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Directed motion generated by heat bath nonlinearly driven by external noise

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Abstract

Based on the heat bath system approach where the bath is nonlinearly modulated by an external Gaussian random force, we propose a new microscopic model to study directed motion in the overdamped limit for a nonequilibrium open system. Making use of the coupling between the heat bath and the external modulation as a small perturbation, we construct a Langevin equation with multiplicative noise- and space-dependent dissipation and the corresponding Fokker–Planck–Smoluchowski equation in the overdamped limit. We examine the thermodynamic consistency condition and explore the possibility of observing a phase-induced current as a consequence of statedependent diffusion and, necessarily, nonlinear driving of the heat bath by the external noise.

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In recent times, the phenomena of noise-induced transport under nonequilibrium conditions have gained wide interdisciplinary interest where the interplay of fluctuations and nonlinearity of the system plays an important role [1–5]. Exploitation of the nonequilibrium fluctuations present in the medium helps us to generate phase-induced-directed motion of the Brownian particle. The presence of spatial anisotropy in the potential together with nonequilibrium perturbations enables one to extract the useful work from random fluctuations without violating the second law of thermodynamics [3]. This led us to its wide applicability in explaining the dynamics of molecular motors [2, 6], directed transport in photovoltaic and photoreflective materials [7], and the efficiency of tiny molecular machines in a highly stochastic environment [4, 5, 8], realization of the ratchet effect in cold atom [9], and the construction of artificial

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molecular rotors that produce controlled directional motion mimicking molecular motor protein [10]. In some special cases, one can generate directed motion even in a symmetric potential due to state-dependent diffusion. For such systems, the state-dependent diffusion coefficient, D(q), felt by the Brownian particle could arise either due to the space-dependent friction or the presence of local hotspots [2, 3, 11, 12].

To the best of our knowledge, in almost all the above-mentioned cases the corresponding Langevin equation is either written phenomenologically or is constructed from a microscopic system heat bath Hamiltonian model where the associated heat bath is in thermal equilibrium. To generate directed motion one then applies an external perturbation, time periodic force or correlated random force, to break the symmetry of the force field as equilibrium thermal fluctuations are unable to create spontaneous symmetry breaking. Symmetry breaking can also be achieved by considering a nonlinear coupling between the Brownian particle and thermal heat bath thereby generating a multiplicative noise term in the resulting Langevin equation which in turn gives a position-dependent diffusion term effectively creating a phase-induced bias in the dynamics. In the present paper, we propose a system heat bath model where the heat bath is weakly modulated by an external noise. Although the microscopic model we present here has a close kinship to our earlier approach [13] to study escape from a metastable state within the context of external noise-modulated heat bath, the present formalism differs from our earlier model in the following way. The heat bath-external noise coupling is considered to be nonlinear and in addition to that the system is also nonlinearly coupled with the heat bath thereby resulting in a nonlinear multiplicative Langevin equation and the corresponding Fokker-Planck-Smoluchowski equation with space-dependent diffusion. We then explore the possibility of observing directed transport as a result of phase difference between the coupling function and the periodic potential in which the Brownian particle is moving. Our theoretical model can be tested experimentally to study the directional motion of artificial chemical rotors in photoactive solvent [10]. To observe the effect of external stochastic modulation, one can carry out the experiment in a photochemically active solvent (the heat bath) where the solvent is under the influence of external monochromatic light with fluctuating intensity of a wavelength which is absorbed solely by the solvent molecules. As a result of this, the modulated solvent heats up due to the conversion of light energy into heat energy by radiationless relaxation process and an effective temperature-like quantity develops due to the constant input of energy. Since the fluctuations in the light intensity result in the polarization of the solvent molecules, the effective reaction field around the reactants gets modified [14].

To start with, we consider a classical particle of unit mass bilinearly coupled to a heat bath consisting of N mass-weighted harmonic oscillators characterized by the frequency set ω_j . In addition to that, the heat bath is nonlinearly driven by an external noise $\epsilon(t)$. The Hamiltonian for the composite system is

$$H = H_S + H_B + H_{SB} + H_{\text{int}},\tag{1}$$

where $H_S = (p^2/2) + V(q)$, is the system's Hamiltonian with q and p being the coordinate and momentum of the system particle, respectively, and V(q) is the potential energy function of the system. $H_B + H_{SB} = \sum_{j=1}^{N} \left[(p_j^2/2) + (\omega_j^2/2) \{x_j - c_j f(q)\}^2 \right]$, where $\{x_j, p_j\}$ are the variables for the *j*th bath oscillator. The system–heat bath interaction is given by the coupling term $c_j \omega_j f(q)$, with c_j being the coupling strength. We consider the interaction, $H_{\text{int}} = \sum_{j=1}^{N} \kappa_j g(x_j) \epsilon(t)$, between the heat bath and the external noise $\epsilon(t)$, where κ_j denotes the strength of the interaction and $g(x_j)$ is an arbitrary analytic function of the bath variables, in general nonlinear. This type of interaction makes the bath variables explicitly time-dependent. A large class of phenomenologically modeled stochastic differential equation may be obtained from a microscopic Hamiltonian for particular choice of coupling function $g(x_j)$. In what follows we have chosen $g(x_j) = x_j^2/2$, which makes the spring constants of the bath oscillators time-dependent. The external noise is stationary, Gaussian with the properties $\langle \epsilon(t) \rangle_e = 0$ and $\langle \epsilon(t) \epsilon(t') \rangle_e = 2D\delta(t - t')$, where *D* is the strength of the external noise and $\langle \cdot \rangle_e$ implies averaging over the external noise processes. From equation (1), we have the dynamical equations for the system and bath variable

$$\ddot{q}(t) = -V'(q(t)) + f'(q(t)) \sum_{j} c_{j} \omega_{j}^{2} \{x_{j}(t) - c_{j} f(q(t))\},$$
(2)

$$\ddot{x}_j(t) + \left\{\omega_j^2 + \kappa_j \epsilon(t)\right\} x_j(t) = c_j \omega_j^2 f(q(t)),$$
(3)

where we have used $g(x_j) = x_j^2/2$. To solve equation (3) for x_j , we assume a solution of the form

$$x_{j}(t) = x_{j}^{0}(t) + \kappa_{j} x_{j}^{1}(t),$$
(4)

where $x_i^0(t)$ is the solution of the unperturbed equation of motion

$$\ddot{x}_{i}^{0}(t) + \omega_{j}^{2} x_{i}^{0}(t) = c_{j} \omega_{j}^{2} f(q(t)).$$
(5)

The physical situation that has been addressed here is the following, we consider that at t = 0, the heat bath is in thermal equilibrium in the absence of the external noise $\epsilon(t)$. At $t = 0_+$, the external noise agency is switched on and the heat bath is modulated by $\epsilon(t)$ [13]. Then, $x_i^{1}(t)$ must satisfy the equation

$$\ddot{x}_{j}^{1}(t) + \omega_{j}^{2} x_{j}^{1}(t) = -x_{j}^{0}(t)\epsilon(t),$$
(6)

with the initial conditions $x_i^1(0) = p_i^1(0) = 0$. The solution of equation (6) is given by

$$x_{j}^{1}(t) = -\frac{1}{\omega_{j}} \int_{0}^{t} dt' \sin \omega_{j}(t-t') x_{j}^{0}(t') \epsilon(t').$$
⁽⁷⁾

The formal solution of equation (5) is given by

$$x_{j}^{0}(t) = x_{j}^{0}(0)\cos\omega_{j}t + \frac{p_{j}^{0}(0)}{\omega_{j}}\sin\omega_{j}t + c_{j}\omega_{j}\int_{0}^{t}dt'\sin\omega_{j}(t-t')f(q(t')),$$
(8)

where $x_j^0(0)$ and $p_j^0(0)$ are the initial position and momentum, respectively, of the *j*th oscillator. Now using this solution in equation (7) we have, after an integration by parts, the equation of motion for $x_j^1(t)$ which gives the equations of motion for the bath variables $x_j(t)$ (from equation (4)) as

$$\begin{aligned} x_{j}(t) &= \left[x_{j}^{0}(0) - c_{j} f(q(0)) \right] \cos \omega_{j} t + \frac{p_{j}^{0}(0)}{\omega_{j}} \sin \omega_{j} t \\ &+ c_{j} \int_{0}^{t} dt' \cos \omega_{j} (t - t') f'(q(t')) \dot{q}(t') - \frac{\kappa_{j}}{\omega_{j}} \int_{0}^{t} dt' \sin \omega_{j} (t - t') \epsilon(t') x_{j}^{0}(t'). \end{aligned}$$

$$(9)$$

Using the above solution in equation (2), we finally obtain the equation of motion for system variable as

$$\ddot{q}(t) = -V'(q(t)) + f'(q(t)) \sum_{j} c_{j} \omega_{j}^{2} \left[\left\{ x_{j}^{0}(0) - c_{j} f(q(0)) \right\} \cos \omega_{j} t + \frac{p_{j}^{0}(0)}{\omega_{j}} \sin \omega_{j} t \right] \\ - \sum_{j} c_{j}^{2} \omega_{j}^{2} f'(q(t)) \int_{0}^{t} dt' \cos \omega_{j} (t - t') f'(q(t')) p(t') \\ - f'(q(t)) \sum_{j} c_{j} \kappa_{j} \omega_{j} \int_{0}^{t} dt' \sin \omega_{j} (t - t') \epsilon(t') x_{j}^{0}(t'),$$
(10)

where $p(t) = \dot{q}(t)$ is the generalized momentum of the system variable. This equation can be rewritten as

$$\ddot{q}(t) = -V'(q(t)) - f'(q(t)) \int_0^t dt' \gamma(t-t') f'[q(t')] p(t') + f'(q(t)) F(t) -f'(q(t)) \sum_j^N c_j \kappa_j \omega_j \int_0^t dt' \sin \omega_j (t-t') x_j^0(t') \epsilon(t'),$$
(11)

where we have defined $\gamma(t)$ and F(t) as, $\gamma(t) = \sum_{j=1}^{N} c_j^2 \omega_j^2 \cos \omega_j(t)$ and $F(t) = \sum_{j=1}^{N} c_j \omega_j^2 [\{x_j(0) - c_j f(q(0))\} \cos \omega_j t + (p_j(0)/\omega_j) \sin \omega_j t]$. At this point, we note that the forcing term F(t) is deterministic as expected. It ceases to be deterministic when it is not possible to specify all the $x_j^0(0)$'s and $p_j^0(0)$'s, i.e., the initial conditions of all the bath variables, exactly. The standard procedure to overcome this problem is to consider a distribution of $x_j^0(0)$ and $p_j^0(0)$ to specify the statistical properties of the bath-dependent forcing term F(t). The distribution of the bath oscillators is assumed to be a canonical distribution of the Gaussian form

$$W[x_j^0(0), p_j^0(0)] = Z^{-1} \exp\left[-\frac{H_B + H_{SB}}{k_B T}\right],$$
(12)

where Z is the bath-partition function. This choice of the distribution function of bath variables makes the internal noise F(t) Gaussian. It is now easy to verify the statistical properties of F(t) as $\langle F(t) \rangle = 0$ and $\langle F(t)F(t') \rangle = 2k_B T \gamma (t - t')$, where k_B is the Boltzmann constant and T is the equilibrium temperature. $\langle \cdot \rangle$ implies the average over the initial distributions of bath variables which is assumed to be a canonical distribution of the Gaussian form as given in equation (12). The second relation is the celebrated fluctuation–dissipation relation [15] which ensures that the bath was in thermal equilibrium at t = 0.

To identify equation (11) as a generalized Langevin equation we must impose some conditions on the coupling coefficients c_i and κ_i , on the bath frequencies ω_i and on the number N of the bath oscillators that will ensure that $\gamma(t)$ is indeed dissipative and the last term in equation (11) is finite for $N \to \infty$. A sufficient condition for $\gamma(t)$ to be dissipative is that it is positive definite and decreases monotonically with time. These conditions are achieved if $N \to \infty$ and if $c_j \omega_j^2$ and ω_j are sufficiently smooth functions of j [17]. As $N \to \infty$, one replaces the sum by an integral over ω weighted by a density of state $\rho(\omega)$. Thus, to obtain a finite result in the continuum limit the coupling function $c_i = c(\omega)$ and $\kappa_i = \kappa(\omega)$ are chosen [13, 16] as $c(\omega) = c_0/\omega\sqrt{\tau_c}$ and $\kappa(\omega) = \kappa_0$, where c_0 and κ_0 are constants and τ_c is the correlation time of the heat bath. The choice $\kappa(\omega) = \kappa_0$ is the simplest one where we assume that every bath mode is excited with the same intensity. This simple choice makes the relevant term finite for $N \to \infty$. Consequently, $\gamma(t)$ becomes, $\gamma(t) = \left(c_0^2/\tau_c\right) \int d\omega \rho(\omega) \cos \omega t$; $1/\tau_c$ may be characterized as the cutoff frequency of the bath oscillators. The density of modes $\rho(\omega)$ of the heat bath is assumed to be Lorentzian, $\rho(\omega) = (2/\pi) \left[\tau_c / (1 + \omega^2 \tau_c^2) \right]$. The above assumption resembles broadly the behavior of the hydrodynamical modes in a macroscopic system [18]. With these forms of $\rho(\omega), c(\omega)$ and $\kappa(\omega)$ we have the expression for $\gamma(t)$ as $\gamma(t) = (c_0^2/\tau_c) \exp(-t/\tau_c)$, which reduces to $\gamma(t) = 2c_0^2 \delta(t)$ for vanishingly small correlation time τ_c and consequently one obtains a δ -correlated noise process.

Taking into consideration all the above assumptions and assuming that the system variable evolves much more slowly in comparison to the external noise $\epsilon(t)$, in the limit $\tau_c \rightarrow 0$, equation (11) reduces to

$$\ddot{q}(t) = -V'(q(t)) - \gamma [f'(q(t))]^2 \dot{q}(t) + f'(q(t))F(t) + \gamma \kappa_0 f(q(t))f'(q(t))\epsilon(t),$$
(13)

where $\gamma = c_0^2$ is the dissipation constant and the Langevin force F(t) is characterized by the statistical properties

$$\langle F(t) \rangle = 0, \qquad \langle F(t)F(t') \rangle = 2\gamma k_B T \delta(t - t').$$
 (14)

Equation (13) is the generalized Langevin equation for the system variable. At this juncture, it is noteworthy that for f(q) = q, equation (13) reduces to $\ddot{q}(t) = -V'(q(t)) - \gamma \dot{q}(t) + F(t) + \gamma \kappa_0 q(t) \epsilon(t)$. Thus, for linear system–bath coupling (i.e. for f(q) = q), our Hamiltonian given by equation (1) may be the starting point for the construction of a Langevin equation with both additive and multiplicative noise, which has numerous applications in various fields of physics, e.g. phase transition, etc. For harmonic potential, this equation has been extensively studied by many authors in various contexts [19].

In the Langevin equation (13), the noise terms (internal and external) appear multiplicatively and the dissipation is space-dependent. Using the method of van Kampen [19] for nonlinear stochastic differential equations, the Fokker–Planck equation corresponding to the Langevin equation (13) is given by [13, 19]

$$\frac{\partial P}{\partial t} = -\frac{\partial}{\partial q}(pP) + \frac{\partial}{\partial p}\{\lambda(q)p + V'(q)\}P + \{\lambda(q)k_BT + \gamma^2\kappa_0^2D[f(q)f'(q)]^2\}\frac{\partial^2 P}{\partial p^2},$$
(15)

where P = P(q, p, t) is the phase space probability density function and $\lambda(q) = \gamma [f'(q)]^2$ is the space-dependent dissipation function. Instead of handling two noise processes (internal and external) independently, one can define an *effective* noise process $\xi(t)$ and an auxiliary function G(q) to obtain the same Fokker–Planck equation (15) from the following Langevin equation:

$$\ddot{q} = -V'(q) - \lambda(q)\dot{q} + G(q)\xi(t), \tag{16}$$

with

$$\langle \xi(t) \rangle = 0, \qquad \langle \xi(t)\xi(t') \rangle = 2\delta(t - t'), \tag{17}$$

$$\lambda(q) = \gamma [f'(q)]^2, \qquad G(q) = f'(q) \sqrt{\gamma k_B T} + D(\gamma \kappa_0)^2 f^2(q).$$
(18)

That the Langevin equation (16) gives the same Fokker–Planck equation (15) can be verified by using van Kampen's methodology [19]. The construction of Langevin equation using an effective noise term and an auxiliary function has been done earlier in the configuration space by Wu *et al* [20], whereas we have written the Langevin equation (16) in the phase space. Thus, as far as the equation for the evolution of probability density function is concerned, equation (16) is the equivalent description of the stochastic differential equation (13). Equation (16) is one of the *key results* of this work as it incorporates the effects of thermal noise F(t)and the external noise $\epsilon(t)$ in an unified way even when the underlying noise processes are multiplicative due to the nonlinear system–bath coupling and nonlinear modulation of the heat bath by an external noise. It is important to mention here that equation (16) describes a thermodynamically open system where there is no fluctuation–dissipation relation so that the system will not reach at usual thermal equilibrium, instead, a steady state is attainable for large t [13, 19]. From the computational point of view, generation of a single multiplicative noise processes is much more economical than to generate two separate multiplicative noise processes.

In equation (16), the noise is multiplicative and the dissipation is space-dependent. In the case of large dissipation, one eliminates the fast variables adiabatically to get a simpler description of the system dynamics. The traditional approach to the elimination of fast

variables for multiplicative noise processes does not always give the correct description. In order to get the correct Langevin equation in the overdamped limit, we follow the method of Sancho *et al* [21] and then using van Kampen's lemma [22] and Novikov's theorem [23] we get the Fokker–Planck–Smoluchowski equation corresponding to equation (16) for the probability density P(q, t) in the configuration space [21]:

$$\frac{\partial P(q,t)}{\partial t} = \frac{\partial}{\partial q} \frac{1}{\lambda(q)} \left[V'(q) + \frac{\partial}{\partial q} \frac{G^2(q)}{\lambda(q)} \right] P(q,t).$$
(19)

In the ordinary Stratonovich description [21], the Langevin equation corresponding to the Fokker–Planck equation (19) is

$$\dot{q} = -\frac{V'(q)}{\lambda(q)} - \frac{G(q)G'(q)}{[\lambda(q)]^2} + \frac{G(q)}{\lambda(q)}\xi(t).$$
(20)

Equation (20) differs from the Langevin equation, obtained by using the traditional way of adiabatic elimination of fast variable, due to the presence of the second term on the right-hand side. This term, $G(q)G'(q)/[\lambda(q)]^2$, represents the effect of multiplicative noise in the process of elimination of fast variable [21].

The stationary solution of equation (19) contains inhomogeneous effective temperaturelike term, a generalization of the Boltzmann factor for state-dependent diffusion in open system, which arises due to the entanglement of the external driving with the nonlinearity of the system heat bath coupling, a well-known effect in several contexts, e.g., Landauer Blow torch effect [11]. In the absence of external bath modulation, i.e., when $G(q) = f'(q)\sqrt{\gamma k_B T}$, equation (19) gives the correct equilibrium distribution function, $P_{eq}(q) = \mathcal{N} \exp[-V(q)/k_B T]$, with \mathcal{N} being the normalization constant. In the overdamped limit, we then have the stationary current as

$$J = -\frac{1}{\lambda(q)} \left[V'(q) + \frac{\mathrm{d}}{\mathrm{d}q} \left(\frac{G^2(q)}{\lambda(q)} \right) \right] P_{\mathrm{st}}(q).$$
(21)

Integrating the above equation, we have the expression of stationary probability distribution in terms of stationary current

$$P_{\rm st}(q) = \frac{e^{-\phi(q)}}{G^2(q)/\lambda(q)} \left[\frac{G^2(0)}{\lambda(0)} P_{\rm st}(0) - J \int_0^q \lambda(q') e^{\phi(q')} \, \mathrm{d}q' \right],\tag{22}$$

where

$$\phi(q) = \int_0^q \frac{V'(q')}{G^2(q')/\lambda(q')} \, \mathrm{d}q' = \int_0^q \frac{V'(q')}{k_B T + D\gamma \kappa_0^2 f^2(q')} \, \mathrm{d}q'. \tag{23}$$

We then consider a symmetric periodic potential with periodicity 2π , $V(q) = V(q+2\pi)$, and the periodic coupling function with the same periodicity as the potential, $f(q) = f(q+2\pi)$. Now applying the periodic boundary condition on $P_{st}(q)$, $P_{st}(q) = P_{st}(q+2\pi)$, and the normalization condition on stationary probability distribution we have the expression for stationary current [24]

$$J = [1 - e^{\phi(2\pi)}] / \left\{ \int_0^{2\pi} \frac{\lambda(q)}{G^2(q)} e^{-\phi(q)} dq \int_0^{2\pi} \lambda(q') e^{\phi(q')} dq' - [1 - e^{\phi(2\pi)}] \right. \\ \left. \times \int_0^{2\pi} \frac{\lambda(q)}{G^2(q)} e^{-\phi(q)} \int_0^q \lambda(q') e^{\phi(q')} dq' dq \right\}.$$
(24)

From the condition of periodicity it is clear that for the periodic potential and the periodic derivative of coupling function with same periodicity $V'(q)/[G^2(q)/\lambda(q)]$ is periodic with same periodicity. This makes the effective potential $\phi(2\pi)$ equal to zero so that the numerator



Figure 1. Variation of current, *J*, as a function of phase difference, θ , for different values κ_0^2 and for the parameter set $\alpha = 0.5$, $k_B T = 0.1$, $\gamma = 1.0$ and D = 1.0.



Figure 2. Plot of the generalized potential $\phi(q)$ as a function of the coordinate q for different values of κ_0^2 and for the parameter set $\alpha = 0.5$, $k_B T = 0.1$, $\gamma = 1.0$, D = 1.0 and $\theta = 0.5\pi$.

of equation (24) reduces to zero. Thus, there is no occurrence of current for a periodic potential and periodic derivative of coupling function with same periodicity and hence there is no violation of the second law of thermodynamics. The thermodynamic consistency based on symmetry consideration ensures the validity of the present formalism. Büttiker [25] have shown that a overdamped particle subjected to a drift force field with sinusoidal space dependence and also a sinusoidally modulated space-dependent diffusion with the same period as the drift experiences a net driving force. The resulting current depends on the amplitude of the modulation of diffusion and is a periodic function of phase difference between the sinusoidal drift and the sinusoidal modulation of the diffusion.

Let us consider that the particle is moving in a sinusoidal symmetric potential of the form

$$V(q) = V_0 [1 + \cos(q + \theta)],$$
(25)

where V_0 is constant and may be taken as barrier height and θ is the phase factor which can be controlled externally. The coupling function is chosen as $f(q) = q + \alpha \cos q$, where α is the modulation parameter. We now calculate the current given by equation (24). In figure 1, the variation of current as a function of phase difference is shown for different values of the coupling constant κ_0 . Since κ_0 is the perturbation parameter in our analysis we have kept its maximum value low, i.e., $\sim k_B T$. For the value of the other parameters we have chosen a particular set from the complete parameter space. An extensive analysis using the full parameter space will be given in our future communication. The current shown in figure 1 is basically due to the phase difference between the symmetric periodic potential and the spacedependent diffusion caused by the nonlinear modulation of the heat bath by external noise. The current does vanish when the phase difference is either zero or integral multiple of π . When the heat bath is linearly modulated by external noise source, it is easy to observe that the effective potential $\phi(q)$ is integrable and there will be no asymmetry in the effective potential as the noise in the corresponding Langevin equation appears additively and the diffusion coefficient becomes space-independent. Thus, when the heat bath is driven nonlinearly by the external noise agency there is a net directed motion or phase-induced current. This is because of the fact that when the external noise drives the heat bath nonlinearly the phase bias gives a tilt to the effective potential $\phi(q)$ which makes the transition between left to right and right to left unequal. In figure 2, we plot the generalized potential $\phi(q)$ for various coupling constant κ_0^2 . The phase difference (hence the nonlinear driving of the heat bath) breaks the detailed balance of the system. When the phase difference is zero or the heat bath is driven linearly there is no net drift velocity. Thus, when we drive the heat bath linearly with δ -correlated external noise, even in the presence of phase difference between V(q) and f'(q), there is no net current. For net drift, apart from phase difference, nonlinear driving of the heat bath is required. This is the *central result of this paper*.

In conclusion, we have proposed a new microscopic analysis to study the generation of directed motion for a nonlinearly driven heat bath by an external noise. Making use of a perturbative treatment we have derived an effective Langevin equation with space-dependent dissipation and multiplicative noise. Using the corresponding Fokker–Planck–Smoluchowski equation with a space-dependent diffusion coefficient, we have checked the thermodynamic consistency condition and have shown that to observe a phase-induced current one necessarily needs a nonlinear driving of the heat bath by an external Gaussian noise. In our future venture in this direction, we wish to compare our analytical result with stochastic simulation using the complete parameter space.

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