbf{r},t) + \nabla \cdot [-\hat{D}(\rho)\nabla\rho(\mathbf{r},t) + \boldsymbol{\xi}(\mathbf{r},t)] = 0, \qquad (1)$$

with $\mathbf{r} \in \Lambda \equiv [0,1]^d$. The field $\mathbf{j}(\mathbf{r},t) \equiv -\hat{D}(\rho)\nabla\rho(\mathbf{r},t) + \boldsymbol{\xi}(\mathbf{r},t)$ is the fluctuating current, with local average given by Fick's or Fourier's law with a diffusivity matrix $\hat{D}(\rho)$, and $\boldsymbol{\xi}(\mathbf{r},t)$ is a Gaussian white noise with $\langle\boldsymbol{\xi}(\mathbf{r},t)\rangle = 0$, and characterized by a mobility matrix $\hat{\sigma}(\rho)$

$$\langle \xi_\alpha(\mathbf{r},t)\xi_\beta(\mathbf{r}',t')\rangle = L^{-d}\sigma_\alpha(\rho)\delta_{\alpha\beta}\delta(\mathbf{r}-\mathbf{r}')\delta(t-t'),$$

with L is the system size in natural units and $\alpha,\beta \in [1,d]$. This (conserved) noise term accounts for the many fast microscopic degrees of freedom which are averaged out in the coarse-graining procedure resulting in Eq. (1). The diffusion and mobility transport matrices are diagonal, with components $D_\alpha(\rho)$ and $\sigma_\alpha(\rho)$, respectively, being related via a local Einstein relation $\hat{D}(\rho) = f_0''(\rho)\hat{\sigma}(\rho)$, with $f_0(\rho)$ the *equilibrium* free energy of the system at hand. To

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completely define the problem, the evolution Eq. (1) must be supplemented with appropriate boundary conditions, which typically include an external gradient along a given direction (say $\hat{x}$), $\rho(\mathbf{r},t)|_{x=0,1} = \rho_{L,R}$, which drives the system out of equilibrium for $\rho_L \neq \rho_R$, and periodic boundaries along all other $(d-1)$ directions.

The probability of observing a given history $\{\rho(\mathbf{r},t),\mathbf{j}(\mathbf{r},t)\}_0^\tau$ of duration τ for the density and current fields can be written using path integrals as [28]

$$P\big(\{\rho,\mathbf{j}\}_0^\tau\big) \sim \exp(+L^d I_\tau[\rho,\mathbf{j}]),$$

with an action $I_\tau[\rho,\mathbf{j}] = -\int_0^\tau dt \int_\Lambda d\mathbf{r}\, \mathcal{L}(\rho,\mathbf{j})$ and

$$\mathcal{L}(\rho,\mathbf{j}) = \tfrac{1}{2}[\mathbf{j} + \hat{D}(\rho)\nabla\rho]\cdot\hat{\Sigma}(\rho)[\mathbf{j} + \hat{D}(\rho)\nabla\rho].$$

The matrix $\hat{\Sigma}(\rho)$ is diagonal with components $\Sigma_\alpha(\rho) \equiv \sigma_\alpha^{-1}(\rho)$, and the fields $\rho(\mathbf{r},t)$ and $\mathbf{j}(\mathbf{r},t)$ are coupled via the continuity equation [see also Eq. (1)]

$$\partial_t\rho(\mathbf{r},t) + \nabla\cdot\mathbf{j}(\mathbf{r},t) = 0. \tag{2}$$

In any other case $I_\tau[\rho,\mathbf{j}] \to -\infty$. The probability $P_\tau(\mathbf{J})$ of observing an averaged empirical current $\mathbf{J}$, defined as

$$\mathbf{J} = \frac{1}{\tau}\int_0^\tau dt \int_\Lambda d\mathbf{r}\,\mathbf{j}(\mathbf{r},t), \tag{3}$$

scales for long times as $P_\tau(\mathbf{J}) \sim \exp[+\tau L^d G(\mathbf{J})]$, and the current large deviation function (LDF) $G(\mathbf{J})$ can be related to $I_\tau[\rho,\mathbf{j}]$ via a simple saddle-point calculation in the long-time limit, $G(\mathbf{J}) = \lim_{\tau\to\infty}\tau^{-1}\max_{\{\rho,\mathbf{j}\}} I_\tau[\rho,\mathbf{j}]$, subject to constraints (2) and (3) and the fixed boundary conditions. The density and current fields solution of this variational problem, denoted here as $\bar{\rho}(\mathbf{r},t;\mathbf{J})$ and $\bar{\mathbf{j}}(\mathbf{r},t;\mathbf{J})$, are just the optimal path the system follows to sustain a long-time current fluctuation $\mathbf{J}$.

This is a complex spatiotemporal variational problem whose solution remains challenging in most cases [3,4,24–28,31,32,50–53,68], so simplifying hypotheses are required. Inspired by results from 1D [3,4,50–53], we now propose a weak version of the additivity principle (or wAP in short) which consists in two main hypotheses, namely, that (i) the dominant paths responsible for a given current fluctuation are indeed time independent [69], i.e., $\rho(\mathbf{r})$ and $\mathbf{j}(\mathbf{r})$, and (ii) the relevant fields exhibit structure only along the gradient direction, so $\rho(x)$ and $\mathbf{j}(x)$ in our convention. Clearly (ii) is expected on physical grounds due to periodicity along all directions orthogonal to the gradient. To make clear the simplifying power of the wAP, note that (i) implies, via the continuity Eq. (2), that the relevant current vector fields are divergence-free, $\nabla\cdot\mathbf{j}(\mathbf{r}) = 0$, and this, together with (ii) above and constraint (3), leads to current fields $\mathbf{j}(x) = (J_\parallel,\mathbf{j}_\perp(x))$, with

$$\mathbf{J}_\perp = \int_0^1 dx\,\mathbf{j}_\perp(x), \tag{4}$$

and where we have decomposed $\mathbf{J} = (J_\parallel,\mathbf{J}_\perp)$ along the gradient ($\parallel$) and all other, $(d-1)$ directions ($\perp$). The wAP thus leads to the following simplified variational problem for the current LDF:

$$G_{\rm w}(\mathbf{J}) = -\min_{\substack{\rho(x)\\ \mathbf{j}_\perp(x)}} \int_0^1 dx\,\mathcal{L}_{\rm w}(\rho,\mathbf{j}_\perp;\mathbf{J}),$$

$$\mathcal{L}_{\rm w}(\rho,\mathbf{j}_\perp;\mathbf{J}) = \frac{[J_\parallel + D_1(\rho)\rho'(x)]^2}{2\sigma_1(\rho)} + \sum_{\alpha=2}^d \frac{{j_\perp^{(\alpha)}(x)}^2}{2\sigma_\alpha(\rho)},$$

and subject to the constraints (4) and the imposed boundary conditions. To explicitly take into account the constraints, we now introduce $(d-1)$ Lagrange multipliers and define a modified functional $\mathcal{L}_{\rm w}^{(\boldsymbol{\nu}_\perp)}(\rho,\mathbf{j}_\perp;\mathbf{J}) \equiv \mathcal{L}_{\rm w}(\rho,\mathbf{j}_\perp;\mathbf{J}) - \boldsymbol{\nu}_\perp\cdot\mathbf{j}_\perp(x)$. Standard variational calculus thus leads to the following differential equation for the optimal density profile $\bar{\rho}_{\rm w}(x;\mathbf{J})$ [53]:

$$D_1(\rho)^2\rho'(x)^2 = {J_\parallel}^2 + \sigma_1(\rho)\left[2K - \sum_{\alpha=2}^d {\nu_\perp^{(\alpha)}}^2\sigma_\alpha(\rho)\right],$$

where K is an integration constant which guarantees the correct boundary conditions [53]. The optimal current field also follows as $\bar{\mathbf{j}}_{\rm w}(x;\mathbf{J}) = [J_\parallel,\bar{\mathbf{j}}_{{\rm w},\perp}(x;\mathbf{J})]$ with

$$\bar{j}_{{\rm w},\perp}^{(\alpha)}(x;\mathbf{J}) = \nu_\perp^{(\alpha)}\sigma_\alpha(\bar{\rho}_{\rm w}), \quad \alpha\in[2,d], \tag{5}$$

with the Lagrange multipliers fixed via (4) to $\nu_\perp^{(\alpha)} = J_\perp^{(\alpha)}/\int_0^1 dx\,\sigma_\alpha(\bar{\rho}_{\rm w})$. Equation (5) shows that the optimal, divergence-free current vector field exhibits structure along the gradient direction in all orthogonal components, and this structure is coupled to the optimal density profile via the mobility transport coefficient.

This result should be compared with the straightforward extension of the 1D-AP to high dimensions, which amounts to assume, together with (i) and (ii) above, that the optimal current field is constant across space and hence equals $\mathbf{J}$ due to (3). This strong additivity principle (or sAP in short) leads to an even simpler variational problem for the current LDF, $G_{\rm s}(\mathbf{J}) = -\min_{\rho(x)}\int_0^1 dx\,\mathcal{L}_{\rm s}(\rho;\mathbf{J})$, with

$$\mathcal{L}_{\rm s}(\rho;\mathbf{J}) = \frac{[J_\parallel + D_1(\rho)\rho'(x)]^2}{2\sigma_1(\rho)} + \sum_{\alpha=2}^d \frac{{J_\perp^{(\alpha)}}^2}{2\sigma_\alpha(\rho)},$$

whose optimal solution is denoted here as $\bar{\rho}_{\rm s}(x;\mathbf{J})$. Note that, for $\mathbf{J}$ fixed, we expect $\bar{\rho}_{\rm s}(x;\mathbf{J}) \neq \bar{\rho}_{\rm w}(x;\mathbf{J})$ in general, and the question remains as to which hypothesis (wAP or sAP) yields a maximal $G(\mathbf{J})$. Intuition suggests that the wAP should offer a better solution as it includes additional degrees of freedom that the system at hand can *put at work* to improve its rate function. To confirm rigorously this argument, note first that the optimal current field $\bar{\mathbf{j}}_{\rm w}(x;\mathbf{J})$ is a functional of the optimal density $\bar{\rho}_{\rm w}(x;\mathbf{J})$ [see Eq. (5)], so we can always write $G_{\rm w}(\mathbf{J}) = \mathcal{F}_{\rm w}(\bar{\rho}_{\rm w};\mathbf{J})$, where we have defined the functional $\mathcal{F}_\ell(\psi;\mathbf{J}) \equiv -\int_0^1 dx\,\mathcal{L}_\ell(\psi;\mathbf{J})$, with $\ell = {\rm w, s}$, for any function $\psi(x)$ obeying the boundary conditions. Similarly, we may write $G_{\rm s}(\mathbf{J}) = \mathcal{F}_{\rm s}(\bar{\rho}_{\rm s};\mathbf{J})$. Since $\bar{\rho}_{\rm w}(x;\mathbf{J})$ is the maximizer of the wAP action, clearly $\mathcal{F}_{\rm w}(\bar{\rho}_{\rm w};\mathbf{J}) \geqslant \mathcal{F}_{\rm w}(\psi;\mathbf{J})\ \forall\psi(x) \neq \bar{\rho}_{\rm w}(x;\mathbf{J})$. Next, we compare both functionals $\mathcal{F}_{\rm w,s}$ applied to *the same* profile $\bar{\rho}_{\rm s}$ at fixed $\mathbf{J}$, i.e., we define

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$\Delta_{\rm ws} \equiv \mathcal{F}_{\rm w}(\bar\rho_{\rm s};\mathbf{J}) - \mathcal{F}_{\rm s}(\bar\rho_{\rm s};\mathbf{J})$ and find

$$\Delta_{\rm ws} = \sum_{\alpha=2}^{d} \frac{J_\perp^{(\alpha)2}}{2}\left[\int_0^1 dx\,\frac{1}{\sigma_\alpha(\bar\rho_{\rm s})} - \frac{1}{\int_0^1 dx\,\sigma_\alpha(\bar\rho_{\rm s})}\right] \geqslant 0.$$

The last inequality arises because $\int_0^1 dx\,\sigma_\alpha^{-1}(\bar\rho_{\rm s}) \geqslant [\int_0^1 dx\sigma_\alpha(\bar\rho_{\rm s})]^{-1}$, which is a particular instance of the reverse Hölder's inequality [70]. In this way, $\mathcal{F}_{\rm w}(\bar\rho_{\rm w};\mathbf{J}) \geqslant \mathcal{F}_{\rm w}(\bar\rho_{\rm s};\mathbf{J}) \geqslant \mathcal{F}_{\rm s}(\bar\rho_{\rm s};\mathbf{J})$ and hence $G_{\rm w}(\mathbf{J}) \geqslant G_{\rm s}(\mathbf{J})$. This proves that, when compared to the strong AP, the weak AP always yields a better minimizer of the macroscopic fluctuation theory action for currents. This result therefore singles out the wAP as the relevant simplifying hypothesis to study current statistics in general d-dimensional systems. Interestingly, the previous proof shows that both the sAP and wAP yield the same result only for constant mobility, $\sigma_\alpha(\rho) = \sigma_\alpha\ \forall\alpha$, or for current fluctuations parallel to the gradient direction, $\mathbf{J} = (J_\parallel, \mathbf{J}_\perp = 0)$. This observation helps in making sense of previous, seemingly contradictory results [71–73].

Our aim now is to verify the wAP predictions against both numerical simulations of rare events and microscopic exact calculations of various paradigmatic models of diffusive transport in $d = 2$. Our first model of choice is the widely studied ZRP [65,66], a model of interacting particles amenable to exact computations due to the factorization property of its stationary measure. The ZRP is defined on a d-dimensional lattice of linear size L whose sites i may be occupied by an arbitrary number of particles $n_i \in \mathbb{N}$ which jump to randomly chosen neighbors at a rate $\omega_\alpha(n_i) = h_\alpha f(n_i)$, with $f(n_i)$ the interaction function (which depends only on the population of the departure site) and h_α the (constant) hopping rate along the α direction, $\alpha \in [1,d]$. Different interaction functions model varying physical situations, but for concreteness we focus here on a constant $f(n) = 1$, which mimics an effective attraction between particles on each site [65]. When coupled to particle reservoirs at the left and right boundaries at densities ρ_L and ρ_R, respectively [65,66], with $\rho_L \neq \rho_R$, the so-defined ZRP sustains a net average current of particles $\langle\mathbf{J}\rangle = \hat{x}h_1(\rho_L - \rho_R)/[(1+\rho_L)(1+\rho_R)]$ described by Fick's law with a diffusivity matrix with components $D_\alpha(\rho) = h_\alpha/(1+\rho)^2$. Moreover, the mobility coefficient has components $\sigma_\alpha(\rho) = 2h_\alpha\rho/(1+\rho)$, and together these transport coefficients can be used to solve numerically the MFT problem for currents under the wAP conjecture (see [62] for the 1D case). We compare these theoretical predictions with exact results for the ZRP current LDF and the associated optimal density profiles, which can be obtained within the so-called quantum Hamiltonian formalism for the master equation [16,60–62]. Within this picture, the current LDF is obtained from the lowest eigenvalue of a *tilted Hamiltonian*, a spectral problem which reduces to a $L \times L$ system of linear equations due to the factorization property of ZRP [16,60–62] (see Appendix A in the Supplemental Material [74]). Optimal density profiles are then related to the left and right eigenvectors associated to the lowest eigenvalue [52,53,59]. Figure 1 shows our results for $G(\mathbf{J})$ (top) and $\bar\rho(x;\mathbf{J})$ [bottom, after subtracting the steady-state profile $\rho_{\rm av}(x)$ [75]] for parameters $\rho_L = 1$, $\rho_R = 0.1$, and isotropic hopping rates $h_\alpha = 1/2\ \forall\alpha$. The agreement between wAP predictions and exact matrix computations for $L = 10^5$ is excellent in all cases, while sAP predictions fail outside the gradient direction, the discrepancy being maximal for orthogonal fluctuations and increasing with $|\mathbf{J}|$. Appendix B in the Supplemental Material [74] presents similar data for an anisotropic ZRP, as well as for a fluid of random walkers, and in all cases the agreement between wAP predictions and matrix data for $L = 10^5$ is remarkable.

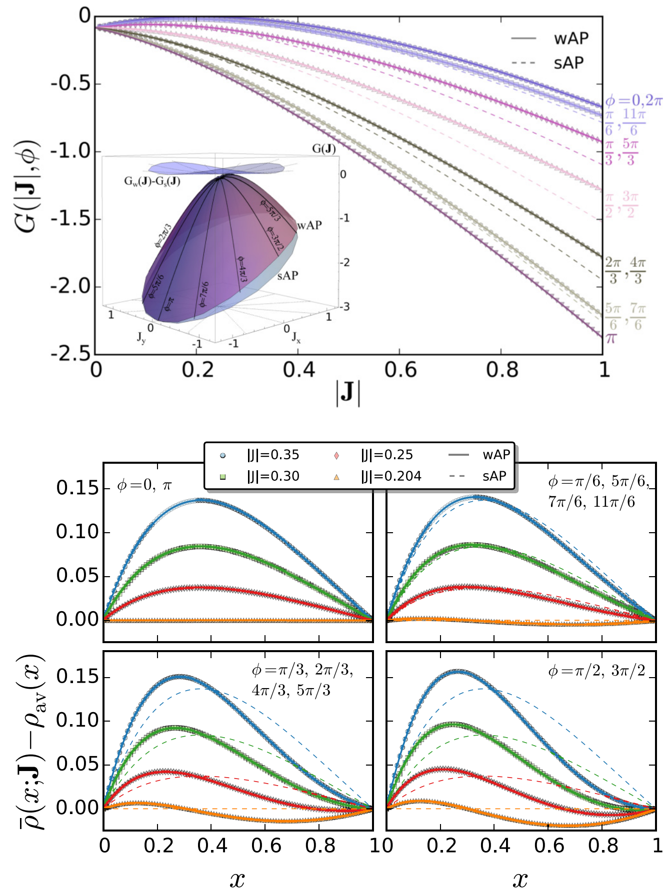

FIG. 1. Top: Current LDF for the isotropic ZRP vs $|\mathbf{J}|$ for different angles $\phi = \tan^{-1}(J_y/J_x)$. Inset: $G(\mathbf{J})$ from MFT under wAP and sAP. Clearly, $G_{\rm w}(\mathbf{J}) \geqslant G_{\rm s}(\mathbf{J})$. Bottom: Excess optimal density profiles for different $|\mathbf{J}|$ and ϕ. Symbols stand for exact matrix computations for $L = 10^5$, while solid (dashed) lines represent wAP (sAP) predictions.

The previous results are restricted to transport models with a factorizable stationary measure [65]. We now focus on the more complex 2D-KMP model of heat transport [64], defined on a square lattice of linear size L whose sites i contain certain amount of energy $\rho_i \in \mathbb{R}_+$. Dynamics proceeds via random energy exchanges between neighbors, such that the pair energy is conserved, and we couple the system to two thermal baths at the left and right ends at temperatures $T_{L,R}$, respectively [53,64], with periodic boundary conditions in the y direction. At the macroscopic level this model obeys Fourier's law with a scalar conductivity $D(\rho) = 1/2$ and a mobility $\sigma(\rho) = \rho^2$, and for $T_L \neq T_R$ it develops a linear temperature profile $\rho_{\rm av}(x) = T_L + x\,(T_R - T_L)$ with a nonzero average current $\langle\mathbf{J}\rangle = \hat{x}(T_L - T_R)/2$. For this nonfactorizable model the quantum Hamiltonian matrix approach does not yield useful results. Instead, we measure the full current

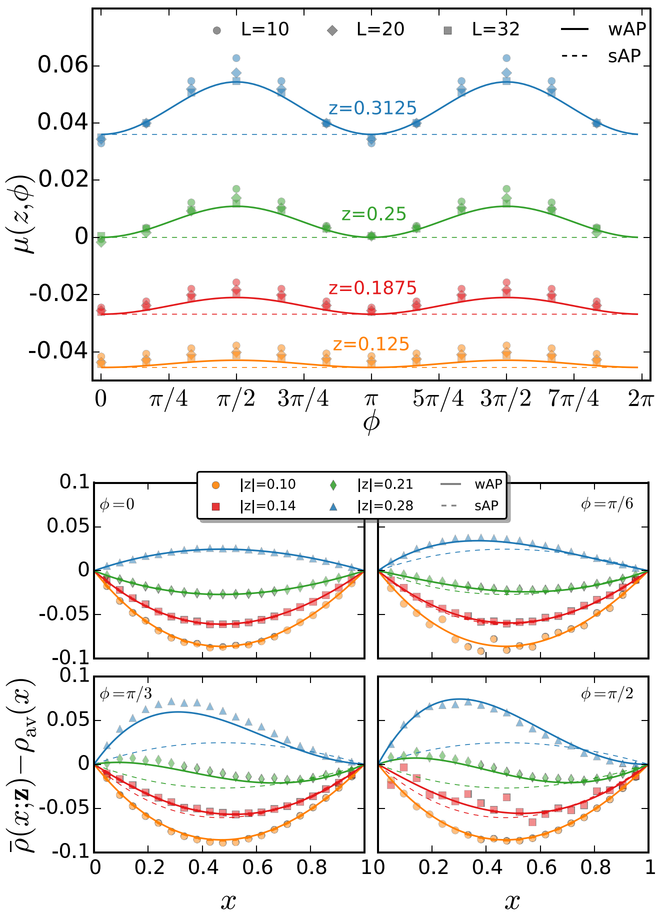

FIG. 2. Top: Legendre transform of the current LDF for the KMP model vs ϕ for different values of $z \equiv |\mathbf{z}|$ and varying L. Convergence to the wAP prediction as L increases is apparent. Bottom: Excess optimal density profiles for different z and ϕ as measured for $L = 20$. Symbols stand for cloning simulation results, while solid (dashed) lines represent wAP (sAP) predictions.

statistics using advanced cloning Monte Carlo simulations particularly designed for this task [15,52,53,55–58]. This method, which works well for not too large L, yields the Legendre-Fenchel transform of the current LDF, $\mu(\boldsymbol{\lambda}) = \max_{\mathbf{J}}[G(\mathbf{J}) + \boldsymbol{\lambda}\cdot\mathbf{J}]$. Figure 2 shows the measured $\mu(\boldsymbol{\lambda})$ for $T_L = 2$, $T_R = 1$ and different L, as a function of the current angle ϕ for different values of $|\mathbf{z}|$, with $\mathbf{z} \equiv \boldsymbol{\lambda} + \boldsymbol{\epsilon}$ and $\boldsymbol{\epsilon} = \frac{1}{2}(T_R^{-1} - T_L^{-1})$, corresponding to a broad range of current fluctuations [15]. While the sAP predicts a ϕ-independent $\mu(\boldsymbol{\lambda})$ for fixed $|\mathbf{z}|$, we observe a double-bump structure in ϕ as predicted by wAP [76]. Moreover, finite-size data clearly converge to the wAP prediction as L increases, while sAP only yields the correct prediction for $\phi = 0,\pi$, as expected. Note that similar finite-size corrections are observed for the ZRP (see Appendix B in the Supplemental Material [74]). Data for optimal density profiles also fit nicely the theoretical wAP curves, overall demonstrating the superior predictive power of the weak additivity principle presented in this Rapid Communication.

In summary, we have extended the additivity principle to general d-dimensional driven diffusive systems, demonstrating the key role played by a structured current field (coupled to the local density via the mobility coefficient) to understand current statistics in $d > 1$. Predictions from the so-called weak additivity principle have been tested against both exact matrix results and simulations of rare events in different paradigmatic models of transport in $d = 2$, and a remarkable agreement is found in all cases. Moreover, we have also proven that the wAP (and not the sAP) offers a better minimizer of the MFT action for currents, except for current fluctuations along the gradient direction, where both wAP and sAP yield equivalent results. This explains previous apparent validations of the sAP in d-dimensional systems [71–73], as these works focus on a scalar current parallel to the gradient. However, in the general vectorial-current case the role of the structured, divergence-free optimal current field associated to the wAP cannot be overlooked. Indeed, our general findings agree with very recent microscopic results for the ZRP which highlight the importance of the local structure of the current field in this model [77]. An interesting issue for future study concerns the stability of the wAP solution against space and time perturbations in d-dimensional boundary driven systems [78]. Finally, we mention that additivity violations are known to happen in 1D periodic systems via a dynamic phase transition to a traveling-wave phase with broken symmetries [25,28,31–33,68,79–81]. The natural question of course concerns the nature of this transition for $d > 1$. We anticipate that a similar spontaneous symmetry-breaking phenomenon exists at the fluctuation level in d dimensions, for which a form of weak additivity in terms of a structured current field also plays a crucial role [76].

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