Nonequilibrium relation between potential and stationary distribution for driven diffusion

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We investigate the relation between an applied potential and the corresponding stationary-state occupation for nonequilibrium and overdamped diffusion processes. This relation typically becomes long ranged resulting in global changes for the relative density when the potential is locally perturbed, and inversely, we find that the potential needs to be wholly rearranged for the purpose of creating a locally changed density. The direct question, determining the density as a function of the potential, comes under the response theory out of equilibrium. The inverse problem of determining the potential that produces a given stationary distribution naturally arises in the study of dynamical fluctuations. This link to the fluctuation theory results in a variational characterization of the stationary density upon a given potential and vice versa.

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I. INTRODUCTION

Imagine independent colloidal particles in a potential field and subject to friction and noise as imposed by a thermal reservoir or background fluid. In thermal equilibrium at inverse temperature β, $\text{Prob}(x) \propto \exp[-\beta V(x)]$, where V is the potential on the states x. Typical examples include the Laplace barometric formula but also the distribution of particles in a fluid undergoing rigid rotation. We now add an external forcing and we wait until a steady regime gets installed. The stationary statistics depends on the potential, but most certainly and because of the forcing the resulting time-invariant distribution of velocities and positions of the particles gets modified with respect to the Maxwell-Boltzmann statistics. The relation between potential and stationary distribution is far from understood for generic nonequilibrium systems, beyond its general specification as being for example a solution to the time-independent Fokker-Planck-Smoluchowski equation.

We show here that small local variations in the potential can globally affect the relative density, provided a nongradient driving is present. That effect already arises in linear order around equilibrium. For the inverse relation, we are asking to reconstruct the potential which, under a known driving, realizes a stationary distribution. In equilibrium, the change in the potential needed to change the density $\rho \to \rho \exp(-A)$ is simply equal to A—not so in nonequilibrium. It is then a genuine problem what potential field can produce a given particle density at a fixed driving. Beyond obvious applications in interpreting observational data, this question also naturally emerges in dynamical fluctuation theory, cf. [1]. In particular, the large fluctuations of certain time averages around their stationary values are governed by a functional (sometimes called an effective potential) that is given in terms of the potential of the inverse problem. We will give two possible approaches to finding the potential, one of which is analytical and the other one is based on a variational formula.

The specific examples we treat in this paper and for which the analysis can be applied are those of diffusing particles in a background rotational velocity field. Diffusion in rotating media is one of the central objects in geophysical and astrophysical applications. The question of nonlocal and irreversible effects is of particular interest for galactic dynamics, where according to Chandrasekhar's theory the huge number of relatively small-size gravitational encounters gives rise to an effective Brownian motion for test stars, cf. [2]; see also [3] for an account in the context of galaxy formation. Arguably, also experimentally a most realistic scenario for maintaining a constant nonconservative force is via differential rotation. One can think of concentric cylinders rotating at different angular frequencies which are imposed on the fluid by stick boundary conditions. Far from equilibrium and under a general angular (possibly angle-dependent) driving one can expect not only that currents are being maintained but also that the time-symmetric aspects of diffusion can be essentially changed. It is known that the diffusion phenomenon itself may be influenced by rotation, even by rigid rotation [4]. Related considerations on nonequilibrium diffusion also apply to other scenarios, including, e.g., shear flow [5–8] and oscillatory flows [9], and stochastic models of particle transport in turbulent media necessarily include discussions of driven diffusion phenomena [10]. Colloidal particles in harmonic wells and driven by shear flow have been explicitly treated for the violation of the fluctuation-dissipation relation in [11].

The relation between stationary density and potential is generically nonlocal or long range but as our particles are mutually independent, that obviously says nothing about the generic long-range correlations in nonequilibrium systems. As we will see however, the mathematical mechanisms are not unrelated. Several of these nonlocal effects and generic long-range correlations under nonequilibrium conditions have been discussed in similar contexts of interacting particle systems, most recently from the point of fluctuation theory [12–14], in perturbation theory for the stationary density [15], and as a result of the breaking of the fluctuation-dissipation relation [16–18]. It was originally the mode-coupling theory in hydrodynamic studies for a fluid not in thermal equilibrium that revealed the (macroscopic) long-

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range correlations between fluctuations. Light scattering experiments can reveal these correlations [19–22]. In contrast, the present work analyzes the nonlocality on a mesoscopic length scale and that does not result from particle interactions but as is already present in a single-particle distribution (or, equivalently, in a density or an ensemble of independent particles), due to the imposed nonequilibrium driving.

In Sec. II, we specify our dynamical model: independent particles undergoing an overdamped diffusive motion in a confining potential and under driving. The nonlocality in the relation between potential and distribution is discussed throughout Sec. III. The latter already speaks about the inverse problem of determining the potential for a given density, which is then elaborated in Sec. IV, in the context of variational principles and for the purpose of the dynamical fluctuation theory. In Appendixes A–C we add further details about the McLennan's interpretation of nonequilibrium distributions, about the Green's functions encountered in the response problem, and about the dynamical fluctuation origin of the variational principles under consideration.

II. DIFFUSION IN A TWO-DIMENSIONAL ROTATIONAL FLUID

Restricting ourselves for the moment to the two-dimensional plane with points labeled by the polar coordinates $x=(r,\theta)$, we consider an ensemble of independent test particles subject to a rotation-symmetric force with potential $U(r)$, sufficiently confining so that

$$Z = 2\pi \int_0^{+\infty} e^{-U} r dr < +\infty.$$

The particles are suspended in a nonequilibrium fluid exerting an additional force that can have some conservative component with potential $\Phi(r,\theta)$ and a nonconservative force $v=(v_r,v_\theta)$ for which we assume that the radial component $v_r=0$ vanishes. The angular driving force v_θ can be associated with the local velocity of the background fluid which is maintained in a differential rotation state. We assume a thermally homogeneous background (setting the temperature to one), modeled by a Gaussian and temporally white noise. Given that the motion is noninertial, it satisfies the Langevin equation

$$dx_t = v dt - \nabla(U+\Phi)dt + \sqrt{2} dB_t \tag{2.1}$$

with B_t standard two-dimensional Brownian motion.

An implicit assumption in the above construction is the smoothness of the functions U, Φ, and v_θ on the domain taken here as the entire two-dimensional plane. Yet, interesting modifications arise when the origin $r=0$ is not accessible and the particles can only move in the nonsimply connected domain obtained by removing the latter. This allows for possible singularities when approaching the origin and the existence of a potential for the driving force v is no longer equivalent to the condition $\nabla \times v = 0$; the rotational field of the form $v=(0,v_\theta)$, $v_\theta \propto 1/r$ serving as example. The exclusion of the origin can be ensured, e.g., by an infinitely repellent potential therein or via suitable boundary conditions at the origin.

Note that in the absence of a potential, $U=\Phi=0$, dynamics (2.1) does continue to make sense, although a normalizable stationary distribution no longer exists. The transient regime is still relevant and has been studied in detail [23].

The stationary distribution for dynamics (2.1) has density ρ verifying the Fokker-Planck-Smoluchowski equation

$$\nabla \cdot J = 0, \quad J = \rho v - \rho \nabla (U+\Phi) - \nabla \rho. \tag{2.2}$$

We refer also to [8,24] for more thermodynamic and kinetic gas considerations in the derivation of that nonequilibrium dynamical equation. In polar coordinates the probability current $J=(J_r,J_\theta)$ takes the form

$$J_r = -\rho \frac{\partial(U+\Phi)}{\partial r} - \frac{\partial \rho}{\partial r}, \quad J_\theta = \rho v_\theta - \frac{\rho}{r}\frac{\partial \Phi}{\partial \theta} - \frac{1}{r}\frac{\partial \rho}{\partial \theta}. \tag{2.3}$$

By turning on the driving v_θ, typically not only an angular current J_θ is generated but also a nonzero radial component J_r does get maintained. This is *a priori* not in contradiction with the existence of a stationary distribution; its normalizability essentially depends on the imposed potential $U+\Phi$ and on the boundary conditions.

Our general aim is to analyze the relation between test potentials Φ and stationary densities ρ, under a given confining rotation-symmetric potential U and as mediated by the rotational field v_θ. First, we examine the issue of spatial nonlocality.

III. LONG-RANGE RESPONSE TO CHANGING THE POTENTIAL

Nonlocal features have been widely discussed in the nonequilibrium literature. Mostly however deals with the presence of long-range correlations, cf. [13,16,19,25–27] for time-separated viewpoints, or with models of self-organized criticality, cf. [28]. In our case, we have independent particles; hence there are no correlations between the particles and correlations between spatial points only appear because of fixing the number of particles or by fixing the mass. We think of the spatial dependence in the density as it is affected by local changes in the external potential, and vice versa.

In the absence of driving, $v=0$, stationarity equation (2.1) has the usual equilibrium solution $\rho \propto e^{-U-\Phi}$, $J=0$, which is manifestly a local functional of the test potentials Φ in the sense that the response

$$\frac{\delta}{\delta \Phi(z)}\left[\log \frac{\rho(x)}{\rho(y)}\right] = \delta(z-y) - \delta(z-x)$$

is insensitive to perturbing Φ away from both points x and y.

One can ask to what extent this is an equilibrium property but, in fact, it is easy to devise special nonequilibrium conditions where such a locality still holds. As a simple example, take $\Phi=0$ and let the angular driving velocity be rotationally symmetric, $v_\theta=u(r)$. Then, the stationary density and current become

$$\rho = \frac{1}{Z}e^{-U}, \quad J = \left(0, \frac{u}{Z}e^{-U}\right). \tag{3.1}$$

Although the stationary density coincides with the equilibrium solution and is perfectly local in the potential U, it now corresponds to a current-carrying steady state. Thus one cannot unambiguously decide just from the stationary distribution itself whether the system rests in equilibrium or whether irreversible flows are present.

Yet, generic nonequilibrium distributions do get modified due to driving and, as a result, they typically pick up some nonlocality. Next comes a simple demonstration.

A. Exactly solvable model

In the example above the radial currents are absent and the steady state is rotation symmetric. A simple exactly solvable case where the rotation symmetry is broken can be obtained for an angular driving of the form $v_\theta = f(\theta)/r$ and for test potentials that are constant along radials, $\Phi(r,\theta) = \Psi(\theta)$. The origin is excluded by the boundary condition $J_r(0)=0$. In this case, the stationary density is found to be of the form

$$\rho(r,\theta) = p(r)q(\theta), \quad p(r) = \frac{1}{Z}e^{-U(r)}, \tag{3.2}$$

which is under the given assumptions the general form for a density with everywhere vanishing radial current, $J_r=0$. The steady state decomposes into separated concentric motions and the angular distribution $q(\theta)$ in Eq. (3.2) is determined from stationarity condition (2.2), which reads $J_\theta(r,\theta) = j(r)$ for some rotation-symmetric function $j(r)$ that can be determined. Explicitly, from Eq. (2.3),

$$\{f(\theta) - \Psi'(\theta)\}q(\theta) - q'(\theta) = \frac{rj(r)}{p(r)}, \tag{3.3}$$

which decouples the polar coordinates and confirms ansatz (3.2). The angular current $j(r)$ is obtained by dividing Eq. (3.3) by q and integrating over the angle variable, which yields, always for $v_\theta(r,\theta) = f(\theta)/r$,

$$j(r) = \frac{p(r)}{r} \frac{\displaystyle\int_0^{2\pi} f(\theta)d\theta}{\displaystyle\int_0^{2\pi} q^{-1}(\theta)d\theta}. \tag{3.4}$$

As expected, a nonzero steady current is maintained whenever the angular driving does not allow for a potential, i.e., if the work performed over concentric circles is nonzero, $w = \int_0^{2\pi} f d\theta \neq 0$. Using the normalization condition $\int_0^{2\pi} q(\theta)d\theta = 1$, the solution of Eq. (3.3) is obtained in the form

$$q(\theta) = \frac{1}{\Omega}\int_0^{2\pi} e^{W(\theta',\theta)}d\theta',$$
$$\Omega = \int_0^{2\pi}\int_0^{2\pi} e^{W(\theta',\theta)}d\theta' d\theta \tag{3.5}$$

with the work function

$$W(\theta',\theta) = \Psi(\theta') - \Psi(\theta) + \oint_{\theta'}^{\theta} f\, d\xi.$$

Here we have used the notation $\oint_{\theta'}^{\theta}$ for the integral performed along the positively oriented path $\theta' \to \theta$ on the circle, i.e., it coincides with $\int_{\theta'}^{\theta}$ for $\theta' \leq \theta$ whereas it equals to $\int_{\theta'}^{2\pi} + \int_0^{\theta}$ otherwise. In the sequel we also employ the shorthand $\oint$ for the integral $\int_0^{2\pi}$.

Equivalently, the same solution to Eq. (3.3) can also be obtained in terms of the current $j(r)$; this leads to the next explicit expression for the latter,

$$j(r) = \frac{p(r)}{\Omega r}(e^w - 1). \tag{3.6}$$

The equilibrium angular distribution is recovered for $w=0$ (or $j=0$), in which case the work function $W(\theta',\theta)$ derives from a potential and formulas (3.5) boils down to the Boltzmann-Gibbs form.

For $w \neq 0$ the character of the stationary density becomes modified, as can be read from the response to changes in the test potential $\Phi = \Psi(\theta)$ that we take to depend on the angle θ only. We take the functional derivative for changes in the value of Ψ at fixed angle η,

$$\frac{\delta}{\delta\Psi(\eta)}\left[\log\frac{\rho(r,\theta)}{\rho(r,\theta')}\right] = Y(\eta,\theta') - Y(\eta,\theta), \tag{3.7}$$

where

$$Y(\eta,\theta) = \delta(\eta - \theta) - \frac{e^{W(\eta,\theta)}}{\displaystyle\oint e^{W(\eta',\theta)}d\eta'}.$$

It is the second term that generates the nonlocality as its reciprocal

$$\oint e^{W(\eta',\theta) - W(\eta,\theta)}d\eta' = \int e^{\Psi(\eta) - \Psi(\eta') + \oint_{\eta}^{\eta'}\{f - w\delta(\xi-\theta)\}d\xi}d\eta' \tag{3.8}$$

still depends on θ. Note also that since the work function $W(\eta,\theta)$ is discontinuous at $\theta=\eta$, so is the nonlocal contribution in the response [Eq. (3.7)] at $\eta=\theta$ and $\eta=\theta'$.

That nonlocal term is manifestly a correction of order $O(w)$; hence, some more explicit information can be obtained within the weak driving approximation, considering the driving force $f(\theta)$ (or total work per cycle w) small. This yields, up to $O(w)$,

$$\frac{\delta}{\delta\Psi(\eta)}\left[\log\frac{\rho(r,\theta)}{\rho(r,\theta')}\right] = \delta(\eta-\theta') - \delta(\eta-\theta) + wq_*(\eta) \times \begin{cases} \displaystyle\oint_{\theta'}^{\theta} q_* d\xi, & \text{if } \eta \in (\theta \to \theta') \\ \displaystyle\oint_{\theta}^{\theta'} -q_* d\xi, & \text{if } \eta \in (\theta' \to \theta), \end{cases}$$

where $q_*(\eta)$ stands for the auxiliary density

$$q_*(\eta) = \frac{e^{\Psi(\eta)}}{\oint e^{\Psi} d\xi}$$

and $\eta \in (\theta \to \theta')$ indicates that η belongs to the positively oriented path from θ to θ'. This explicitly confirms the nonlocal and discontinuous structure of the response: *The relative density $\rho(r,\theta)/\rho(r,\theta')$ of our weakly driven system remains (strongly) sensitive to locally modifying the potential, $\Psi(\theta) \to \Psi(\theta) + \epsilon\delta(\theta - \eta)$, at an arbitrary angle η. The effect disappears at equilibrium*, $w=0$.

Note that this special example is essentially one dimensional and we have so far only considered the response to an r-constant change in the potential. The response to a strictly local perturbation will be discussed in the next section by a more general method.

The nonlocality of the inverse problem for this specific example, potential as function of the density, is continued around Eqs. (3.13)–(3.15).

B. General linear theory

Having observed that the nonlocal features of nonequilibrium states already emerge in the lowest order of the driving strength, we can now follow the linear analysis more systematically. The method is by now well known; we refer to earlier work of McLennan and others [29,30]. The analysis starts from the overdamped form [Eq. (2.1)], and again for simplicity we keep in mind diffusion in the entire plane under natural boundary conditions (decay at infinity).

One takes the reference equilibrium distribution (for $v=0$) as

$$\rho_o(x) = \frac{1}{\mathcal{Z}} e^{-V(x)}, \tag{3.9}$$

where we combine $V=U+\Phi$ and $\mathcal{Z}$ is the normalization. Assume now that the driving velocity field v is uniformly small, $|v|=O(\varepsilon)$.

The solution of the stationarity equation (2.2) to linear order in ε reads

$$\log \frac{\rho}{\rho_o} = \frac{1}{L_V}(\nabla \cdot v - v \cdot \nabla V), \tag{3.10}$$

where $L_V = -\nabla V \cdot \nabla + \Delta$, which is recognized as the generator of a reversible diffusion in potential V; see Appendix A for more details and for a physical interpretation in terms of the McLennan's theory [29]. Writing Eq. (3.10) in the form

$$\Delta \nu - \nabla V \cdot \nabla \nu = \nabla \cdot v - v \cdot \nabla V \tag{3.11}$$

with $\nu = \log(\rho/\rho_o)$, its variation along $V \to V + \delta V$ is

$$\Delta \delta\nu - \nabla V \cdot \nabla \delta\nu - \nabla \delta V \cdot \nabla \nu = - v \cdot \nabla \delta V.$$

In terms of the equilibrium generator L_V and the stationary current $J = \rho(v - \nabla V) - \nabla \rho$, this reads

$$L_V \delta\nu = -\frac{J}{\rho} \cdot \nabla \delta V \tag{3.12}$$

always up to terms $O(\varepsilon^2)$; in the same order the density ρ on the right-hand side can be replaced by ρ_o. This is a Poisson equation for $\delta\nu$ in which the Laplacian (free diffusion) is modified with a drift term in potential V. Note that since $L_V = \frac{1}{\rho_0}\nabla \cdot (\rho_0 \nabla)$ and $\nabla \cdot J = 0$, this problem is equivalent to studying the electrostatic potential in an inhomogeneous dielectric environment as generated by a source with zero total charge. Whereas the local component of the response to δV is already hidden in the V dependence of the equilibrium density ρ_o, the nonlocal character of solutions to Eq. (3.12) follows from general features of elliptic operators. The solution of the free Poisson equation (with only the Laplacian and natural boundary conditions at infinity) is explicit and manifestly long range. The potential V or the finiteness of the system introduces an extra confinement and the claim needs to be refined. One expects that within the confinement region where the density ρ_o is approximately constant and near its maximal value, the response $\delta\nu(x)$ at x to a local perturbation δV (both localized within that region) can be well estimated by replacing L_V with the free Laplacian $L_0 = \Delta$. This intuition is indeed correct as we shortly explain in Appendix B. In that region, *the response $\delta\nu(x)$ to a local perturbation δV derives from the Green's function for d-dimensional Brownian motion, weighted by the local mean velocity J/ρ*. In this sense the nonlocal response is intrinsically a nonequilibrium feature.

Although the above linear analysis can formally be extended far from equilibrium and one obtains a generalization of response formula (3.12), the linear operator replacing L_V is no longer symmetric, in agreement with the breakdown of Onsager reciprocity relations. We will see in the next section that an inverse formulation of our linear-response question does not suffer from the above complication and it also becomes remarkably easier to study outside the weak driving regime.

C. Local response to nonlocal perturbation

In this section we discuss long-range aspects in the inverse problem, namely, how the test potential Φ that makes a *given* density ρ stationary is affected by a local change in ρ. The relevance of this question and some other approaches are considered in Sec. IV.

We start by revisiting the exactly solvable model of Sec. III A. The confining potential $U(r)$ and the driving $v(r,\theta) = [0, f(\theta)/r]$ are always considered fixed. For the class of radial-angular uncorrelated densities, $\rho(r,\theta) = p(r)q(\theta)$, the stationary equation (2.2) is satisfied for the test potential of the form $\Phi(r,\theta) = \Phi_0(r) + \Psi(\theta)$, with the radial part

$$\Phi_0 = -\log p - U \tag{3.13}$$

and with the angular part equal to

$$\Psi = -\log q + \int_{\theta_0}^{\theta} \left(f - \frac{C}{q}\right) d\xi. \tag{3.14}$$

Here θ_0 is an arbitrary fixed angle and the constant C is determined from

$$C = \frac{\oint f\, d\theta}{\oint q^{-1} d\theta}. \tag{3.15}$$

The latter specifies the corresponding stationary current field as $J=(0,C/r)$. Away from equilibrium, i.e., for $w=\oint f d\theta \neq 0$, the angular component $\Psi(\theta)$ apparently becomes a nonlocal functional of the angular density $q(\theta)$, similar to what we have observed for the functional dependence $\rho[\Psi]$.

In the general case, we are asked to find the potential Φ that solves the stationarity equation (2.2) as a function of density ρ for given velocity field v and confining potential U, say on d-dimensional space. By changing $\rho \to \rho + \delta\rho$ with $\int \delta\rho(x) dx = 0$, we get the linear-response equation for $G=U+\Phi+\log\rho$,

$$\frac{1}{\rho}\nabla \cdot (\rho \nabla \delta G) = \frac{J}{\rho} \cdot \nabla \delta\nu \tag{3.16}$$

with $\nu=\log\rho$ and $J=\rho(v-\nabla G)$ the stationary current. We recognize in the left-hand side of Eq. (3.16) the action of the generator

$$L_\rho f(x) = \Delta f(x) + \nabla \log \rho \cdot \nabla f$$

for the function $f=\delta G$. The linear operator L_ρ generates a *reversible* diffusion in potential $-\log\rho$, i.e., an equilibrium process. The analysis is now exactly similar as from Eq. (3.12), but with ν replacing $-V$, and now restricting to a confinement region where $\rho(x)$ is approximately constant and maximal. The source is nonzero by the presence of $J\neq 0$ in the right-hand side of Eq. (3.16). We refer again to Appendix B for the analysis, but the conclusion remains that *a generic local change in density $\delta\rho$ in the confinement region requires a nonlocal adjustment of the potential and the corresponding response function derives from the Green's function for the d-dimensional Laplacian.*

Remark that no weak driving or small current assumption was employed in the above argument. In fact, the presence of the (auxiliary) reversible diffusion generated by L_ρ suggests that, even far from equilibrium, there are symmetries in the response functions. This is indeed true; see Sec. B 3 of Appendix B for such a reciprocity relation.

IV. MORE ABOUT THE INVERSE PROBLEM

One can ask how to actually construct the test potential Φ that makes a *given* density ρ stationary, i.e., solving Eq. (2.2). An immediate application is found in dynamical fluctuation theory; a brief review is left in Appendix C. In the following we present a general procedure to solve the inverse stationary problem for a class of densities. Next, a variational formulation suitable for numerical implementation will be given.

A. General solution

We are back to the setup of Sec. II for two-dimensional rotational diffusion. We restrict to those densities ρ that are everywhere bounded from zero and for which all (nonempty) equilevel lines, $\rho(r,\theta)=\text{const}$, are closed curves. We also stick to trivial boundary conditions at infinity, as guaranteed by a sufficient decay of all the fields ρ, U, and v. The auxiliary velocity

$$c = v - \nabla(U + \Phi + \nu), \quad \nu = \log \rho \tag{4.1}$$

shares with the driving field $v(r,\theta)$ an equal vorticity,

$$\nabla \times c = \nabla \times v. \tag{4.2}$$

The probability current is $J=\rho c$, and stationarity condition (2.2) reads

$$\nabla \cdot c + c \cdot \nabla \nu = 0. \tag{4.3}$$

We only need to find the vector field $c(r,\theta)$; then the potential $\Phi(r,\theta)$ can be calculated as

$$\Phi(x) = -\nu(x) - U(x) + \int_{\gamma: x_0 \rightsquigarrow x} (v - c) \cdot d\ell \tag{4.4}$$

modulo a constant, where the integral is taken along an arbitrary curve connecting a fixed initial point x_0 with x.

To determine $c(r,\theta)$ solving Eqs. (4.2) and (4.3), we first observe that it is unique by the Helmholtz decomposition theorem when supplying the boundary condition that the difference $c-v$ goes to zero at infinity. Still another boundary condition has to be added in the case the origin is not accessible and excluded from the domain.

In the following we restrict ourselves again to the two-dimensional plane. Equation (4.3) is solved by any vector field of the form

$$c(r,\theta) = g[\nu(r,\theta)]\left(-\frac{1}{r}\frac{\partial \nu}{\partial \theta}, \frac{\partial \nu}{\partial r}\right), \tag{4.5}$$

with g an arbitrary function. The latter is fixed by condition (4.2),

$$\nabla \times \left\{ g[\nu(r,\theta)]\left(-\frac{1}{r}\frac{\partial \nu}{\partial \theta}, \frac{\partial \nu}{\partial r}\right)\right\} = \nabla \times v, \tag{4.6}$$

which after integration over the surface enclosed by any equilateral curve of the density, $\nu(r,\theta)=a$, and using Stokes' theorem yields

$$\oint_{\nu=a} v \cdot d\ell = g(a) \oint_{\nu=a} \left(-\frac{1}{r}\frac{\partial \nu}{\partial \theta}, \frac{\partial \nu}{\partial r}\right) \cdot d\ell. \tag{4.7}$$

Parametrizing the curve $\nu(r,\theta)=a$ by its proper length so that

$$d\ell = \left[\frac{1}{r^2}\left(\frac{\partial \nu}{\partial \theta}\right)^2 + \left(\frac{\partial \nu}{\partial r}\right)^2\right]^{-1/2} \left(-\frac{1}{r}\frac{\partial \nu}{\partial \theta}, \frac{\partial \nu}{\partial r}\right) ds,$$

we finally get

$$g(a) = \frac{\oint_{\nu=a} v \cdot d\ell}{\oint_{\nu=a} \left[\frac{1}{r^2}\left(\frac{\partial \nu}{\partial \theta}\right)^2 + \left(\frac{\partial \nu}{\partial r}\right)^2 \right]^{1/2} ds}. \tag{4.8}$$

Formulas (4.4), (4.5), and (4.8) together provide an explicit solution for the test potential Φ.

As a check we take the example Eq. (3.1); there

$$c = [0, u(r)] = v$$

and the curves $\nu = a$ are concentric, corresponding to the equipotential lines for $U(r)$, assuming that it is monotone in r. Therefore Eq. (4.8) gives $g(a) = -u(r)/U'(r)$ for $a = -U(r) - \log Z$.

Further, the more general example of Sec. III A has $c = [0, j(r)/q(\theta)]$ with nonvanishing divergence whenever q is not a constant, in contrast with form (4.5). The point is that this example has a velocity field which is not defined at the origin, it being excluded from the domain. Hence, Stokes' theorem in the form of Eq. (4.7) cannot be used and a modification is needed; we omit details.

The above solution, basically obtained by a suitable deformation of polar coordinates, provides a class of examples with nonvanishing radial current. The latter is generally the case whenever ν does not decompose into independent radial and angular parts; compare with the model of Sec. III A.

B. Variational approach

Write now Fokker-Planck-Smoluchowski equation (2.2), considered again as the inverse stationary problem for the test potential Φ, in the form

$$\nabla \cdot (J_0 - \rho \nabla \Phi) = 0 \tag{4.9}$$

with $J_0 = J_0(\rho)$ the Φ-independent part of the probability current J,

$$J_0(\rho) = \rho(v - \nabla U) - \nabla \rho. \tag{4.10}$$

Recalling that it is an elliptic partial differential equation for Φ, its solution coincides with the minimizer of the quadratic functional

$$\mathcal{F}_\rho[\Psi] = \frac{1}{2}\int \rho \nabla \Psi \cdot \nabla \Psi dx + \int \Psi \nabla \cdot J_0(\rho) dx \tag{4.11}$$

under the unchanged boundary conditions if present. This formulation is suitable for numerical computations; see, e.g., via [31].

There are other variational principles of physical importance that appear intimately related to our inverse stationary problem. To explain those, consider the functional

$$\mathcal{G}[\mu, j] = \frac{1}{4}\int \mu^{-1}[j - J_0(\mu)] \cdot [j - J_0(\mu)] dx \tag{4.12}$$

defined for all normalized densities μ and all divergenceless currents j, $\nabla \cdot j = 0$; see Appendix C for its meaning within the dynamical fluctuations theory. This functional is manifestly positive and zero only if μ and j coincide with the stationary density, respectively, the stationary current (for the case $\Phi = 0$). It can be used to construct the variational functional

$$\mathcal{I}[\mu] = \inf_{j:\nabla \cdot j = 0} \mathcal{G}[\mu, j] \tag{4.13}$$

with minimizer equal to the stationary density. This is a constrained variational problem that can be solved by Lagrange multipliers; the solution reads

$$\mathcal{I}[\mu] = \frac{1}{4}\int \mu \nabla \Phi \cdot \nabla \Phi dx \tag{4.14}$$

with Φ the test potential that makes the density μ stationary, cf. Eq. (4.9),

$$\nabla \cdot [J_0(\mu) - \mu \nabla \Phi] = 0. \tag{4.15}$$

In this way, the solution to the inverse stationary problem is an essential step in constructing the variational functional $\mathcal{I}[\mu]$ on densities.

Finally, recall that Eq. (4.15) is equivalent to the variational problem $\mathcal{F}_\mu[\Psi] = \min$ with $\mathcal{F}_\mu$ introduced in Eq. (4.11). Combining with Eq. (4.14) we have the relation

$$\inf_\Psi \mathcal{F}_\mu[\Psi] = \mathcal{F}_\mu[\Phi] = -2\mathcal{I}[\mu] \tag{4.16}$$

that yields the next expression for the functional $\mathcal{I}[\mu]$ (changing $\Psi \to 2\Psi$ for convenience and integrating by parts),

$$\mathcal{I}[\mu] = \sup_\Psi \int \nabla \Psi \cdot [J_0(\mu) - \mu \nabla \Psi] dx. \tag{4.17}$$

This *unconstrained* variational formula is apparently more useful for numerical computations than Eq. (4.13) above.

V. CONCLUSION

The relation between potential and stationary density in mesoscopic (stochastic) systems appears to be generically long ranged whenever there is a true nonequilibrium driving. That long-range effect is *a priori* distinct from the long-range correlations under conservative dynamics extensively studied before, and it occurs already for free particles. In models of overdamped diffusions considered in this paper, we have linked that long-range effect to the slow spatial decay of the Green's function for a certain equilibrium diffusion process (in the first order around equilibrium).

Vice versa, a similar nonlocal change of potential is generically needed to create a local change in the stationary density. This issue appears relevant for the inverse stationary problem that naturally emerges in the context of dynamical fluctuations and nonequilibrium variational principles. We have indicated how these specific issues become mutually related, together with comparing some numerically feasible schemes based on the dynamical fluctuation theory that might be of use in applications.

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APPENDIX A: McLENNAN THEORY OF STATIONARY DISTRIBUTIONS

It is useful to see how the original McLennan reasoning [29] can be used to provide some physical interpretation for the stationary density of a weakly driven diffusion. We can write formula (3.10) in the equivalent form, always to linear order in ϵ,

$$\rho(x) = \rho_o(x)\exp\int_0^{+\infty} dt\langle v(x_t)\cdot\nabla V(x_t) - \nabla\cdot v(x_t)\rangle_x^o, \tag{A1}$$

where $\langle\cdot\rangle_x^o$ denotes expectation over the equilibrium process [that is process (2.1) with $v=0$] started from position x. (For a mathematical discussion on how to take the limits $\varepsilon\to 0$, $T\to+\infty$, we refer to [32].) It is interesting to recognize here the linear part in the irreversible entropy flux. When the density of the test particles is μ then the instantaneous mean work done by the background field v is

$$\mathcal{W} = \int v\cdot[(v-\nabla V)\mu - \nabla\mu]dx$$

as the expression between square brackets is the current profile at density μ. Clearly, for small driving that equals

$$\mathcal{W} = -\int (v\cdot\nabla V - \nabla\cdot v)\mu dx + O(\varepsilon^2).$$

In other words, to linear order in the nonequilibrium background, $-v(x)\cdot\nabla V(x)+\nabla\cdot v(x)$ equals the mean dissipated work per unit time provided the particle is at x. (Incompressibility of the background fluid can be imposed by letting $\nabla\cdot v=0$.) That linear term is exactly what appears in the expectation in Eq. (A1). Therefore, the linear nonequilibrium correction to the Boltzmann distribution corresponds to the total dissipated work under the equilibrium relaxation process as started from different initial configurations.

APPENDIX B: MORE TECHNICAL ASPECTS OF THE NONLOCALITY

1. Nonlocality in (equilibrium) transient distributions

The nonlocal features as discussed in the present paper refer to fluctuations and responses in steady nonequilibria. Nevertheless, their origin takes us to Poisson equations for reversible dynamics; see Eqs. (3.12) and (3.16). We therefore start here with a look at equilibrium dynamics but in the transient regime.

Take a reversible ($v=0$) diffusion in a potential landscape V at equilibrium, $\nu=\log\rho=-V$ (up to an irrelevant constant). Perturb the system by changing the potential at time $t=0$ to $V+\delta V$ and let the system relax toward a new equilibrium. The evolved distribution at time t be $\mu_t=\rho+\delta\mu_t$, corresponding to the effective time-dependent potential $\nu+\delta\nu_t$, $\delta\nu_t=\delta\mu_t/\rho$. By the linear-response theory,

$$\frac{d}{dt}\delta\nu_t = L_V\delta\nu_t + \frac{1}{\rho}\nabla\cdot(\rho\nabla\delta V), \quad \delta\nu_0 = 0. \tag{B1}$$

Using that the second term on the right-hand side equals

$$\frac{1}{\rho}\nabla\cdot(\rho\nabla\delta V) = L_V\delta V,$$

we find

$$\delta\nu_t = \left(\int_0^t e^{sL_V}ds\right)L_V\delta V = (e^{tL_V}-1)\delta V, \tag{B2}$$

where the equilibrium condition has been used. As a result, denoting with $p_t(x,y)$ the transition kernel,

$$\delta\nu_t(x) = -\delta V(x) + \int dy p_t(x,y)\delta V(y)$$

or

$$\frac{\delta\nu_t(x)}{\delta V(y)} = -\delta(x-y) + p_t(x,y). \tag{B3}$$

Remember that $\delta\nu_t$ is only determined up to a constant, which explains why $\lim_{t\to\infty}\delta\nu_t=-\delta V+\langle\delta V\rangle_\rho$ differs from the "naturally expected" value $-\delta V$; in the above the additive constant has been fixed by the initial condition $\delta\nu_0=0$. *The nonlocal part in the linear response for fixed time t, thus, exactly equals the transition-probability density $p_t(x,y)$. It is nonlocal in the sense that over distances where ρ is approximately constant and maximal (or around the minimum of V), there is only slow decay in $|x-y|$. As time grows larger, that effect typically dies out, restoring a strictly local response in the infinite-time limit.*

As an example, the standard one-dimensional Ornstein-Uhlenbeck process (or, oscillator process) corresponding to the potential $V(x)=x^2/2$ has a response function with the large-time asymptotics

$$\frac{\delta}{\delta V(y)}[\nu_t(x)-\nu_t(x')] = \delta(x'-y) - \delta(x-y) + e^{-t}(x'-x)y\rho(y) + O(e^{-2t}), \tag{B4}$$

the nonlocal component of which has a weight exponentially damped in time.

2. Green's function in confinement region

The response analysis in Secs. III B and III C reduces the problem to finding the Green's function,

$$L_\rho^{(x)}\mathcal{G}(x,y) = -\,\delta(x-y), \tag{B5}$$

with $L_\rho = \frac{1}{\rho}\nabla\cdot(\rho\nabla)$ generating diffusion in the potential $-\log\rho$. It has an explicit solution in terms of the transition kernel (or transition-probability density),

$$\mathcal{G}(x,y) = \int_0^{+\infty}[p_t(x,y) - \rho(y)]dt. \tag{B6}$$

In a confinement region where ρ is approximately constant around its maximum, one expects that $\mathcal{G}(x,y)$ is essentially determined by a free diffusion. To asses this conjecture, we need to understand how the inhomogeneities in ρ outside the confinement region influence the Green's function inside it and, more basically, how to make sense to the generally ill-defined expression Eq. (B6) for the free diffusion.

As well known [33], for a free diffusion (related to the Brownian motion as $\sqrt{2}B_t$) in dimension d, with the transition kernel

$$p_t^{\text{free}}(0,x) = (4\pi t)^{-d/2}e^{-|x|^2/4t}, \tag{B7}$$

the Green's function $\mathcal{G}^{\text{free}}(x) = \int_0^\infty p_t(0,x)dt$ only exists in the transient case, $d \geq 3$. For $d=1,2$ the divergence cannot be "renormalized" via a stationary density like in Eq. (B6) as the latter does not exist. Yet, its divergent part is in fact x independent and one has in *all* dimensions well-defined differences,

$$\int_0^\infty [p_t^{\text{free}}(0,x) - p_t^{\text{free}}(0,x')]dt = \begin{cases} \frac{1}{2}(|x'| - |x|), & \text{if } d=1 \\ \frac{1}{2\pi}(\log|x'| - \log|x|), & \text{if } d=2 \\ \frac{1}{4}\pi^{-d/2}\Gamma(d/2-1)(|x|^{2-d} - |x'|^{2-d}), & \text{if } d\geq 3. \end{cases} \tag{B8}$$

Hence, the free diffusion Green's function is well defined up to a possibly infinite additive constant. However the latter becomes irrelevant due to the "dipole" character of the source term in Eq. (3.12) and (3.16); cf. also Eq. (B20) below.

It remains to see in what sense the exterior of a confinement region enters the properties of the (true) Green's function. To simulate that, we consider the (standard) diffusion in a cube $[-L/2,L/2]^d$ with reflexive boundary conditions. The transition kernel is $p_t(x,y) = \Pi_{i=1}^d q_t(x_i,y_i)$ with

$$q_t(x_i,y_i) = \frac{1}{L} + \frac{2}{L}\sum_{n\geq 1}\cos\left[\pi n\left(\frac{x_i}{L}+\frac{1}{2}\right)\right] \times\cos\left[\pi n\left(\frac{y_i}{L}+\frac{1}{2}\right)\right]e^{-\pi^2 n^2/L^2 t} \tag{B9}$$

For $d=1$ the Green's function can be obtained explicitly,

$$\mathcal{G}(x,y) = \int_0^\infty [p_t(x,y) - \rho(y)]dt = \frac{L}{12} - \frac{1}{2}|y-x| + \frac{1}{2L}(x^2+y^2). \tag{B10}$$

Clearly, up to a correction $O(1/L)$ it coincides with the Green's function for free diffusion; moreover, the "infinite" additive constant has been regularized and fixed by the length of the region.

In general one has

$$p_t(0,x) = \frac{1}{L^d}\sum_k \exp\{ik\cdot x - |k|^2 t\} \tag{B11}$$

with the summation over the dual lattice, $k_i = \ldots, -2\pi/L, 0, 2\pi/L, \ldots$. Hence,

$$\mathcal{G}(0,x) = \frac{1}{L^d}\sum_{k\neq 0}\frac{1}{|k|^2}e^{ik\cdot x}, \tag{B12}$$

which is to be compared with the free diffusion for which, formally,

$$\mathcal{G}^{\text{free}}(0,x) = \frac{1}{(2\pi)^d}\int \frac{dk}{|k|^2}e^{ik\cdot x}. \tag{B13}$$

The latter is "infrared divergent" for $d \leq 2$ and the above finite lattice version just provides its particular regularization (above all it provides a cutoff of the neighborhood of $k=0$). Note that an alternative (and more standard) way of regularizing the free Green's function is to add a "positive mass:" for $d=2$ one obtains

$$\mathcal{G}_\epsilon(0,x) = \frac{1}{4\pi^2}\int \frac{dk}{|k|^2+\epsilon^2}e^{ik\cdot x} = \frac{1}{2\pi}\int_0^\infty \frac{uJ_0(u|x|)}{u^2+\epsilon^2}du = \frac{1}{2\pi}K_0(\epsilon|x|) \tag{B14}$$

with J_0 and K_0 the Bessel functions of the first and of the second kind, respectively. Its short-distance asymptotics is

$$\mathcal{G}_\epsilon(0,x) = \frac{\log 2 - \gamma}{2\pi} - \frac{1}{2\pi}\log(\epsilon|x|) + o(1) \tag{B15}$$

(γ being the Euler constant).

These calculations indicate what the "boundary effects" on the Green's function in a region with approximatively constant density profile are: the difference from the free Green's function becomes negligible on length scales much smaller than size of the region. Although this comparison includes the removal of an infrared divergence in low dimensions, the latter is well "renormalizable" in the above sense of finite differences. Our conclusion is that one could for the present purposes deal just with the free Green's function (although as such being ill defined).

As a specific example we consider the Ornstein-Uhlenbeck process for the diffusion in a quadratic spherically symmetric potential. Its Green's function can be found by solving the Eq. (B5) with $\rho(x) \propto \exp[-V(x)] \equiv \exp(-\epsilon^2|x|^2/2)$ (for simplicity we restrict here to a source located at the origin). Again in two dimensions, this has a solution

$$\mathcal{G}_{\mathrm{OU}}(0,x) = -\frac{1}{2\pi}\int_{1/\epsilon}^{|x|}\frac{dr}{r}e^{V(r)} \tag{B16}$$

up to an arbitrary additive constant. For $\epsilon|x| \ll 1$, what we have called the confinement region, it reads

$$\mathcal{G}_{\mathrm{OU}}(0,x) = -\frac{1}{2\pi}\log(\epsilon|x|) + o(1), \tag{B17}$$

in agreement with either of the two above regularization procedures. Similarly, for dimensions $d>2$ one gets

$$\mathcal{G}_{\mathrm{OU}}(0,x) = -\frac{\Gamma(d/2)}{2\pi^{d/2}}\int_{1/\epsilon}^{|x|}\frac{dr}{r^{d-1}}e^{V(r)}, \tag{B18}$$

yielding a power-law decay $|x|^{2-d}$ if $\epsilon|x| \ll 1$.

3. "Reciprocity relations" in the inverse problem

In contrast to Sec. III B, the analysis of Sec. III C does not make any use of close-to-equilibrium assumptions while all the same, in Eq. (3.16) and for the inverse problem, the linear response is given in terms of a *reversible* process. A solution to Eq. (3.16) can be written as

$$\delta G(x) = -\int dy \mathcal{G}(x,y)\left(\frac{J}{\rho}\cdot\nabla\delta\nu\right)(y), \tag{B19}$$

where $\mathcal{G}(x,y)$ is the Green's function, Eqs. (B5) and (B6). Since the transition probabilities satisfy detailed balance, the Green's function exhibits the same symmetry: $\rho(x)\mathcal{G}(x,y) = \rho(y)\mathcal{G}(y,x)$.

We now propose a partial integration which is allowed if the current J decays sufficiently fast at infinity; using moreover that J is divergenceless and that δG is physically determined only modulo a constant, one can then write Eq. (B19) as

$$\delta G(x) = \int dy \nabla_y \frac{\mathcal{G}(x,y)}{\rho(y)}\cdot(J\delta\nu)(y) \tag{B20}$$

and therefore

$$J(x)\cdot\nabla_x\frac{\delta G}{\delta\nu(y)} = J(y)\cdot\nabla_y\frac{\delta G}{\delta\nu(x)}. \tag{B21}$$

That relation vaguely resembles an Onsager reciprocity: $-\frac{\delta}{\delta\nu(y)}\nabla_x G$ can be interpreted as the extra (gradient) force at x needed to have a delta-function-like response at y.

APPENDIX C: DYNAMICAL FLUCTUATIONS

Variational principles often arise in the context of fluctuation theory. For example, the entropy and related thermodynamic potentials play a role both as important equilibrium variational functionals (second law) and as functionals governing the equilibrium fluctuations (Einstein's fluctuation theory). Here we sketch how the functionals $\mathcal{G}$ and $\mathcal{I}$ introduced in Sec. IV B also fit such a scheme; a more technical account of this problem for overdamped diffusions can be found in [1].

We consider the diffusion process [Eq. (2.1)] with the test potential Φ set to zero. For any random realization x_t, $t \ge 0$, of this process we introduce the empirical occupation density

$$\bar{\rho}_T(z) = \frac{1}{T}\int_0^T \delta(x_t - z)dt \tag{C1}$$

that counts the relative time spent at each point z. Apparently, $\bar{\rho}_T(z)$ is the random density dependent on the realized history. In the limit $T\to\infty$ it converges to the stationary density ρ, with probability one by the ergodic theorem. The main result reads that for large but finite times T, the probability of fluctuations of $\bar{\rho}_T$ has the asymptotics given by the large deviation law

$$\boldsymbol{P}(\bar{\rho}_T = \mu) \propto e^{-T\mathcal{I}[\mu]}, \tag{C2}$$

in which the functional $\mathcal{I}[\mu]$ of Sec. IV B is recognized as an exponential decay rate. Then, the variational inequality $\mathcal{I}[\mu] \ge \mathcal{I}[\rho] = 0$ is a mere consequence of fluctuation law (C2). As observed before, finding $\mathcal{I}[\mu]$ amounts to solving inverse stationary problems (4.14) and (4.15) or, equivalently, to evaluating variational expression (4.17).

Similarly, functional (4.12) reveals to be the exponential decay rate in the large deviation asymptotics of the joint probability law for the empirical occupation times and the empirical current. For proofs and for more details see [1].

The large deviation theory for stochastic systems has been started and rigorously established by Donsker and Varadhan [34,35]. In the physics literature, these methods go back to the seminal work of Onsager and Machlup [36].

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