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Microscopic origin of hydrodynamic behavior: Entropy production and the steady state*

Gregory L. Eyink and Joel L. Lebowitz
Rutgers University, USA

Herbert Spohn
Theoretische Physik, Universität München, FRG

Abstract. We study the relation between the microscopic dynamics of systems of particles and the hydrodynamic laws they obey on a macroscopic scale. Our focus is the steady state of particle systems in contact with reservoirs at different values of temperature, chemical potential, etc. The validity of the stationary transport law in this case presumably requires some features of "stochasticity" or "chaos" in the microscopic dynamics. Here, we incorporate such features *by hand* by considering actual stochastic dynamics, in order to concentrate on the essential aspects of the transition from microscopic to macroscopic. As further simplifications, we study discrete systems on a lattice. Modeling the reservoirs by appropriate stochastic boundary dynamics, we show there are unique stationary distributions. These stationary ensembles are further shown to have a certain canonical form, especially promoted by Zubarev, from which the proper macroscopic transport law may be inferred. We next define and study the microscopic entropy production for our models. In particular, we show there is also a unique state of minimum entropy production and we study its relation to the unique steady state, well known as the principle of minimum entropy production. Finally, we review the role of entropy production in recent progress on the proof of hydrodynamics for stochastic models and in the characterization of the steady state by a variational principle.

1. Introduction

The subject of this article has a history which predates by some time the "standard" subject of this conference, the origin of chaotic behavior in systems with few degrees of freedom whose dynamics is governed by

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simple, deterministic equations. We want to discuss instead the origin of collective, orderly behavior of macroscopic matter described by simple deterministic equations, from the chaotic, essentially random motions of the atoms or molecules which are their microscopic constituents. To put it in another way, we investigate the connection between the motions of atoms whose mean free paths are typically measured in angstroms and hydrodynamic behavior usually observed on the scale of millimeter or larger: a ratio of macro to micro scales of at least 10^5. We shall generally call the spatial ratio ϵ^{-1}.

Now it is a remarkable fact that there is a hierarchical structure in nature which makes it possible, even necessary, to study different levels independently. This explains how the hydrodynamic equations of fluids could be established before the atomistic structure of matter was fully understood and survived intact the transformation from classical to quantum mechanics. The macroscopic level of description is a "contracted" one, involving a small number of local variables that very often correspond to the microscopically conserved quantities of the underlying dynamics.* Nevertheless, the problem of explaining how such a "contracted" description can be a closed and causal one, dubbed by G. E. Uhlenbeck the "macroscopic causality problem,"[1] is not fully elucidated even today.

Important progress on this problem has been made in the past several years in the case where the microscopic dynamics consists of particles randomly moving on a discrete lattice with some stochastic interactions. We refer the reader to several recent review articles on the derivation of time-dependent macroscopic equations from microscopic model systems (Refs. 4–6). Here, as indicated by the subtitle of this article, we focus on another aspect of the problem: the connection between the microscopic and macroscopic descriptions of nonequilibrium stationary states. In such systems, steady currents are maintained by contact with infinite particle and heat reservoirs ("heat baths"). There is also in such systems a continuous, time-independent production of entropy. In fact, the entropy production has been found to play a crucial role in the analysis of these states. It has been known for a long time, cf. Prigogine (Ref. 7), that stationary nonequilibrium states—at least in the linear regime, close to global equilibrium—are characterized at the macroscopic level by a minimum of entropy production, compatible with the external contraints

*There are model systems, such as the voter model, for which there is a hydrodynamic description even without a conserved quantity[2]; in realistic systems, hydrodynamic Goldstone modes do not correspond to a microscopic conservation law.[3]

imposed on the system. More recently, entropy production has appeared as the key technical tool in the method of Guo, Papanicolau, and Varadhan for deriving hydrodynamic limits of particle systems with stochastic dynamics.[8] This method has subsequently been adapted to study the hydrodynamics (more properly, "hydrostatics") of the steady states of such systems interacting with model reservoirs.[9] Here we shall discuss all of these connections, not only because of the permanent value of what has been already discovered, but also because of the promise these ideas and methods have for future work.

In Sec. 2, we introduce the stochastic, interacting particle models which are our object of study. With reservoirs modeled by appropriate stochastic boundary dynamics, these systems are shown to have unique stationary states. These stationary ensembles are further shown to have a certain "canonical" form, analogous to the Gibbs formulas for the equilibrium ensembles. In Sec. 3, we define the microscopic entropy production for our models and establish its chief properties. It is shown that there is a unique state of minimum entropy production, and the connection of that state with the steady state is studied both at the macroscopic and microscopic levels. In Sec. 4, we discuss in an expository, nontechnical way the recent progress in applying entropy production arguments to the proof of hydrodynamical limits. We also describe briefly how the principle of minimal entropy production should play an important role in removing a major technical restriction of the present proofs. Finally, we briefly review the current status of proposed variational principles for nonequilibrium steady states.

2. Steady states of particle models with stochastic dynamics

The mathematical models we consider are of a type which have been the subject of intense scrutiny for the past several years (for a review see Refs. 4 and 5 and, for the latest complete exposition, the monograph of H. Spohn[6]). These are discrete lattice systems with stochastic dynamics, which arguably play the same role for nonequilibrium statistical mechanics which Ising-type models have played for equilibrium. To be more precise, the models we consider in our context are continuous-time Markov processes on the finite state space $\Omega = \{0,1\}^{\Lambda}$, where $\Lambda = ([-M,M] \cap \mathbb{Z})^d$ is a cubic lattice of $(2M+1)^d$ sites. Here, the ratio of scales parameter $\epsilon = M^{-1}$. The components $\eta(x)$, $x \in \Lambda$, of the state vector $\eta \in \Omega$ denote the occupation numbers of the sites x (1 = occupied, 0 = unoccupied). To specify the dynamics we prescribe rates $c(x,y;\eta)$, $x,y \in \Lambda$, $c(x,\eta)$, $x \in \partial\Lambda = \{x: x_1 = \pm M\}$, where $c(x,y;\eta)$

gives the probability per unit (microscopic) time for a particle–hole exchange between sites x and y and $c(x,\eta)$ gives the corresponding rate for particle creation/annihilation at a boundary site x. Then, the evolution of any random variable for the systems is given by the Markov semigroup $(e^{L_M t}f)(\eta) = E^{\eta}[f(\eta_t)]$, with

$$(L_M f)(\eta) = \frac{1}{2}\sum_{x,y\in\Lambda} c(x,y;\eta)[f(\eta^{xy}) - f(\eta)] + \sum_{x\in\partial\Lambda} c(x,\eta)[f(\eta^{x}) - f(\eta)] \tag{2.1}$$

defining the generator of the process. In Eq. (2.1) η^{xy} denotes η with the occupancies at x,y interchanged and η^{x} denotes η with the occupancy at the single site x switched ($0\leftrightarrow 1$).

For simplicity, we shall choose here the exchange dynamics to allow only nearest-neighbor jumps: i.e., $c(x,y;\eta)=0$ unless $|x-y|=1$. More essential restrictions on the exchange rates $c(x,y;\eta)$ are the following:

(a) *Finite range*: $c(x,y;\eta)$ depends on η only through $\{\eta_z \,|\, |z-x|<R, |z-y|<R\}$.

(b) *Translation-invariance*: Let τ_a be the shift by $a\in\mathbb{Z}^d$ on $\mathbb{Z}^d$, $\tau_a\eta(x) = \eta(x-a)$.

Then, for all $x,y\in\Lambda$, $\eta\in\Omega$, $a\in\mathbb{Z}^d$:

$$c(x,y;\eta) = c(x+a, y+a; \tau_a\eta) \tag{2.2}$$

for $|(x+a)_1 \pm M| > R$, $|(y+a)_1 \pm M| > R$. We adopt periodic boundary conditions except in the 1-direction.

(c) *Detailed balance*: We associate to each configuration $\eta\in\Omega$ an energy $H(\eta)$ so that

$$c(x,y;\eta) = c(x,y;\eta^{xy}) e^{-(\Delta_{x,y}H)(\eta)}, \tag{2.3}$$

with $(\Delta_{x,y}H)(\eta) = H(\eta^{xy}) - H(\eta)$. We assume here further that $H(\eta)$ is defined in terms of a finite-range, translation-invariant potential.

(d) *Nondegeneracy*:

$$c(x,y;\eta) > 0 \quad \text{for} \quad \eta(x)\neq\eta(y). \tag{2.4}$$

The exchange rates $c(x,y;\eta)$ in the boundary regions $|x_1 \pm M| < R$, $|y_1 \pm M| < R$ may be chosen arbitrarily subject to conditions (a), (c), (d) [i.e., (b) is not required].

The bulk dynamics we have defined clearly conserves the total particle number:

$$N(\eta) = \sum_{x\in\Lambda} \eta_x. \tag{2.5}$$

The boundary rates $c(x,\eta)$, on the other hand, correspond to particle creation and annihilation at the sites x: $x_1 = \pm M$. They represent in an idealized way the interaction of the system with infinite particle reservoirs in equilibrium at chemical potentials $\lambda_\pm$ and are thus required to satisfy the detailed balance conditions[10]:

$$c(x,\eta) = c(x;\eta^x) e^{-(\Delta_x H)(\eta) + \lambda_x(1-2\eta_x)}, \quad x = (\pm M, x_1) \tag{2.6}$$

with $(\Delta_x H)(\eta) \equiv H(\eta^x) - H(\eta)$ and $\lambda_{(\pm M, x_1)} = \lambda_\pm$. We also assume for these rates the finite range condition analogous to (a) above, and nondegeneracy: $c(x,\eta) > 0$ for all $x\in\partial\Lambda$, $\eta\in\Omega$. However, we make no further assumptions or special choice for the boundary rates.

With our assumptions on the rates, particularly the nondegeneracy conditions, the state space Ω forms a single ergodic class and standard theorems on stationary Markov processes with finite state space (see, for example, Ref. 11) imply that there is a unique stationary probability measure μ_{ss} on Ω, which, in fact, is approached at an exponential rate starting from any initial configuration $\eta\in\Omega$.

We would now like to discuss the expected macroscopic behavior of this model. That is, we wish to understand the large-scale structure of the stationary measure in the hydrodynamical scaling limit as $\epsilon \equiv 1/M \to 0$ (see Refs. 4–6). A particular object of interest is the expected value of the particle number current:

$$j_{x,y}(\eta) = c(x,y;\eta)[\eta(x) - \eta(y)] \tag{2.7}$$

in the stationary measure. Note $j_{x,y}(\eta)$ gives the systematic part of the particle transport from site x to y per unit time in the configuration η. According to Fick's law of diffusion, the steady-state current at the macroscopic point $q\in[-1,1]$ should be related to the local density gradient as

$$j_\mu(q) = -D_{\mu\nu}[\rho(q)] \frac{\partial\rho(q)}{\partial q^\nu}, \tag{2.8}$$

where $D_{\mu\nu}$ is the bulk diffusion (matrix), which depends only on the local density. To prove Eq. (2.8) for our microscopic model, we should establish the hydrodynamic limit:

$$\lim_{\epsilon\to 0} \epsilon^{-1} \langle j_{[\epsilon^{-1}q], [\epsilon^{-1}q]+e_1} \rangle^{\epsilon}_{ss} = -D_{11}[\rho_{ss}(q)] \frac{\partial\rho_{ss}}{\partial q_1}(q). \tag{2.9}$$

We have denoted expectation in the stationary measure μ^{ϵ}_{ss} for system size $M = \epsilon^{-1}$ by $\langle\cdot\rangle^{\epsilon}_{ss}$. The macroscopic density profile $\rho_{ss}(q)$ on $[-1,1]$ appearing in Eq. (2.9) is the *stationary* solution of the nonlinear diffusion equation:

$$\frac{\partial}{\partial t}\rho(q,t)=\frac{\partial}{\partial q^{\mu}}\left[D_{\mu\nu}[\rho(q)]\,\frac{\partial}{\partial q^{\nu}}\rho(q)\right] \tag{2.10}$$

[obtained by substituting Eq. (2.8) into the continuity equation $\partial\rho(q,t)/\partial t = -\partial j_{\mu}(q)/\partial q_{\mu}$], subject to the boundary conditions:

$$\rho_{ss}(\pm 1)=\rho(\lambda_{\pm})\equiv\rho_{\pm}. \tag{2.11}$$

Here, $\rho(\lambda)$ gives the usual thermodynamic equilibrium connection between chemical potential and density for the statistical mechanical system with Hamiltonian $H(\eta)$ as above. That is, restating the above, subject to Eq. (2.11),

$$\frac{\partial}{\partial q^{\mu}}\left[D_{\mu\nu}[\rho_{ss}(q)]\,\frac{\partial}{\partial q^{\nu}}\rho_{ss}(q)\right]=0. \tag{2.12}$$

Notice that Eq. (2.9) contains, in particular, the statement that $\langle j_1([\epsilon^{-1}q])\rangle_{ss}^{\epsilon}\sim\text{const}\times\epsilon$, which is often called the property of *normal transport.*

To make a connection of these macroscopic considerations with the microscopic model it is useful to introduce certain explicit formulas for the stationary measures μ_{ss}^{ϵ}. The expressions of the sort we shall discuss were discovered nearly simultaneously 30 years ago by several authors,[12-14] and have since been plausibly argued to represent the analog for the nonequilibrium steady state of the Gibbs formulas for the thermal equilibrium state.[15,16] For the derivation of these formulas, we consider any smooth chemical potential profile $\lambda(q)$ on $[-1,1]$ with $\lambda(\pm 1)=\lambda_{\pm}$ [the stationary profile $\lambda_{ss}(q)$ would be most natural, but any other will do as well]. Then, for system size M, we write $\lambda_x=\lambda(\epsilon x)$ for each lattice site $x\in\Lambda$. If L_M^* is the adjoint of L_M with respect to counting measure on Ω, then the convergence theorem cited above and the fundamental theorem of the calculus give

$$\mu_{ss}(\eta)=\lim_{t\to+\infty}(e^{tL_M^*}\mu_{1e})(\eta)=\mu_{1e}(\eta)+\int_0^{\infty}dt(e^{tL_M^*}L_M^*\mu_{1e})(\eta), \tag{2.13}$$

where $\mu_{1e}(\eta)$ is the *local equilibrium distribution*:

$$\mu_{1e}(\eta)=\frac{1}{Z_{1e}}e^{-H(\eta)+\sum_{x\in\Lambda}\lambda_x\eta(x)} \tag{2.14}$$

formed from λ_x. Of course, Eq. (2.13) is true with *any* initial probability measure μ_0 replacing μ_{1e}. However, for $\mu_0=\mu_{1e}$ an explicit calculation in our model gives

$$(L_M^*\mu_{1e})(\eta)=\mu_{1e}(\eta)(\nabla\lambda\cdot I)_{\Lambda}(\eta), \tag{2.15}$$

with

$$(\nabla\lambda\cdot I)_{\Lambda}(\eta)=\sum_{\substack{x\in\Lambda,\\ x+e_1\in\Lambda}}(\lambda_{x+e_1}-\lambda_x)I_{x,x+e_1}(\eta) \tag{2.16}$$

and

$$I_{(x,x+e_1)}(\eta)=c(x,x+e_1;\eta)\left(\frac{e^{(\lambda_{x+e_1}-\lambda_x)(\eta_x-\eta_{x+e_1})}-1}{\lambda_{x+e_1}-\lambda_x}\right). \tag{2.17}$$

Note that $I_{(x,x+e_1)}(\eta)=J_{x,x+e_1}(\eta)+0(\nabla\lambda)$, so that we refer to $I_{(x,x+e_1)}$ as a *modified current.* Notice, if $(\cdot)_{1e}$ denotes expectation with respect to μ_{1e}, then by exploiting detailed balance $I_{x,x+e_1}$ has the property:

$$(I_{(x,x+e_1)})_{1e}=0. \tag{2.18}$$

Thus, we arrive finally at the expression:

$$\mu_{ss}(\eta)=\mu_{1e}(\eta)+\int_0^{\infty}dt[e^{tL_M^*}\mu_{1e}(\nabla\lambda\cdot I)_{\Lambda}](\eta). \tag{2.19}$$

We refer to such formulas for the stationary measures μ_{ss} as the *Zubarev distributions,* since that author, in particular, has advertised them and systematically exploited them over the years.

To investigate the normal transport properties of our system, we substitute into $(\cdot)_{ss}$, given by Eq. (2.19), the bulk-averaged current $J_{\Lambda,1}/|\Lambda|$ with

$$J_{\Lambda,1}(\eta)=\sum_{\substack{x\in\Lambda,\\ x+e_1\in\Lambda}}j_{x,x+e_1}(\eta). \tag{2.20}$$

Just because μ_{1e} is a local equilibrium distribution, we find that

$$\lim_{\epsilon\to 0}\left\langle\frac{J_{\Lambda,1}}{|\Lambda|}\right\rangle_{1e}^{\epsilon}=\frac{1}{2}\int_{-1}^{1}dq\langle j_{0,e_1}\rangle_{\lambda(q)}. \tag{2.21}$$

In fact, Eq. (2.21) *vanishes,* since $\langle j_{0,e_1}\rangle_{\lambda}=0$ by detailed balance: we are therefore interested in the next-order correction to this limit. By exploiting the explicit expression for μ_{1e}^{ϵ} and its good spatial clustering properties, we can prove further that

$$\lim_{\epsilon\to 0}\epsilon^{-1}\left\langle\frac{J_{\Lambda,1}}{|\Lambda|}\right\rangle_{1\epsilon}^{\epsilon}=\frac{1}{2}\int_{-1}^{1}dq(\partial_1\lambda)(q)\sum_{x\in\mathbb{Z}^d}x_1\langle\eta_x j_{0,e_1}\rangle_{\lambda(q)}$$

$$=-\frac{1}{2}\int_{-1}^{1}dq(\partial_1\lambda)(q)\langle c(0,e_1;\eta)\rangle_{\lambda(q)}, \tag{2.22}$$

where the second equality again follows from detailed balance. The second term in Eq. (2.19) is considered similarly. Ignoring for the moment the time integral, we note that

$$\lim_{\epsilon\to 0}\epsilon^{-1}\langle((\nabla\lambda\cdot I)_\Lambda e^{L_M t}J_\Lambda)\rangle_{1\epsilon}^{\epsilon}=\int_{-1}^{1}dq(\partial_1\lambda)(q)$$

$$\times\sum_{x\in\mathbb{Z}^d}\langle j(x,x+e_1)e^{Lt}j(0,e_1)\rangle_{\lambda(q)}. \tag{2.23}$$

Here we have introduced the generator L for the infinite-volume, bulk dynamics, defined for strictly local functions f by

$$(Lf)(\eta)=\frac{1}{2}\sum_{x,y\in\mathbb{Z}^d}c(x,y;\eta)[f(\eta^{xy})-f(\eta)]. \tag{2.24}$$

To prove Eq. (2.23) we exploited again the good spatial decay properties of $\mu_{1\epsilon}$, the quasilocal character of $(e^{Lt}f)(\eta)$ for local functions f and finite times, and the good convergence of the finite-volume dynamics to the infinite-volume dynamics at finite times, as expressed by an inequality of the form:

$$\sup_\eta|(e^{L_M t}f)(\eta_M)-(e^{Lt}f)(\eta)|<\text{const}\,|||f|||\exp[Ct+M\log(Ct)-M\log M] \tag{2.25}$$

(see Ref. 17). Here, η_M is the restriction of the infinite-volume configuration η to the finite-volume Λ and $|||\cdot|||$ is a suitable norm. Let us *assume* that the expression $\epsilon^{-1}\langle((\nabla\lambda\cdot I)_\Lambda e^{L_M t}J_\Lambda)\rangle_{1\epsilon}^{\epsilon}$ is integrable in t uniformly in the system size M. Then, we may apply dominated convergence to infer that

$$\lim_{\epsilon\to 0}\epsilon^{-1}\left\langle\frac{J_{\Lambda,1}}{|\Lambda|}\right\rangle_{ss}^{\epsilon}=-\int_{-1}^{1}dq(\partial_1\lambda)(q)\left[\tfrac{1}{2}\langle c(0,e_1)\rangle_{\lambda(q)}\right.$$

$$\left.-\int_0^\infty dt\sum_{x\in\mathbb{Z}^d}\langle j(x,x+e_1)e^{Lt}j(0,e_1)\rangle_{\lambda(q)}\right]$$

$$=-\int_{-1}^{1}dq(\partial_1\rho)(q)D_{11}[\rho(q)] \tag{2.26}$$

The last equality involves a change of variables from the chemical potential $\lambda(q)$ to the density $\rho(q)$, and the diffusion constant $D_{11}(\rho)$ is given by

$$D_{11}(\rho)\equiv\frac{1}{2\chi(\rho)}\langle c(0,e_1)\rangle_\rho$$

$$-\frac{1}{\chi(\rho)}\int_0^\infty dt\sum_{x\in\mathbb{Z}^d}\langle j(x,x+e_1)e^{Lt}j(0,e_1)\rangle_\rho, \tag{2.27}$$

where $\chi(\rho)=[\lambda'(\rho)]^{-1}$ is the equilibrium susceptibility. Hence, we arrive at a bulk-averaged form of Fick's law [Eq. (2.2)] with an explicit *Green–Kubo formula* [Eq. (2.27)] for the bulk diffusion coefficient $D_{11}(\rho)$. We remark, as an aside, that this bulk-averaged form is independent of the particular smooth profile $\rho(q)$ chosen to interpolate between ρ_- and ρ_+. However, if we choose $\rho=\rho_{ss}$, then $j_{ss}(q)=-\partial_1\rho_{ss}(q)D_{11}[\rho_{ss}(q)]$ is, in fact, independent of q by particle number conservation and, likewise, $\langle J_{\Lambda,1}/|\Lambda|\rangle_{ss}^{\epsilon}=\langle j_1([\epsilon^{-1}q])\rangle_{ss}^{\epsilon}$, so that Eq. (2.26) is equivalent to a *local* statement:

$$\lim_{\epsilon\to 0}(2\epsilon)^{-1}\langle j_1([\epsilon^{-1}q])\rangle_{ss}^{\epsilon}=-D_{11}[\rho_{ss}(q)]\partial_1\rho_{ss}(q). \tag{2.28}$$

The bulk diffusion coefficient $D_{11}(\rho)$ as given by Eq. (2.27) can be shown without difficulty to be non-negative (see Refs. 4 and 6). The above argument thus establishes a normal transport property for these systems and, further, Fick's law as an asymptotic statement.

We emphasize that our derivation of Eqs. (2.26)–(2.28) is based on the *assumption* of the integrability of the finite-volume Green–Kubo integrand in Eq. (2.23) *uniformly* in the system size M. It is an eminently reasonable assumption: for each fixed M, the integrand in fact decays exponentially in t and, further, the non-negativity of D implies automatically [cf. Eq. (2.27)] the integrability of the infinte-volume integrand $\Sigma_{x\in\mathbb{Z}^d}\langle j(x,x+e_1)e^{Lt}j(0,e_1)\rangle_\rho$. Therefore, one *expects* that the time decay behavior of the infinite-volume integrand will dominate uniformly the

finite-volume integrands. However, this must be proved. We want to assert, on the other hand, that we are not concerned here with a mere fine point of rigor, but a real issue of physics. Indeed, the "derivation" of the transport law we gave above may be repeated in a nearly identical fashion for actual Hamiltonian mechanical systems,[15,16] much of it even in a rigorous fashion.[18] However, that "derivation" applies even to a system such as the harmonic crystal which is known *not* to have a normal transport property.[19] Therefore, our *assumption* is certainly false in that case. What goes wrong there is that even the infinite-volume Green–Kubo integrand is not integrable in time: in fact, it tends asymptotically to a nonzero *constant* as $t \to +\infty$. The problem of establishing decay laws of the infinite-volume Green–Kubo integrands is a notoriously difficult one and at this stage it is not understood at all for real systems what dynamical properties could guarantee the validity of our assumption. What one can do with the Zubarev distribution is to give a natural condition which is apparently sufficient (for stochastic particle models, actually sufficient) for the normal transport property: the integrability of the Green–Kubo autocorrelation function uniformly in the system size.

In Sec. 4 we shall review what is presently known rigorously about the transport properties of our models. Under an additional technical restriction, we shall state a theorem which establishes much stronger results than the average transport law expressed in Eq. (2.9).

3. The principle of minimal entropy production

There have been many attempts to theoretically define analogs of equilibrium free energies for nonequilibrium steady states and to formulate associated variational principles. Perhaps the earliest effort was the 1848 work of Kirchoff,[20] in which the electric potential in a bounded region was shown to distribute itself so as to dissipate the least possible heat for given voltages applied on the boundary. This was an example of what is today termed the *principle of minimum entropy production*. Other such examples in disparate contexts were discovered by Helmholtz, Rayleigh, and Lorentz, but it seems to have been Prigogine, in his treatise on irreversible thermodynamics,[7] who first formulated the principle in a general way. (For a historical review of the principle, see the paper of E. T. Jaynes.[21]) We shall study here the principle in the context of stochastic lattice gases.

To analyze the entropy production of our model, it is important to remember that our system is in contact with a thermal reservoir (at uniform inverse temperature $\beta \equiv 1$) and also with particle reservoirs at

the boundary with chemical potentials $\lambda_\pm$. One cannot, therefore, expect that the entropy production of the system *alone* will necessarily be positive. After all, it is quite possible that, depending on initial conditions, the system will on the average transfer entropy to the reservoirs (e.g., if the system is started at a high temperature). It is only the *total* entropy which can be expected to increase. The entropy change in the thermal reservoir equals the amount of energy transferred to it, divided through by its absolute temperature. Likewise, the entropy change in the particle reservoir equals the number of particles transferred to it, multiplied by its "chemical potential" $\lambda_\pm = \beta\mu_\pm$. Thus,

$$\sigma = \frac{dS_{\text{tot}}}{dt} = \dot{S} - \beta\dot{H} + \lambda_+ J_+ + \lambda_- J_-, \tag{3.1}$$

where $J_\pm$ are the particle fluxes *into* the reservoirs. Microscopically, we have, therefore,

$$\sigma[\mu] = -\frac{d}{dt}\sum_\eta \mu_t(\eta)\log\mu_t(\eta)\,|_{t=0} - \frac{d}{dt}\sum_\eta \mu_t(\eta)H(\eta)\,|_{t=0}$$
$$+\lambda_+ \sum_\eta \mu(\eta)J_+(\eta) + \lambda_- \sum_\eta \mu(\eta)J_-(\eta). \tag{3.2}$$

Here, $\mu_t(\eta)$ is the solution of the "master equation":

$$\frac{d}{dt}\mu_t(\eta) = (L^*\mu_t)(\eta)$$
$$\equiv \frac{1}{2}\sum_{\substack{x,y\in\Lambda \\ |x-y|=1}} [c(x,y;\eta^{xy})\mu_t(\eta^{xy}) - c(x,y;\eta)\mu_t(\eta)]$$
$$+ \sum_{x\in\partial\Lambda} [c(x,\eta^x)\mu_t(\eta^x) - c(x,\eta)\mu_t(\eta)], \tag{3.3}$$

with $\mu_0 = \mu$, and the boundary currents $J_\pm$ are defined by

$$J_\pm(\eta) = \sum_{x:x_1=\pm M} c(x,\eta)(2\eta_x - 1). \tag{3.4}$$

An explicit calculation yields

$$\sigma[\mu]=\frac{1}{4}\sum_{\substack{x,y\in\Lambda\\|x-y|=1}}\sum_{\eta}[c(x,y;\eta^{xy})\mu(\eta^{xy})$$

$$-c(x,y;\eta)\mu(\eta)]\log\left[\frac{c(x,y;\eta^{xy})\mu(\eta^{xy})}{c(x,y;\eta)\mu(\eta)}\right]$$

$$+\frac{1}{2}\sum_{x\in\partial\Lambda}\sum_{\eta}[c(x,\eta^{x})\eta(\eta^{x})-c(x,\eta)\mu(\eta)]\log\left[\frac{c(x,\eta^{x})\mu(\eta^{x})}{c(x,\eta)\mu(\eta)}\right]$$

$$=\frac{1}{4}\sum_{\substack{x,y\in\Lambda\\|x-y|=1}}\sum_{\eta}c(x,y;\eta)[e^{\Delta_{x,y}H(\eta)}\mu(\eta^{xy})-\mu(\eta)]$$

$$\times\log\left[\frac{e^{\Delta_{x,y}H(\eta)}\mu(\eta^{xy})}{\mu(\eta)}\right]$$

$$+\frac{1}{2}\sum_{x\in\partial\Lambda}\sum_{\eta}c(x,\eta)[e^{\Delta_{x}H(\eta)+\lambda_{x}(2\eta_{x}-1)}\mu(\eta^{x})-\mu(\eta)]$$

$$\times\log\left[\frac{e^{\Delta_{x}H(\eta)+\lambda_{x}(2\eta_{x}-1)}\mu(\eta^{x})}{\mu(\eta)}\right]. \tag{3.5}$$

The entropy production functional given in Eq. (3.5) has some important properties, which we point out. We note that the function $F(z)=F(x,y)\equiv(x-y)\log(x/y)$, satisfies $F(z)\geq 0$, $F(\lambda z)=\lambda F(z)$ for $\lambda>0$, and $F(z)$ is convex. The functional $\sigma[\mu]$ inherits these properties:

$$(1)\quad\text{(positivity)}\quad \sigma[\mu]\geq 0 \tag{3.6}$$

$$(2)\quad\text{(homogeneity)}\quad \sigma[\lambda\mu]=\lambda\sigma[\mu],\quad \lambda>0 \tag{3.7}$$

$$(3)\quad\text{(convexity)}\quad \sigma[\lambda\mu_1+(1-\lambda)\mu_2]\leq\lambda\sigma[\mu_1]+(1-\lambda)\sigma[\mu_2],\quad \text{for } 0\leq\lambda\leq 1. \tag{3.8}$$

Note that σ is defined on $\mathscr{D}$, the set of non-negative measures on $\{0,1\}^{\Lambda}$. Let $\mathscr{P}$ be the closed convex subset of probability measures on $\{0,1\}^{\Lambda}$. Then, $\partial\mathscr{P}=\{\mu\in\mathscr{P}\,|\,\mu(\eta)=0 \text{ for some } \eta\in\{0,1\}^{\Lambda}\}$. Since σ is non-negative and convex, it achieves a minimum on every closed subset of $\mathscr{D}$: in particular, on $\mathscr{P}$. Furthermore, we observe

Proposition 1. $\sigma[\mu]=+\infty$ for $\mu\in\partial\mathscr{P}$.

Proof: Suppose that $\mu(\eta)=0$ for some η. On the other hand, there must be some configuration, ζ, with $\mu(\zeta)>0$, and furthermore a sequence of *allowed transitions* [i.e., exchanges with $c(x,y)>0$ or creation/annihilations with $c(x)>0$] such that

$$\eta\equiv\eta_0\to\eta_1\to\eta_2\to\cdots\to\eta_{k-1}\to\eta_k\equiv\zeta. \tag{3.9}$$

There must exist some i such that $\mu(\eta_i)=0$ but $\mu(\eta_{i+1})>0$. Suppose, e.g., the transition $\eta_i\to\eta_{i+1}$ is via an exchange of occupancies at x,y (the argument is the same for a creation–annihilation transition). Then,

$$c(x,y;\eta_i)[e^{\Delta_{x,y}H(\eta_i)}\mu(\eta_{i+1})-\mu(\eta_i)]\log\left[\frac{e^{\Delta_{x,y}H(\eta_i)}\mu(\eta_{i+1})}{\mu(\eta_i)}\right]=+\infty. \tag{3.10}$$

Since all the terms of $\sigma[\mu]$ are non-negative it follows that $\sigma[\mu]=+\infty$.■

There are certainly μ for which $\sigma[\mu]<+\infty$, so Proposition 1 has the implication that the minimum entropy production is achieved on the interior Int $\mathscr{P}$ of $\mathscr{P}$. Furthermore, we have

Proposition 2. σ is strictly convex on Int $\mathscr{P}$.

Proof: Note $F[\lambda z_1+(1-\lambda)z_2]=\lambda F(z_1)+(1-\lambda)F(z_2)$ for $0<\lambda<1$ iff $z_1=0$, $z_2=0$ or $z_1=\alpha z_2$ for $\alpha>0$. Hence, for $\mu_1,\mu_2\in$ Int $\mathscr{P}$, $\sigma[\lambda\mu_1+(1-\lambda)\mu_2]=\lambda\sigma[\mu_1]+(1-\lambda)\sigma[\mu_2]$ with $0<\lambda<1$ implies

$$[\mu_1(\eta^{xy}),\mu_1(\eta)]=\alpha_{xy}(\eta)[\mu_2(\eta^{xy}),\mu_2(\eta)] \tag{3.11}$$

for all η,x,y such that $c(x,y;\eta)>0$ and

$$[\mu_1(\eta^{x}),\mu_1(\eta)]=\alpha_{x}(\eta)[\mu_2(\eta^{x}),\mu_2(\eta)] \tag{3.12}$$

for all $\eta,x\in\partial\Lambda$ such that $c(x,\eta)>0$. Since, for any ζ,η, there exists a sequence of allowed transitions $\eta\to\cdots\to\zeta$ and since for each transition $\eta_i\to\eta_{i+1}$, $\mu_1(\eta_{i+1})/\mu_2(\eta_{i+1})=\mu_1(\eta_i)/\mu_2(\eta_i)$, it follows that $\mu_1(\eta)/\mu_2(\eta)=$ const independent of η. In fact, $\mu_1=\mu_2$ by the normalization condition.■

By Proposition 2, there is a unique $\mu_{\min}\in$Int $\mathscr{P}$ at which the minimum of σ is achieved. Since there is also a unique stationary measure $\mu_{ss}\in$Int $\mathscr{P}$, it is tempting to conjecture that $\mu_{\min}=\mu_{ss}$: unfortunately, this is almost never true. Nevertheless, there *is* a relation between the stationary state and the state of minimal entropy production, well known in linear nonequilibrium thermodynamics as the *principle of minimum entropy production*.[7,22] Remarkably, this principle holds not only at the level of macroscopic thermodynamics (as a direct consequence of the Onsager reciprocity relations), but also for microscopic probability measures. (To use a common terminology, it is a level-3 principle, not merely level-1.) We now discuss this connection, first, at the macroscopic, hydrodynamical level and then at the microscopic, statistical level of description for our model.

The steady-state density profile of the purely diffusive systems we discuss is given at the macroscopic level by the solution of the nonlinear transport equation (2.12):

$$\frac{\partial}{\partial q}\cdot\left[D[\rho_{ss}(q)]\frac{\partial}{\partial q}\rho_{ss}(q)\right]=0, \tag{3.13}$$

with boundary conditions $\rho_{ss}(\pm 1)=\rho_{\pm}$. Here, it is convenient to work with the equivalent equation for the chemical potential profile:

$$\frac{\partial}{\partial q}\cdot\left[(\chi D)[\lambda_{ss}(q)]\frac{\partial}{\partial q}\lambda_{ss}(q)\right]=0, \tag{3.14}$$

with boundary condition $\lambda_{ss}(\pm 1)=\lambda_{\pm}$ (χ is the equilibrium susceptibility, $\chi=d\rho/d\lambda$). On the other hand nonequilibrium thermodynamics gives for the entropy production of this system (in terms of the chemical potential):

$$\sigma[\lambda]=\int_{-1}^{1}dq(\chi D)[\lambda(q)]\left[\frac{\partial}{\partial q}\lambda(q)\right]^2. \tag{3.15}$$

Note that this functional of the potential profile is given as an integral over a local entropy production without reference to the particle reservoirs. The macroscopic profile which minimizes the entropy production is given by the solution of the equation:

$$\frac{\delta\sigma}{\delta\lambda(q)}[\lambda_{\min}]=(\chi D)'[\lambda_{\min}(q)]\left[\frac{\partial}{\partial q}\lambda_{\min}(q)\right]^2$$
$$-2\frac{\partial}{\partial q}\cdot\left[(\chi D)[\lambda_{\min}(q)]\frac{\partial}{\partial q}\lambda_{\min}(q)\right]=0. \tag{3.16}$$

Clearly, Eqs. (3.14) and (3.16) are distinct, unless the Onsager coefficient χD is independent of the chemical potential λ, a situation which rarely (if ever) occurs in practice.

On the other hand, even if χD depends upon λ, we may always consider the situation where the deviation from global equilibrium is small, i.e.,

$$\lambda_{\pm}=\lambda\pm\delta, \tag{3.17}$$

and expand both profiles in the small parameter δ:

$$\lambda_{ss}^{(\delta)}=\lambda+\lambda_{ss}^{(1)}\cdot\delta+\lambda_{ss}^{(2)}\cdot\delta^2+\dots, \tag{3.18}$$

$$\lambda_{\min}^{(\delta)}=\lambda+\lambda_{\min}^{(1)}\cdot\delta+\lambda_{\min}^{(2)}\cdot\delta^2+\dots. \tag{3.19}$$

We have anticipated that to zeroth order in δ, both λ_{ss} and $\lambda_{\min}$ are, of course, given by the constant profile $\lambda(q)\equiv\lambda$. However, also to first order in δ, we find that

$$\lambda_{ss}^{(1)}=\lambda_{\min}^{(1)}, \tag{3.20}$$

both being given by the solution of the Laplace equation:

$$(\Delta\lambda^{(1)})(q)=0 \tag{3.21}$$

in $[-1,1]$ with boundary conditions $\lambda^{(1)}(\pm 1)=\pm 1$, i.e., the linear profile $\lambda^{(1)}(q)=q$. We observe that to second order the two profiles will no longer agree. However, the precise content of the thermodynamic principle of minimum entropy production, which holds quite generally, is that the two agree to first order, i.e., Eq. (3.20).

Now let us consider the microscopic situation. Since the unique minimum of $\sigma[\mu]$ occurs at the interior of $\mathscr{P}$, it may be found as the solution of the variational equation:

$$\frac{\delta\tilde{\sigma}}{\delta\mu(\eta)}[\mu_{\min},\alpha_{\min}]=0, \tag{3.22}$$

where we have defined

$$\tilde{\sigma}[\mu,\lambda]\equiv\sigma[\mu]+\alpha\left[\sum_{\eta}\mu(\eta)-1\right], \tag{3.23}$$

which incorporates the normalization constraint by the Lagrange multiplier α. Clearly, Eqs. (3.22) and (3.23) are equivalent to

$$\frac{\delta\sigma}{\delta\mu(\eta)}[\mu_{\min}]=\alpha_{\min}=\text{const (independent of }\eta). \tag{3.24}$$

The value of the Lagrange multiplier is easy to evaluate, since the homogeneity of the entropy production (3.7) implies the Euler relation:

$$\sigma[\mu]=\sum_{\eta}\mu(\eta)\frac{\delta\sigma}{\delta\mu(\eta)}[\mu]. \tag{3.25}$$

Together, Eqs. (3.24) and (3.25) yield

$$\sigma[\mu_{\min}]=\sum_{\eta}\mu_{\min}(\eta)\frac{\delta\sigma}{\delta\mu(\eta)}[\mu_{\min}]=\alpha\sum_{\eta}\mu_{\min}(\eta)=\alpha. \tag{3.26}$$

Hence, the variational equation for $\mu_{\min}$ becomes

$$\frac{\delta\sigma}{\delta\mu(\eta)}[\mu_{\min}]=\sigma[\mu_{\min}]. \tag{3.27}$$

A relationship between $\mu_{\min}$ and μ_{ss} can be inferred from the following inequality:

$$\frac{\delta\sigma}{\delta\mu(\eta)}[\mu]\geq-2\frac{(L^*\mu)(\eta)}{\mu(\eta)}, \tag{3.28}$$

which follows from the explicit computation for our model:

$$\frac{\delta\sigma}{\delta\mu(\eta)}[\mu]=\frac{1}{2}\sum_{x,y\in\Lambda}c(x,y;\eta)\phi\left[1-e^{\Delta_{x,y}H(\eta)}\frac{\mu(\eta^{xy})}{\mu(\eta)}\right]$$

$$+\sum_{x\in\partial\Lambda}c(x,\eta)\phi\left[1-e^{\Delta_x H(\eta)+\lambda_x(2\eta_x-1)}\frac{\mu(\eta^x)}{\mu(\eta)}\right], \tag{3.29}$$

with

$$\phi(u)\equiv\frac{u-\log(1-u)}{2}>u. \tag{3.30}$$

In the case where $\sigma[\mu_{\min}]=0$, Eqs. (3.27) and (3.28) imply that

$$(L^*\mu_{\min})(\eta)\geqslant 0. \tag{3.31}$$

However, this implies, in fact, that

$$(L^*\mu_{\min})(\eta)\equiv 0, \tag{3.32}$$

since conservation of normalization gives

$$\sum_{\eta}(L^*\mu_{\min})(\eta)=0. \tag{3.33}$$

Thus, for $\sigma[\mu_{\min}]=0$,

$$\mu_{\min}=\mu_{ss}. \tag{3.34}$$

However, the condition $\sigma[\mu_{\min}]=0$ holds essentially only in the case of homogeneous equilibrium. Observe that from the definition (3.2):

$$\sigma[\mu_{ss}]=-\sum_{\eta}(L^*\mu_{ss})(\eta)[\log\mu_{ss}(\eta)+1]-\sum_{\eta}(L^*\mu_{ss})(\eta)H(\eta)$$

$$+\lambda_+\sum_{\eta}\mu_{ss}(\eta)j_+(\eta)+\lambda_-\sum_{\eta}\mu_{ss}(\eta)j_-(\eta)$$

$$=(\lambda_+-\lambda_-)\langle j^{(0)}(\eta)\rangle_{ss}, \tag{3.35}$$

where, for $m=-M,\ldots,M-1$,

$$j^{(m)}(\eta)\equiv\sum_{\substack{x,y\in\Lambda:\\ x_1=m}}j_{(x,y)}(\eta). \tag{3.36}$$

We have employed the consequence of stationarity and conservation of particle number:

$$\langle j_+\rangle_{ss}=-\langle j_-\rangle_{ss}=\langle j^{(m)}\rangle_{ss}. \tag{3.37}$$

We see, in particular, that $\sigma[\mu_{ss}]=0$ implies either $\lambda_+=\lambda_-$ or $\langle j^{(0)}\rangle_{ss}=0$, i.e., the equilibrium situation. This may be compared with the macroscopic thermodynamic situation. If $\sigma[\mu_{\min}]>0$, no conclusion may be drawn from the inequality (3.28).

Instead, we may proceed as before and expand in the parameter δ, which measures the deviation from global equilibrium. For this purpose it is convenient to introduce the density f of the measure μ relative to the (grand canonical) Gibbs measure ν_λ at chemical potential λ: $\mu=f\nu_\lambda$. In terms of the density f,

$$\sigma[f]=\frac{1}{4}\sum_{x,y\in\Lambda}\left\langle c(x,y;\eta)[f(\eta^{xy})-f(\eta)]\log\left[\frac{f(\eta^{xy})}{f(\eta)}\right]\right\rangle_\lambda$$

$$+\frac{1}{2}\sum_{x\in\partial\Lambda}\left\langle c^{(\delta)}(x,\eta)[e^{\delta_x(2\eta_x-1)}f(\eta^x)-f(\eta)]\right.$$

$$\left.\times\log\left[\frac{e^{\delta_x(2\eta_x-1)}f(\eta^x)}{f(\eta)}\right]\right\rangle_\lambda \tag{3.38}$$

and

$$\frac{\delta\sigma}{\delta f(\eta)}[f]=\frac{1}{4}\sum_{x,y\in\Lambda}c(x,y;\eta)\{f(\eta^{xy})-f(\eta)$$

$$+f(\eta)[\log f(\eta^{xy})-\log f(\eta)]\}\nu_\lambda(\eta)$$

$$+\frac{1}{2}\sum_{x\in\partial\Lambda}c^{(\delta)}(x;\eta)\{e^{\delta_x(2\eta_x-1)}f(\eta^x)-f(\eta)$$

$$+f(\eta)[\log f(\eta^x)-\log f(\eta)+\delta_x(2\eta_x-1)]\}\nu_\lambda(\eta), \tag{3.39}$$

where $\delta_x=\lambda_x-\lambda$ and the δ-dependence of the boundary rates has been explicitly indicated. Then, we may expand all quantities in powers of δ (for fixed M, everything in sight is analytic in δ):

$$f_{\min}^{(\delta)}=1+\delta\cdot f_{\min}^{(1)}+\delta^2\cdot f_{\min}^{(2)}+\cdots, \tag{3.40}$$

$$c^{(\delta)}(x,\eta)=c^{(0)}(x,\eta)+\delta\cdot c^{(1)}(x,\eta)+\cdots, \tag{3.41}$$

and so forth. Now, it is easy to check that $\sigma[f_{\min}^{(\delta)}]=0(\delta^2)$. Thus, the variational equation (3.27) to $0(\delta)$ reads (with $\epsilon_x=\operatorname{sgn}x_1$):

$$\frac{1}{4}\sum_{x,y\in\Lambda}c(x,y;\eta)[f_{\min}^{(1)}(\eta^{xy})-f_{\min}^{(1)}(\eta)]+\frac{1}{2}\sum_{x\in\partial\Lambda}c^{(0)}(x;\eta)[f_{\min}^{(1)}(\eta^x)$$

$$-f_{\min}^{(1)}(\eta)+\epsilon_x(2\eta_x-1)]=0. \tag{3.42}$$

We separate out the term:

$$\sum_{x\in\partial\Lambda} \epsilon_x c^{(0)}(x;\eta)(2\eta_x - 1) = \sum_{x_\perp} [\, j_+^{(0)}(M,x_\perp;\eta) - j_-^{(0)}(-M,x_\perp;\eta)\,]. \tag{3.43}$$

To evaluate the difference in boundary currents, we use the conservation law:

$$L\eta_x = -\sum_{y\in\Lambda} j_{(x,y)}(\eta) - \delta_{x_1,M} j_+(x;\eta) - \delta_{x_1,-M} j_-(x;\eta), \tag{3.44}$$

to derive

$$\sum_{x_\perp} [\, j_+^{(0)}(M,x_\perp;\eta) - j_-^{(0)}(-M,x_\perp;\eta)\,] = \frac{1}{M}\Big[J_{\Lambda,1}(\eta) - L_0 \sum_{x\in\Lambda} x_1\eta_x \Big], \tag{3.45}$$

with $J_{\Lambda,1}$ the bulk current in the 1-direction:

$$J_{\Lambda,1}(\eta) = \sum_{\substack{x\in\Lambda \\ x+e_1\in\Lambda}} j_{x,x+e_1}(\eta). \tag{3.46}$$

This allows us to rewrite Eq. (3.42) as

$$(L_0 f_{\min}^{(1)})(\eta) = \frac{1}{M}\Big[-J_{\Lambda,1}(\eta) + L_0 \sum_{x\in\Lambda} x_1\eta_x \Big], \tag{3.47}$$

which has the unique solution:

$$f_{\min}^{(1)}(\eta) = \frac{1}{M}\sum_{x\in\Lambda} x_1(\eta_x - \rho) + \frac{1}{M}[(-L_0)^{-1} J_{\Lambda,1}](\eta). \tag{3.48}$$

We wish to compare this expression with the similarly defined quantity $f_{ss}^{(1)}$ for the stationary state. For this purpose, we return to the Zubarev distribution (2.19) for any interpolating profile $\lambda_x^{(\delta)}$ analytic in δ; in particular, $\lambda_x^{(\delta)} = \lambda + \delta\cdot x_1/M$ is convenient. If we expand the density f_{ss} in δ, we find from Eq. (2.19) that

$$f_{ss}^{(1)}(\eta) = \frac{1}{M}\sum_{x\in\Lambda} x_1(\eta_x - \rho) + \frac{1}{M}\int_0^\infty dt(e^{tL_0} J_{\Lambda,1})(\eta). \tag{3.49}$$

We observe immediately the identity of Eqs. (3.48) and (3.49), i.e.,

$$f_{\min}^{(1)} = f_{ss}^{(1)}. \tag{3.50}$$

This is the microscopic version of the principle of minimum entropy production, which extends the macroscopic version [Eq. (3.20)]. Not only the density, but *all* the variables, will have expectations which agree

to first order in δ for the two ensembles. Such a microscopic version has been established earlier in the context of quantum systems weakly coupled to thermal reservoirs.[23] The present proof emends some errors in the proof for a similar stochastic model in Ref. 24.

4. Entropy production and the hydrodynamic limit

Guo, Papanicolaou, and Varadhan[8] have shown that the entropy production [Eq. (3.5)] is a central quantity to consider for analyzing the hydrodynamic limit. In the original work,[8] GPV studied the time-dependent hydrodynamics of a Ginzburg–Landau model on a periodic, one-dimensional lattice. Here we describe the application of their techniques to the stationary hydrodynamics (hydrostatics) of the types of models considered above.[9] We shall first state the, unfortunately restrictive, technical conditions under which the results in Ref. 9 are proved. Then, we shall state the precise results obtained there. Finally, we shall briefly sketch some of the ideas in the proof.

The chief technical restriction under which a hydrodynamic limit has been proved is the so-called *gradient condition*.[4,6] This states that there is a bounded, local function h (of range R) so that the particle current is given by

$$j_{x,y}(\eta) = h_x(\eta) - h_y(\eta) \tag{4.1}$$

[here, $h_x(\eta) = \tau_x h_0(\eta)$, etc.]. This condition states that the microscopic current is a gradient of a local function. This is already close to the macroscopic transport law: all that is needed is to replace the steady-state expectation of $h_x(\eta)$ by an appropriate function of the local density. We may note that nontrivial examples of rates which satisfy all of the imposed conditions, particularly the gradient condition and detailed balance, are known in *one* dimension only. Therefore, we restrict ourselves to one-dimensional models. On the other hand, there is no restriction there on the interactions, i.e., on $H(\eta)$. For each $H(\eta)$, it is always possible to find rates satisfying Eq. (4.1), although the gradient models are not generic.

Now, with these, admittedly heavy, restrictions, the following results are established in Ref. 9:

Theorem 1. Let $X^\epsilon(\phi)$ be the empirical density field defined by

$$X^\epsilon(\phi) = \epsilon \sum_{x=-M}^{M} \phi(\epsilon x)\eta(x) \tag{4.2}$$

for $\phi \epsilon C_0^\infty[-1,1]$ and P^ϵ be the law of that field induced by the stationary measure μ_{ss}^ϵ. Further, let P be the law (delta distribution) of the deterministic density field:

$$X(\phi)=\int_{-1}^{1} dq\, \phi(q)\rho_{ss}(q), \quad \phi \epsilon C_0^\infty[-1,1], \tag{4.3}$$

where $\rho_{ss}(q)$ is the solution of the stationary transport equation (2.12). Then, P is the weak limit of P^ϵ as $\epsilon \to 0$. In particular, $X^\epsilon(\phi)$ converges in probability with respect to P^ϵ to the deterministic density field $X(\phi)$ given by the stationary transport equation.

This result explains why, with overwhelming probability, the empirical density in the steady state will be given by the solution ρ_{ss} of the macroscopic equation (2.12). The proof in fact establishes a stronger result:

Theorem 2. Let $g_0(\eta)$ be any bounded, local function at the origin, $X^\epsilon(g;\phi)$ the empirical extensive field defined by

$$X^\epsilon(g;\phi)=\epsilon \sum_{x=-M}^{M} \phi(\epsilon x) g_x, \tag{4.4}$$

and

$$X(g;\phi)=\int_{-1}^{1} dq\, \phi(q)\langle g_0(\eta)\rangle_{\rho_{ss}(q)}, \quad \phi \epsilon C_0^\infty[-1,1], \tag{4.5}$$

a corresponding deterministic field. Denote by P_g^ϵ the law of $X^\epsilon(g;\phi)$ and by P_g the delta distribution associated to $X(g;\phi)$. Then, P_g is the weak limit of P_g^ϵ as $\epsilon \to 0$.

As a corollary of this result one has also:

Corollary (Fick's law and normal transport). Consider the bounded, local function $j_1(\eta) = c(0,1;\eta)(\eta_0 - \eta_1)$, which is the (systematic) current. Then the law of $\epsilon^{-1}X^\epsilon(j_1;\phi)$ converges weakly to the law of $X(j_1;\phi) \equiv -\int_{-1}^{1} dq\, \phi(q) D[\rho_{ss}(q)]\partial_q \rho_{ss}(q)$; in particular, the current field converges in probability with respect to μ_{ss}^ϵ to the deterministic limit given by Fick's law. Furthermore, for every $q \epsilon [-1,1]$,

$$\lim_{\epsilon \to 0} \epsilon^{-1}\langle j_1([\epsilon^{-1}q])\rangle_{ss}^\epsilon = -D[\rho_{ss}(q)]\partial_q \rho_{ss}(q). \tag{4.6}$$

Finally, the strongest consequence of the entropy production argument is contained in

Theorem 3 (L^2—local equilibrium property). For any bounded local function $g_0(\eta)$,

$$\lim_{\epsilon \to 0} \int_{-1}^{1} dq\, |\mu_{ss}^\epsilon(g_{[\epsilon^{-1}q]}) - \langle g_0\rangle_{\rho_{ss}(q)}|^2 = 0. \tag{4.7}$$

This result states that at most spatial points, the steady-state expectation of a local observable converges as $\epsilon \to 0$ to the expectation in an appropriate local equilibrium distribution.

The proof exploits entropy production in the following way: it is first shown that the total entropy production in the steady state is "small," i.e.,

$$\sigma[\mu_{ss}^\epsilon] = 0(\epsilon). \tag{4.8}$$

This is a consequence of Eq. (3.35). Consider the current:

$$j_{\Lambda',1}(\eta)=\frac{1}{2(M-R)} \sum_{x=-(M-R)}^{M-R} j_{x,x+1}(\eta) \tag{4.9}$$

averaged over the interior block $[-(M-R), M-R]$. By stationarity and conservation of particle number, as in Eq. (3.37), it follows that

$$\langle j^{(0)}(\eta)\rangle_{ss}^\epsilon = \langle j_{\Lambda',1}(\eta)\rangle_{ss}^\epsilon. \tag{4.10}$$

On the other hand, by the gradient condition (4.1):

$$j_{\Lambda',1}(\eta)=\frac{h_{M-R}(\eta)-h_{-(M-R)}(\eta)}{2(M-R)}. \tag{4.11}$$

Because $h_x(\eta)$ is a bounded function uniformly in x,

$$j_{\Lambda',1}(\eta)=0\left(\frac{1}{M}\right) \tag{4.12}$$

for *every* η and, thus, in particular, $\langle j^{(0)}(\eta)\rangle_{ss}^\epsilon = 0(1/M)$ via Eq. (4.10). This and Eq. (3.35) yield the required bound Eq. (4.8).

The point of this estimate is that, by subadditivity of the entropy production, the marginal entropy production in any finite microscopic block of sites is, at most, $0(\epsilon)$ [in fact, it is presumably $0(\epsilon^2)$] and thus vanishes in the limit as $\epsilon \to 0$. Hence, by the properties of the entropy production discussed in Sec. 3, the marginal distribution in that finite microscopic block must converge as $\epsilon \to 0$ to a convex combination of canonical Gibbs measures. By the law of large numbers and equivalence of ensembles, this allows one to replace any sum function in a large microscopic block by a suitable function of the (empirical) density. A separate "two-block estimate" shows that the empirical densities in large microscopic blocks which are macroscopically close are nearly equal, and allow a similar replacement to be made in small macroscopic blocks. This allows one to derive from the identities:

$$L\eta(x) = (\Delta h)_x(\eta) \tag{4.13}$$

and

$$L[\eta(x)\eta(y)] - [L\eta(x)]\eta(y) - \eta(x)[L\eta(y)]$$
$$= (\delta_{x,y} - \delta_{x+1,y})c(x,x+1;\eta) + (\delta_{x,y} - \delta_{x-1,y})c(x,x-1;\eta) \tag{4.14}$$

that, for any weak subsequential limit P^* of P^ϵ,

$$\partial_q^2 E^*\{\hat{h}[\rho(q)]\} = 0 \tag{4.15}$$

and

$$\partial_q^2 E^*\{\hat{h}[\rho(q)]\rho(p)\} + \partial_p^2 E^*\{\rho(q)\hat{h}[\rho(p)]\} = 0 \tag{4.16}$$

hold in a weak sense. We have introduced here the function of density $\hat{h}(\rho) \equiv \langle h_0(\eta)\rangle_\rho$, where the expectation is with respect to an infinite Gibbs measure at density ρ. If one linearizes the latter equation around the stationary profile $\rho_{ss}(q)$ as

$$\rho(q) = \rho_{ss}(q) + \delta\rho(q), \tag{4.17}$$

then one obtains, using also Eq. (4.15):

$$\partial_q^2\{D[\rho_{ss}(q)]E^*[\delta\rho(q)\delta\rho(p)]\}$$
$$+ \partial_p^2\{D[\rho_{ss}(p)]E^*[\delta\rho(q)\delta\rho(p)]\} = 0, \tag{4.18}$$

which has the unique solution subject to Dirichlet boundary conditions

$$E^*[\delta\rho(q)\delta\rho(p)] = 0. \tag{4.19}$$

In Ref. 9, a nonlinear version of the above argument is given which leads to a similar consequence. Note that Eq. (4.19) implies that the density profile $\rho(q)$ in the measure P^* is deterministic and given by $\rho_{ss}(q)$. That, finally, gives Theorem 1. The other results of the paper can be deduced from the above considerations with a little extra work.

5. Concluding remarks

To conclude this paper, we would like to make a series of remarks on the themes we have discussed, particularly to explain their importance for future work.

First, we point out that the principle of minimum entropy production has relevance for the proof of hydrodynamic limits, in order to remove the restriction to gradient models. It turns out that for nongradient models it is important not only to establish the local equilibrium structure of the measure, but, in fact, to have the next-order correction in ϵ to the local equilibrium.[25]

The form of that correction may be guessed from the Zubarev distribution formula in Sec. 2. Choosing a smooth profile $\lambda_{ss}(q)$ and setting $\lambda_x = \lambda_{ss}(\epsilon x)$, we see that $(\nabla_1\lambda) = 0(\epsilon)$. Thus, we conjecture that, for a bounded local observable $g_0(\eta)$,

$$\lim_{\epsilon\to 0} \epsilon^{-1}\Big[\sum_{|\epsilon^{-1}q|} \langle g(\eta)\rangle_{ss}^\epsilon - \langle g_0(\eta)\rangle_{\rho_{ss}(q)}$$
$$- \lambda'_{ss}(q)\sum_{x\in\mathbb{Z}} x_1\langle[\eta_x - \rho_{ss}(q)]g_0(\eta)\rangle_{\rho_{ss}(q)}$$
$$- \lambda'_{ss}(q)\int_0^\infty dt \sum_{x\in\mathbb{Z}} \langle(e^{\mathcal{L}t}J_{x,x+1})\cdot(\eta)g_0(\eta)\rangle_{\rho_{ss}(q)}\Big] = 0. \tag{5.1}$$

(In one dimension, this misses an extra contribution from the long-range correlations: see Ref. 4, Sec. 7.) However, we have already seen in Sec. 3 that, to *first order in* ϵ, the same correction may be guessed by minimizing the entropy production. The advantage is that the correction is then seen to be given by a variational principle. The reader interested in these matters is advised to consult the notes of Spohn (Ref. 6, Sec. 4.5) and the preprint of S. R. S. Varadhan.[25]

A second remark is that, in the book of Zubarev,[15] a quite different variational principle was proposed to characterize the nonequilibrium distributions, namely, a *maximum entropy principle* modeled after the one of Gibbs for the equilibrium distributions. It would, of course, be very attractive if nonequilibrium statistical mechanics were able to be developed along Gibbsian lines. Unfortunately, without mentioning any details, we must report that in examining the formal arguments of Zubarev, we have found problems which we, at least, could not resolve. Here, we have instead characterized the Zubarev distribution, as a first-order correction to local equilibrium, by a principle of minimum entropy production. We must caution also here that we do not expect such a characterization to be valid for steady states of models with deterministic, Hamiltonian dynamics in interaction with stochastic reservoirs, at least if the entropy is defined in terms of the usual Gibbsian expression as in Eq. (3.2) above. Since Hamiltonian dynamics conserves the Gibbs entropy, its production in such models will not have any bulk dynamical contribution and minimum entropy production would not usefully characterize the local structure of the steady state.

Finally, we remark that the principle of minimum entropy production, as we have discussed it, is clearly a principle of limited validity: it only

applies to systems globally near equilibrium. However, there is another closely related principle which may, in fact, be an *exact* result even in far from equilibrium situations. This is the *principle of least dissipation*, introduced by Onsager in 1931.[26] In contrast to Prigogine's principle of minimum entropy production, which attempts to characterize the steady state by a *static* variational principle, the principle of Onsager is explicitly a *dynamical* one. Although rigorous mathematical studies remain to be done, the Onsager principle appears to be a viable candidate for the long sought generalization of the equilibrium variational principles to the nonequilibrium steady state.[27]

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