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Large Deviation of the Density Profile in the Steady State of the Open Symmetric Simple Exclusion Process

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We consider an open one dimensional lattice gas on sites $i = 1,\ldots, N$, with particles jumping independently with rate 1 to neighboring interior empty sites, the *simple symmetric exclusion process*. The particle fluxes at the left and right boundaries, corresponding to exchanges with reservoirs at different chemical potentials, create a stationary nonequilibrium state (SNS) with a steady flux of particles through the system. The mean density profile in this state, which is linear, describes the typical behavior of a macroscopic system, i.e., this profile occurs with probability 1 when $N \to \infty$. The probability of microscopic configurations corresponding to some other profile $\rho(x)$, $x = i/N$, has the asymptotic form $\exp[-N\mathscr{F}(\{\rho\})]$; $\mathscr{F}$ is the *large deviation functional*. In contrast to equilibrium systems, for which $\mathscr{F}_{\text{eq}}(\{\rho\})$ is just the integral of the appropriately normalized local free energy density, the $\mathscr{F}$ we find here for the nonequilibrium system is a nonlocal function of ρ. This gives rise to the long range correlations in the SNS predicted by fluctuating hydrodynamics and suggests similar nonlocal behavior of $\mathscr{F}$ in general SNS, where the long range correlations have been observed experimentally.

KEY WORDS: Large deviations; symmetric simple exclusion process; open system; stationary nonequilibrium state.

1. INTRODUCTION

The extension of the central object of equilibrium statistical mechanics, entropy or free energy, to stationary nonequilibrium systems in which there

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is a transport of matter or energy has proved difficult. One knows from various approximate theories like fluctuating hydrodynamics that such systems exhibit long range correlations very different from those of equilibrium systems.[1–3] These correlations extend over macroscopic distances, as has been established rigorously in some models, and reflect the intrinsic nonadditivity of such systems. They have been measured experimentally in a fluid with a steady heat current.[2,4] Their derivation from a well defined macroscopic functional valid beyond local equilibrium (where there are no such correlations) is clearly desirable. We report here what we believe is the first exact derivation of such a functional for a nonequilibrium model which is relatively simple but exhibits the realistic feature of macroscopically long range correlations.

Before describing our model and results, we review briefly the corresponding results for equilibrium systems.[5–8] Let us ask for the probability of finding an isolated macroscopic equilibrium system, having a given number of particles and energy and contained in a given volume V, in a specified macro state $\mathscr{M}$, that is, of finding the microscopic configuration X of the system in a certain region $\Gamma_{\mathscr{M}}$ of its phase space. According to the basic tenet of equilibrium statistical mechanics, embedded in the Boltzmann–Gibbs–Einstein formalism, this probability is proportional to $\exp[S(\mathscr{M})/k_B]$, where the (Boltzmann) entropy $S(\mathscr{M})$ of the macro state $\mathscr{M}$ is defined by $S(\mathscr{M}) = k_B \log |\Gamma_{\mathscr{M}}|$, with $|\Gamma_{\mathscr{M}}|$ the phase space volume of $\Gamma_{\mathscr{M}}$.[5–9]

When the system is not isolated but is part of a much larger system—a situation idealized by considering the system to be in contact with an infinite thermal reservoir at temperature T and chemical potential ν—then the entropy in the formula above is replaced by an appropriate free energy. Consider in particular a lattice gas in a unit cube containing L^d sites with spacing $1/L$ (similar formulas will hold for continuum systems), and suppose that the macro state of interest is specified by a *density profile* prescribing the density $\rho(x)$ at each macroscopic position x in the cube. Then the probability of finding the system in this macro state is given for large L by

$$P(\{\rho(x)\}) \sim \exp[-L^d \mathscr{F}_{\mathrm{eq}}(\{\rho\})], \tag{1.1}$$

with

$$\mathscr{F}_{\mathrm{eq}}(\{\rho\}) = \int [f_\nu(\rho(x)) - f_\nu(\bar{\rho})]\, dx. \tag{1.2}$$

The integration in (1.2) is over the unit cube, $f_\nu(r) = a(r) - \nu r$, where $a(r)$ is the usual Helmholtz free energy density for a uniform equilibrium system at density r, and the equilibrium density $\bar{\rho} = \bar{\rho}(\nu)$ corresponding to the chemical potential ν is obtained by minimizing f_ν:

$$\nu = \left.\frac{\partial a(r)}{\partial r}\right|_{r = \bar{\rho}(\nu)}. \tag{1.3}$$

Note that $-f_\nu(\bar{\rho})$ is just the pressure in the grand canonical ensemble. We have suppressed the dependence of f and $\mathcal{F}_{\mathrm{eq}}$ on the constant temperature T, and assume for simplicity that neither $\bar{\rho}$ nor $\rho(x)$, for any x, lies in a phase transition region at this temperature.

The challenge is to extend these results to nonequilibrium systems, in particular, to systems which are maintained in a stationary nonequilibrium state (SNS) with a steady flux of particles by contact with two boundary reservoirs at different chemical potentials. We would like to generalize the formula (1.2) for $\mathcal{F}_{\mathrm{eq}}(\{\rho\})$, obtaining a large deviation functional $\mathcal{F}(\{\rho\})$ such that the probability of observing a density profile $\rho(x)$ is given by a formula analogous to (1.1). The typical profile would then correspond to the ρ which minimizes $\mathcal{F}$. A similar analysis and an appropriate $\mathcal{F}$ would certainly be useful for the study of pattern formation in more general SNS. An interesting example is the Bénard system, in which the particle flux is replaced by a heat flux maintained by reservoirs at different temperatures, with the hotter reservoir below the system, and the typical patterns change abruptly from uniform to rolls to hexagonal cells as the fluid is driven away from equilibrium.[10] Open systems of this type have been discussed extensively in the literature from both a microscopic and macroscopic point of view; see refs. 11, 12, and references therein.

Given our current limited understanding of such SNS, however, it is necessary to start with the simplest systems; our results here are for the one dimensional symmetric simple exclusion process (SSEP),[13–15] driven by boundary reservoirs at distinct chemical potentials ν_0 and ν_1. We consider a lattice of N sites, in which each site i is either empty ($\tau_i = 0$) or occupied by a single particle ($\tau_i = 1$), so that each of the 2^N possible configurations of the system is characterized by N binary variables $\tau_1,..., \tau_N$. Each particle independently attempts to jump to its right neighboring site, and to its left neighboring site, in each case at rate 1 (so that there is no preferred direction). It succeeds if the target site is empty; otherwise nothing happens. At the boundary sites, 1 and N, particles are added or removed: a particle is added to site 1, when the site is empty, at rate α, and removed, when the site is occupied, at rate γ; similarly particles are added to site N at rate δ and removed at rate β. This corresponds to the system being in contact with infinite left and right reservoirs having fugacities $z_0 = \exp \nu_0 = \alpha/\gamma$, and $z_1 = \exp \nu_1 = \delta/\beta$, see refs. 16 and 17. We therefore define

$$\rho_0 = \frac{z_0}{1+z_0} = \frac{\alpha}{\gamma+\alpha}, \qquad \rho_1 = \frac{z_1}{1+z_1} = \frac{\delta}{\beta+\delta}, \tag{1.4}$$

and think of these as the densities of the reservoirs. They will in fact be the stationary densities at the left and right ends of the system when $N \to \infty$ (see (7.12) below).

We refer to z_0 and z_1 as fugacities because if we were to place our system in contact with only the left (right) reservoir by limiting particle input and output to just the left (right) side, i.e., by setting $\delta = \beta = 0$ ($\alpha = \gamma = 0$), then its stationary state would be one of equilibrium with fugacity z_0 (z_1), with no net flux of particles. Of course if $z_0 = z_1 = z$ then the system would be in an equilibrium state whether in contact with one or both reservoirs, i.e., in a product measure with uniform density $\rho = z/(1+z)$; this value follows from (1.3), since for this system

$$a(r) = r \log r + (1-r) \log(1-r). \tag{1.5}$$

For the model considered here the typical profile $\bar{\rho}(x, \tilde{t})$, on the macroscopic spatial-temporal scale with variables $(x, \tilde{t})$ defined by $i \to xN$ and $t \to \tilde{t}N^2$, is for $N \to \infty$ governed by the diffusion equation[16–18]

$$\frac{\partial \bar{\rho}(x, \tilde{t})}{\partial \tilde{t}} = \frac{\partial^2 \bar{\rho}(x, \tilde{t})}{\partial x^2}, \qquad \rho(0, \tilde{t}) = \rho_0, \quad \rho(1, \tilde{t}) = \rho_1, \tag{1.6}$$

which gives for the stationary state $\bar{\rho}(x) = \rho_0 + (\rho_1 - \rho_0)\, x$. Spohn[3] (see also ref. 19) computed explicitly, for $\alpha + \gamma = \beta + \delta = 1$, both the expected density profile and the pair correlation in the stationary state, and showed that the results agree, in the above scaling limit, with those obtained from fluctuating hydrodynamics.

While higher order correlations can also be obtained in principle, the difficulty of the computation increases rapidly with the desired order. The complete measure on the microscopic configurations in the steady state may, however, be computed through the so-called matrix method.[20–24] From this measure we would like to determine the probability of seeing an arbitrary macroscopic density profile $\rho(x)$, $x \in [0, 1]$; by definition, this is the sum of the probabilities of all microscopic configurations which are consistent with $\rho(x)$, e.g., all configurations τ such that for any x_0, x_1 with $0 \leqslant x_0 < x_1 \leqslant 1$, $|\frac{1}{N} \sum_{i=x_0 N}^{x_1 N} \tau_i - \int_{x_0}^{x_1} \rho(x)\, dx| < \delta_N$, for some appropriate choice of δ_N with $\delta_N \to 0$ as $N \to \infty$, e.g., $\delta_N = N^{-\kappa}$, $0 < \kappa < 1$.

The deviations of macroscopic systems from typical behavior, e.g., from the profile $\bar{\rho}(x, \tilde{t})$ governed by the diffusion equation, is a central issue of statistical mechanics.[5–8, 11, 12] The time dependent problem was first studied by Onsager and Machlup,[25] who considered space-time fluctuations for Hamiltonian systems in equilibrium (for which $\bar{\rho}$ is constant). The problem of observing a profile $\rho(x, \tilde{t})$ not necessarily close to $\bar{\rho}(x, \tilde{t})$, the so-called problem of large deviations, was later studied rigorously for the SSEP on a torus by Kipnis, Olla, and Varadhan,[26] who found an exact expression for the probability of observing such a profile (see also refs. 15 and 18). An important ingredient in their analysis was the fact that the dynamics satisfied detailed balance with respect to any product measure with constant density, and that such a product measure is in fact the appropriate microscopic measure at each macroscopic position. This corresponds for stochastic systems to reversibility of the microscopic dynamics, which also plays an important role in the Onsager–Machlup theory. There have been various attempts to extend these results to open systems in which the dynamics no longer satisfy detailed balance with respect to the stationary measure.[12, 27–29] Bertini *et al.*[28] have indeed succeeded in doing this for the so-called zero-range process with open boundaries, for which the microscopic stationary state is also a product measure. The problem is more difficult for our system, where it is known[3] that the stationary microscopic state contains long range correlations—correlations expected to be generic for SNS[1, 30–32] and even measured experimentally in some cases.[4] We shall see that this is reflected in a nonlocal structure for $\mathscr{F}(\{\rho\})$. A preliminary version of our results was given in ref. 33, and more recently Bertini *et al.*[29] succeeded in rederiving this result, and obtaining a large deviation functional for space-time profiles, using a semi-macroscopic method (which could be further checked, at least for small fluctuations, by comparing its predictions with the direct calculation of the time dependent correlations given in ref. 34).

2. SUMMARY OF RESULTS

In the present paper we give the exact asymptotic formula for the probability $P_N(\{\rho(x\})$ of seeing a density profile $\rho(x)$, $0 \leqslant \rho(x) \leqslant 1$, in the one dimensional open system with SSEP internal dynamics. (The exact sense in which we establish this formula is sketched later in this section.) Let ρ_0 and ρ_1 be defined as in (1.4); we will assume for definiteness that $\rho_0 > \rho_1$ (results for the case $\rho_0 < \rho_1$ then follow from the right-left symmetry or the particle-hole symmetry, and for the case $\rho_0 = \rho_1$ by taking the limit $\rho_0 \to \rho_1$).

Our main result is then:

$$\lim_{N\to\infty} \frac{\log P_N(\{\rho(x\})}{N} \equiv -\mathscr{F}(\{\rho\}), \tag{2.1}$$

where

$$\mathscr{F}(\{\rho\}) = \int_0^1 dx \left\{ \rho(x) \log\left(\frac{\rho(x)}{F(x)}\right) + (1-\rho(x)) \log\left(\frac{1-\rho(x)}{1-F(x)}\right) + \log\left(\frac{F'(x)}{\rho_1-\rho_0}\right)\right\}. \tag{2.2}$$

The auxiliary function $F(x)$ in (2.2) is given as a function of the density profile $\rho(x)$ by the monotone solution of the nonlinear differential equation

$$\rho(x) = F(x) + \frac{F(x)(1-F(x))\, F''(x)}{F'(x)^2}, \tag{2.3}$$

with the boundary conditions

$$F(0) = \rho_0, \qquad F(1) = \rho_1. \tag{2.4}$$

We will show in Section 5 that such a solution exists and is (at least when $\rho_0 < 1$ and $\rho_1 > 0$) unique.

We now summarize some consequences of (2.2)–(2.4).

(a) Let us denote the right hand side of (2.2), considered as a functional of two independent functions $\rho(x)$ and $F(x)$, by $\mathscr{G}$:

$$\mathscr{G}(\{\rho\}, \{F\})) = \int_0^1 dx \left\{ \rho(x) \log\left(\frac{\rho(x)}{F(x)}\right) + (1-\rho(x)) \log\left(\frac{1-\rho(x)}{1-F(x)}\right) + \log\left(\frac{F'(x)}{\rho_1-\rho_0}\right)\right\}. \tag{2.5}$$

If one looks for a monotone function F, satisfying the constraint (2.4), for which $\mathscr{G}(\{\rho\}, \{F\})$ is an extremum, one obtains (2.3) as the corresponding Euler–Lagrange equation:

$$\frac{\delta\mathscr{G}(\{\rho\}, \{F\})}{\delta F(x)} = 0. \tag{2.6}$$

We will show in Section 5 that the unique monotone solution of (2.3) (or equivalently of (2.6)) is in fact a maximizer of (2.5):

$$\mathcal{F}(\{\rho\}) = \sup_F \mathcal{G}(\{\rho\}, \{F\}). \tag{2.7}$$

We will also show that $\mathcal{F}$ is a convex function of $\{\rho\}$. (More precisely, our derivations will be for the case $1 > \rho_0 > \rho_1 > 0$, but we expect the conclusions to hold in general, that is, for $1 \geqslant \rho_0 > \rho_1 \geqslant 0$ and by symmetry for $1 \geqslant \rho_1 > \rho_0 \geqslant 0$.)

(b) From (2.6) one sees at once that for F the solution of (2.3), (2.4),

$$\frac{\delta \mathcal{F}(\{\rho\})}{\delta \rho(x)} = \frac{\delta \mathcal{G}(\{\rho\}, \{F\})}{\delta \rho(x)} = \log \left[\frac{\rho(x)}{F(x)} \cdot \frac{1-F(x)}{1-\rho(x)} \right], \tag{2.8}$$

and this together with (2.3) implies that the minimum of $\mathcal{F}(\{\rho\})$ occurs for $\rho(x) = F(x) = \bar{\rho}(x)$, where

$$\bar{\rho}(x) = \rho_0(1-x) + \rho_1 x. \tag{2.9}$$

Moreover, from (2.2) and (2.3) one has $\mathcal{F}(\{\bar{\rho}\}) = 0$, confirming that the most likely profile $\bar{\rho}(x)$ is obtained with probability one in the limit $N \to \infty$. Any other profile will have $\mathcal{F}(\{\rho\}) > 0$ and thus, for large N, exponentially small probability. The profile may be discontinuous, or may fail to satisfy the boundary conditions $\rho(0) = \rho_0$ or $\rho(1) = \rho_1$, and still satisfy $\mathcal{F}(\{\rho\}) < \infty$. When $\rho_0 = 0$ or $\rho_1 = 1$ there are some profiles for which $\mathcal{F} = +\infty$; their probability is super-exponentially small in N. For examples, see (d) below and Section 8.

(c) It is natural to contrast the SNS under consideration here with a *local equilibrium* Gibbs measure for the same system—a lattice gas with only hard core exclusion—with no reservoirs at the boundaries but with a spatially varying chemical potential $\nu(x)$[26, 15] which is adjusted to maintain the same optimal profile $\bar{\rho}(x)$. For this system the large deviation functional (free energy) is obtained directly from (1.2), with $f_\nu(r) = r \log r + (1-r) \log(1-r) - \nu r$:

$$\mathcal{F}_{\text{eq}}(\{\rho\}) = \int_0^1 \left\{ \rho(x) \log \frac{\rho(x)}{\bar{\rho}(x)} + [1-\rho(x)] \log \frac{(1-\rho(x))}{(1-\bar{\rho}(x))} \right\} dx. \tag{2.10}$$

In general the two expressions (2.2) and (2.10) are different, and from (2.7),

$$\mathcal{F}(\{\rho\}) = \sup_F \mathcal{G}(\{\rho\}, \{F\}) \geqslant \mathcal{G}(\{\rho\}, \{\bar{\rho}\}) = \mathcal{F}_{\text{eq}}(\{\rho\}). \tag{2.11}$$

$\mathcal{F}(\{\rho\})$ and $\mathcal{F}_{\text{eq}}(\{\rho\})$ agree only for $\rho(x) = \bar{\rho}(x)$ or in the limiting case $\rho_0 = \rho_1$, in which the system is in equilibrium with $\bar{\rho}(x) = \rho_0$. (Equations (2.2)–(2.4) have a well-defined limit for $\rho_1 \nearrow \rho_0$, with $F(x) = \rho_0 + (\rho_1 - \rho_0)\,x + O((\rho_1 - \rho_0)^2)$.) Otherwise $\mathcal{F}(\{\rho\})$ lies above $\mathcal{F}_{\text{eq}}(\{\rho\})$ and thus gives reduced probability for fluctuations away from the typical profile.

Note that the integrand in (2.10) (or (1.2)) is local: changing $\rho(x)$ in some interval $[a, b]$ only changes the value of this integrand inside that interval. This is not true for the integrand of (2.2), because F is determined by the differential equation (2.3) and so $F(x)$ will generally depend on the value of $\rho(y)$ everywhere in $[0, 1]$.

(d) For a constant profile $\rho(x) = r$, the solution F of (2.3) and (2.4) satisfies $F' = AF^r(1-F)^{1-r}$, where A is fixed by (2.4), and

$$\mathcal{F}(\{\rho\}) = \log\left[\int_{\rho_0}^{\rho_1} \left(\frac{r}{z}\right)^r \left(\frac{1-r}{1-z}\right)^{1-r} \frac{dz}{\rho_1 - \rho_0}\right]. \tag{2.12}$$

We see that $\mathcal{F}(\{\rho\}) = \infty$ if $r = 0$ and $\rho_0 = 1$, or $r = 1$ and $\rho_1 = 0$. By contrast $\mathcal{F}_{\text{eq}}(\{\rho\})$ as given in (2.10) would be

$$\mathcal{F}_{\text{eq}}(\{\rho\}) = \int_{\rho_0}^{\rho_1} \log\left[\left(\frac{r}{z}\right)^r \left(\frac{1-r}{1-z}\right)^{1-r}\right] \frac{dz}{\rho_1 - \rho_0}, \tag{2.13}$$

which is finite except in the degenerate cases $\rho_0 = \rho_1 = 1$ and $\rho_0 = \rho_1 = 0$, in which case the measure is concentrated on a single configuration and $\mathcal{F}_{\text{eq}} = \infty$ unless $\rho = \rho_0$.

(e) If we minimize $\mathcal{F}$ subject to the constraint of a fixed mean density $\int_0^1 \rho(x)\,dx$, the right hand side of (2.8) becomes an arbitrary constant, and together with (2.3) one obtains that the most likely profile is exponential: $\rho(x) = A_1 \exp(\theta x) + A_2$ (with $F(x) = 1 - A_2 + A_2(1 - A_2) \exp(-\theta x)/A_1$), the constants being determined by the value of the mean density and the boundary conditions (2.4). (This exponential form, which is the stationary solution of a diffusion equation with drift, was first suggested to us by Errico Presutti).

Similarly, if we impose a fixed mean density in k nonoverlapping intervals, $\int_{a_i}^{b_i} \rho(x)\,dx = c_i$ for $i = 1,..., k$, with no other constraints, then one can show using (2.3) and (2.8) that the optimal profile has an exponential form inside these intervals and is linear outside; it will in general not be continuous at the end points of the intervals.

(f) Using the fact that the exponential is the optimal profile for the case of a fixed mean density in the entire interval, we may compute the distribution of M, the total number of particles in the system, in the steady state for large N. The result for the variance of M which is obtained by applying this computation to small fluctuations agrees with that obtained in [3] directly from the microscopic model (see also Section 7.2) and from fluctuating hydrodynamics [2]:

$$\lim_{N\to\infty} N^{-1}[\langle M^2\rangle_{\text{SNS}} - \langle M\rangle^2]$$

$$= \lim_{N\to\infty} N^{-1}[\langle M^2\rangle_{\text{eq}} - \langle M\rangle^2] - \frac{(\rho_1-\rho_0)^2}{12}. \tag{2.14}$$

(Since $\bar{\rho}$ is given by (2.9) for both systems, $\langle M\rangle_{\text{SNS}} = \langle M\rangle_{\text{eq}} = \langle M\rangle = (\rho_0+\rho_1)/2$.) Note that the variance is reduced in comparison to that in a system in local equilibrium (2.10) with the same $\bar{\rho}$; this reduction of fluctuations was already visible in (2.11). We may also obtain (2.14) by expanding $\mathcal{F}(\rho(x)\})$ about $\bar{\rho}(x)>$ in (2.2); see Section 7.1.

The structure of the rest of the paper is as follows: In Sections 3 and 4 and Appendices A and B we derive our main result (2.2)–(2.4) from the knowledge of the weights of the microscopic configurations as given by their matrix product expressions. Our approach consists in considering the system of N sites as decomposed into n boxes of $N_1, N_2,..., N_n$ sites. We first calculate the generating function of the probability $P_{N_1,..., N_n}(M_1,..., M_n)$, that M_1 particles are located on the first N_1 sites, M_2 particles on the next N_2 sites of the lattice, etc. We then use this generating function to obtain $P_{N_1,..., N_n}(M_1,..., M_n)$. The expression we obtain appears in a parametric form because we extract this probability from the generating function through a Legendre transformation. Then we take the limit of an infinite system which corresponds implicitly to the usual hydrodynamic scaling limit, as explained in great detail in refs. 15 and 18, by first letting $N\to\infty$, keeping $N_i/N = y_i$ fixed, and then letting $y_i\to 0$ to obtain (2.2)–(2.4).

In Section 5 we prove that for any profile $\rho(x)$ there exists a unique monotonic function $F(x)$ which satisfies (2.3) and (2.4). We also establish there, for $1>\rho_0>\rho_1>0$, that $\mathcal{F}(\{\rho\}) = \sup_F \mathcal{G}(\{\rho\}, \{F\})$ and that $\mathcal{F}$ is a convex functional of $\rho(x)$, as discussed in (a) above. In the course of this discussion we describe the behavior of the large deviation functional for piecewise constant density profiles. In Section 6 we calculate optimal profiles under various constraints, as discussed in (e) above. In Section 7 we calculate the correlations of the fluctuations of the density profile around the most probable one and we show that a direct calculation of these correlations agrees with what can be calculated from (2.2)–(2.4). Lastly in Section 8 we exhibit a few examples of density profiles for which one can calculate explicitly the function F and the value of $\mathcal{F}(\{\rho\})$.

3. EXACT GENERATING FUNCTION

For the SSEP with open boundaries as described in the Introduction, the probability of a configuration $\tau = \{\tau_1,..., \tau_N\}$ in the (unique) steady state of our model is given by[20–24, 14]

$$P_N(\tau) = \frac{\omega_N(\tau)}{\langle W|\,(D+E)^N\,|V\rangle}, \tag{3.1}$$

where the weights $\omega_N(\tau)$ are given by

$$\omega_N(\tau) = \langle W|\,\Pi_{i=1}^N (\tau_i D + (1-\tau_i)\,E)\,|V\rangle \tag{3.2}$$

and the matrices D and E and the vectors $|V\rangle$ and $\langle W|$ satisfy

$$DE - ED = D + E, \tag{3.3}$$

$$(\beta D - \delta E)\,|V\rangle = |V\rangle, \tag{3.4}$$

$$\langle W|\,(\alpha E - \gamma D) = \langle W|. \tag{3.5}$$

To obtain the probability of a specified density profile we first calculate the sum $\Omega_{N_1,..., N_n}(M_1, M_2,..., M_n)$ of the weights ω_N of all the configurations with M_1 particles located on the first N_1 sites, M_2 particles on the next N_2 sites, etc. The key to obtaining (2.2) is that the following generating function can be computed exactly:

$$\begin{aligned} Z(\lambda_1,..., \lambda_n; \mu_1,..., \mu_n) &\equiv \sum \frac{\mu_1^{N_1}}{N_1!} \cdots \frac{\mu_n^{N_n}}{N_n!}\, \lambda_1^{M_1} \cdots \lambda_n^{M_n}\, \frac{\Omega_{N_1,..., N_n}(M_1,..., M_n)}{\langle W\,|\,V\rangle} \\ &= \frac{\langle W|\, e^{\mu_1\lambda_1 D + \mu_1 E} \cdots e^{\mu_n\lambda_n D + \mu_n E}\,|V\rangle}{\langle W\,|\,V\rangle}, \end{aligned} \tag{3.6}$$

where the sum is over all N_i, M_i with $0 \leqslant M_i \leqslant N_i$. As shown in Appendix A, Z can be computed explicitly:

$$Z = \left(\frac{\rho_0 - \rho_1}{g}\right)^{a+b} \exp\left[a \sum_{i=1}^{n} \mu_i(1-\lambda_i)\right], \tag{3.7}$$

where ρ_0 and ρ_1 are given by (1.4),

$$a = \frac{1}{\gamma+\alpha}, \qquad b = \frac{1}{\beta+\delta}, \tag{3.8}$$

and

$$g = -\rho_1 + \rho_0 e^{\sum_{i=1}^{n} \mu_i(1-\lambda_i)} + \sum_{i=1}^{n} \frac{1}{\lambda_i - 1} \left(e^{\mu_i(1-\lambda_i)} - 1\right) e^{\sum_{j>i} \mu_j(1-\lambda_j)}. \tag{3.9}$$

Expressions (3.7) and (3.9) are the basis of all the calculations leading to the large deviation functions. As a first step, note that

$$Z(1; \mu) = \frac{\langle W| e^{\mu(D+E)} |V\rangle}{\langle W | V\rangle} = \left(\frac{\rho_0 - \rho_1}{\rho_0 - \rho_1 - \mu}\right)^{a+b}, \tag{3.10}$$

so that one obtains the normalization factor in (3.1):

$$\Omega_0 \equiv \frac{\langle W| (D+E)^N |V\rangle}{\langle W | V\rangle} = \frac{\Gamma(a+b+N)}{\Gamma(a+b)(\rho_0 - \rho_1)^N}. \tag{3.11}$$

4. FROM THE GENERATING FUNCTION TO THE LARGE DEVIATION FUNCTION

It is clear from (3.7) that $Z(\lambda_1,..., \lambda_n; \mu_1,..., \mu_n)$ is singular on the hypersurface

$$g(\mu_1,..., \mu_n; \lambda_1,..., \lambda_n) = 0, \tag{4.1}$$

where g is given by (3.9). Let us consider a very large system of N sites divided into n boxes of $N_1,..., N_n$ sites, with $P_{N_1,..., N_n}(M_1,..., M_n)$ the probability of finding M_1 particles in the first box, M_2 particles in the second box, etc., and let N_i and M_i be proportional to N: $N_i = N y_i$, $M_i = r_i N_i = r_i y_i N$, $i = 1,..., n$. As explained in Appendix B, one can show from the definition of Z that for large N and fixed y_i, r_i,

$$\frac{\log P_{N_1,..., N_n}(M_1,..., M_n)}{N} \simeq \log(\rho_0 - \rho_1) - \sum_{j=1}^{n} y_j \left(\log \frac{\mu_j}{y_j} + r_j \log \lambda_j\right), \tag{4.2}$$

where the box sizes y_j and their particle densities r_j are related to the parameters $\mu_1,..., \mu_n$, $\lambda_1,..., \lambda_n$ by

$$y_j = \frac{\frac{\partial g}{\partial \log \mu_j}}{\sum_{i=1}^{n} \frac{\partial g}{\partial \log \mu_i}}, \tag{4.3}$$

$$r_j = \frac{\frac{\partial g}{\partial \log \lambda_j}}{\frac{\partial g}{\partial \log \mu_j}}, \tag{4.4}$$

with all derivatives calculated on the manifold $g = 0$.

Equation (4.2) gives the large deviation function in a parametric form; the $2n+1$ equations (4.1), (4.3), and (4.4) determine the $2n$ parameters $\mu_1,..., \mu_n, \lambda_1,..., \lambda_n$ in terms of $y_1,..., y_n$ and $r_1,..., r_n$ (since $y_1 + \cdots + y_n = 1$, the n equations (4.3) give only $n-1$ independent conditions, so that the system is not overdetermined). Note from (3.7) and (3.9) that the parameters a and b defined by (3.8) do not appear in the expression for the critical manifold and therefore drop out in the large N limit, i.e., the large deviation functional, like the typical profile, depends only on z_0 and z_1 or ρ_0 and ρ_1.

4.1. Case of a Single Box

One can apply the above results in the case $n = 1$ of a single box. With $\lambda_1 \equiv \lambda$ and $\mu_1 \equiv \mu$, equation (4.1) for the critical manifold becomes

$$g(\mu; \lambda) \equiv -\rho_1 + \rho_0 e^{\mu(1-\lambda)} + \frac{1}{\lambda - 1}(e^{\mu(1-\lambda)} - 1) = 0, \tag{4.5}$$

or more conveniently $\tilde{g}(\mu; \lambda) = 0$, where

$$\tilde{g}(\mu; \lambda) = \mu(1-\lambda) - \log\left(\frac{1-\rho_1+\lambda\rho_1}{1-\rho_0+\lambda\rho_0}\right). \tag{4.6}$$

The function $\tilde{g}$ may be used in place of g in (4.3)–(4.4), because the derivatives there are evaluated on the manifold $g = 0$, so that if the average density $\rho = r_1$ in the box is given by

$$\rho = \frac{-\frac{\lambda}{1-\lambda}\log\left(\frac{1-\rho_1+\lambda\rho_1}{1-\rho_0+\lambda\rho_0}\right) + \frac{\rho_0\lambda}{1-\rho_0+\lambda\rho_0} - \frac{\rho_1\lambda}{1-\rho_1+\lambda\rho_1}}{\log\left(\frac{1-\rho_1+\lambda\rho_1}{1-\rho_0+\lambda\rho_0}\right)}, \tag{4.7}$$

then for large N and $M \simeq \rho N$,

$$\frac{1}{N}\log P_N(M) \simeq -\rho\log\lambda - \log\left[\frac{\log\left(\frac{1-\rho_1+\lambda\rho_1}{1-\rho_0+\lambda\rho_0}\right)}{(\lambda-1)(\rho_1-\rho_0)}\right]. \tag{4.8}$$

Remark. For small fluctuations of the form

$$\rho - \frac{\rho_0+\rho_1}{2} = \delta\rho \ll 1, \tag{4.9}$$

(4.8) gives, again with $M \simeq \rho N$,

$$\frac{1}{N} \log P_N(M) \simeq \frac{-6(\delta\rho)^2}{6\rho_0 + 6\rho_1 - 5\rho_0^2 - 2\rho_0\rho_1 - 5\rho_1^2} + O((\delta\rho)^3). \tag{4.10}$$

For a Bernoulli distribution with average profile (2.9) (the most likely profile, as we will see in Section 6), one would get

$$\frac{1}{N} \log P_N(M) \simeq \frac{-3(\delta\rho)^2}{3\rho_0 + 3\rho_1 - 2\rho_0^2 - 2\rho_0\rho_1 - 2\rho_1^2} + O((\delta\rho)^3); \tag{4.11}$$

from this we can compute the fluctuations of M and obtain (2.14).

4.2. A Finite Number *n* of Large Boxes

Let us calculate $\frac{\partial g}{\partial \log \mu_i}$ on the manifold $g = 0$. From (3.9), we have

$$\begin{aligned}\frac{\partial g}{\partial \log \mu_i} &= \rho_0 \mu_i (1-\lambda_i)\, e^{\sum_{j=1}^n \mu_j(1-\lambda_j)} - \mu_i e^{\sum_{j=i}^n \mu_j(1-\lambda_j)} \\ &\quad + \mu_i(1-\lambda_i) \sum_{j<i} \frac{1}{\lambda_j - 1} (e^{\mu_j(1-\lambda_j)} - 1)\, e^{\sum_{k>j} \mu_k(1-\lambda_k)},\end{aligned} \tag{4.12}$$

which becomes, using (4.1) and (3.9),

$$\begin{aligned}\frac{\partial g}{\partial \log \mu_i} &= -\mu_i e^{\sum_{j>i} \mu_j(1-\lambda_j)} \\ &\quad + \mu_i(1-\lambda_i) \sum_{j>i} \frac{1}{1-\lambda_j} (e^{\mu_j(1-\lambda_j)} - 1)\, e^{\sum_{k>j} \mu_k(1-\lambda_k)} + \rho_1 \mu_i (1-\lambda_i).\end{aligned} \tag{4.13}$$

One can also show that

$$\frac{\partial g}{\partial \log \lambda_i} = -\frac{\lambda_i}{1-\lambda_i} \frac{\partial g}{\partial \log \mu_i} - \frac{\lambda_i}{(\lambda_i - 1)^2} (e^{\mu_i(1-\lambda_i)} - 1)\, e^{\sum_{j>i} \mu_j(1-\lambda_j)}. \tag{4.14}$$

This parametric form can be simplified by replacing the role of the two sequences of parameters μ_i and λ_i by a single sequence of parameters G_i. Let us define the constant C by

$$C = \sum_{i=1}^n \frac{\partial g}{\partial \log \mu_i}, \tag{4.15}$$

and the sequence G_i by

$$G_i = \frac{1}{C} e^{\sum_{j=i}^{n} \mu_j(1-\lambda_j)}, \qquad G_{n+1} = \frac{1}{C}. \tag{4.16}$$

From the very definition of the G_i's it is clear that

$$\mu_i = \frac{\log(G_i/G_{i+1})}{1-\lambda_i}, \tag{4.17}$$

and from (4.3), (4.13), (4.15), and (4.16), we see that

$$\frac{G_{i+1}}{1-\lambda_i} = -\frac{y_i}{\log(G_i/G_{i+1})} + \sum_{j>i} \frac{G_j - G_{j+1}}{1-\lambda_j} + \frac{\rho_1}{C}, \tag{4.18}$$

so that both the μ_i and the λ_i are determined in terms of the sequence G_i, the box sizes y_i and the constant C. The condition (4.1) that $g = 0$ becomes

$$\frac{\rho_1}{C} + \sum_{i=1}^{n} \frac{G_i - G_{i+1}}{1-\lambda_i} = \rho_0 G_1, \tag{4.19}$$

which gives the extra equation needed to determine the constant C (as well as G_{n+1}). Therefore we are left with n free parameters, the G_i's for $1 \leqslant i \leqslant n$.

A more convenient way of writing the λ_i's (i.e., (4.18)) in terms of the G_i's is

$$\frac{1}{\lambda_i - 1} = \frac{1}{G_{i+1}} \frac{y_i}{\log(G_i/G_{i+1})} - \rho_0 + \sum_{j=1}^{i} \left(\frac{1}{G_j} - \frac{1}{G_{j+1}} \right) \frac{y_j}{\log(G_j/G_{j+1})}, \tag{4.20}$$

and the condition (4.19) becomes

$$\rho_0 - \rho_1 = \sum_{j=1}^{n} \left(\frac{1}{G_j} - \frac{1}{G_{j+1}} \right) \frac{y_j}{\log(G_j/G_{j+1})}, \tag{4.21}$$

which can be thought as an equation which determines G_{n+1} in terms of the G_i's.

Once the λ_i are known through (4.20) and (4.21), one gets from (4.4), (4.13), and (4.14) expressions for the r_i's and the large deviation function:

$$r_i = -\frac{\lambda_i}{1-\lambda_i} - \frac{\lambda_i}{(1-\lambda_i)^2} \frac{G_i - G_{i+1}}{y_i}, \tag{4.22}$$

and

$$\frac{\log[P_{N_1,\dots,N_n}(M_1,\dots,M_n)]}{N}$$

$$\simeq -\sum_{i=1}^{n}\left\{y_i \log\left[\frac{\log\left(\frac{G_i}{G_{i+1}}\right)}{y_i(\rho_0-\rho_1)}\right]-y_i\log(1-\lambda_i)+y_i r_i\log(\lambda_i)\right\}. \quad (4.23)$$

Equations (4.20)–(4.23) determine the large deviation function for any specified number n of large boxes, i.e., for fixed y_i, r_i, and $N\to\infty$.

4.3. An Infinite Number of Large Boxes and the Continuous Limit

Letting n become large while keeping each box a small fraction of the total system, i.e., all the y_i's are small or, more formally letting $N\to\infty$ followed by $n\to\infty$ and $y_i\to 0$, one can introduce a continuous variable x, $0\leqslant x\leqslant 1$ and let

$$x_i = y_1+y_2+\cdots+y_i\,. \quad (4.24)$$

All the discrete sequences can now be thought of as functions of x with

$$G_i\equiv G(x_i); \qquad \lambda_i\equiv\lambda(x_i); \qquad r_i\equiv\rho(x_i), \qquad i=1,\dots,n. \quad (4.25)$$

Then using extrapolations to make G, λ, ρ smooth functions of x so that

$$G_{i+1}-G_i\simeq y_i G'(x), \quad (4.26)$$

one finds that (4.20) and (4.21) become

$$\frac{1}{\lambda(x)-1}=\frac{-1}{G'(x)}-\rho_0-\int_0^x\frac{du}{G(u)}, \quad (4.27)$$

$$\rho_0+\int_0^1\frac{du}{G(u)}=\rho_1. \quad (4.28)$$

At this stage it is convenient to replace the function $G(x)$ by another function $F(x)$ defined by

$$F(x)=\rho_0+\int_0^x\frac{du}{G(u)}. \quad (4.29)$$

The expression (4.27) of $\lambda(x)$ becomes then

$$\frac{1}{\lambda(x)-1}=\frac{F'^2(x)}{F''(x)}-F(x). \tag{4.30}$$

Using the above relations we may rewrite (4.22) and (4.23) in terms of F, obtaining (2.2) and (2.3); the boundary conditions (2.4) come from (4.28). The monotonicity of F follows from the uniqueness of the sign of G (see (4.16); note from (4.29) that G is negative in the case $\rho_0 > \rho_1$ that we consider).

5. THE LARGE DEVIATION FUNCTIONAL IN THE CONTINUUM LIMIT

We derive here some properties of Eqs. (2.2)–(2.4). We discuss only the case $1 > \rho_0 > \rho_1 > 0$ and concentrate on results for piecewise constant density profiles, in some instances giving only a sketch of the extension to more general $\rho(x)$. The case in which either $\rho_0 = 1$ or $\rho_1 = 0$ seems technically more difficult; for this case we can show the existence of a solution, but omit the proof here.

5.1. Uniqueness

In this section we show that any monotone solution $F(x)$ of (2.3) and (2.4) is unique. If F and $\hat{F}$ are distinct solutions then necessarily $F'(0) \neq \hat{F}'(0)$, since the standard initial value problem for (2.3), with prescribed values of $F(0)$ and $F'(0)$, has a unique solution. Suppose that $\hat{F}'(0) > F'(0)$; we will show that then $\hat{F}(x) > F(x)$ for $0 < x \leqslant 1$, contradicting $F(1) = \hat{F}(1) = \rho_1$. For otherwise let y to be the smallest positive number for which $F(y) = \hat{F}(y)$, so that

$$F(x) < \hat{F}(x), \qquad 0 < x < y \leqslant 1. \tag{5.1}$$

Let $g(x) = F(x)(1-F(x))/F'(x)$ and $\hat{g}(x) = \hat{F}(x)(1-\hat{F}(x))/\hat{F}'(x)$. Then $g(0) > \hat{g}(0)$ and, from (2.3), which can be written in the form $g'(x) = 1-F(x)-\rho(x)$, and (5.1), $g'(x)-\hat{g}'(x) = \hat{F}(x)-F(x) > 0$ for $0 < x < y$, so that $g(y) > \hat{g}(y)$ and hence $F'(y) < \hat{F}'(y)$, which is inconsistent with (5.1).

5.2. Piecewise Constant Profiles and Extensions

In this section we prove existence of a solution $F_\rho(x)$ of (2.3) and (2.4), and show that this solution maximizes $\mathscr{G}(\{\rho\}, \{F\})$, given by (2.5), for a piecewise constant density profile

$$\rho(x) = r_i \qquad \text{for} \quad x_{i-1} < x < x_i, \tag{5.2}$$

where $0 = x_0 < x_1 < \cdots < x_n = 1$. We will write $y_i = x_i - x_{i-1}$. It follows from (2.3) that $F_\rho(x)$ must satisfy

$$F'_\rho(x) = A_i \psi_i(F_\rho(x)) \tag{5.3}$$

for $x_{i-1} < x < x_i$, where A_i is a (negative) constant and

$$\psi_i(F) = \left(\frac{F}{r_i}\right)^{r_i} \left(\frac{1-F}{1-r_i}\right)^{1-r_i}. \tag{5.4}$$

Continuity of $F_\rho(x)$ and $F'_\rho(x)$ implies that $F_\rho(x_1),..., F_\rho(x_{n-1})$ and the constants $A_1,..., A_n$ must satisfy

$$A_i = \frac{1}{y_i} \int_{F_\rho(x_{i-1})}^{F_\rho(x_i)} \frac{dz}{\psi_i(z)} \tag{5.5}$$

and

$$A_i \psi_i(F_\rho(x_i)) = A_{i+1} \psi_{i+1}(F_\rho(x_i)). \tag{5.6}$$

Conversely, the existence of values $F_\rho(x_1),..., F_\rho(x_{n-1})$ and $A_1,..., A_n$ satisfying (5.5) and (5.6) implies the existence of a solution F_ρ of (2.3) and (2.4), obtained by solving (5.3) on each interval $[x_{i-1}, x_i]$.

So we need to prove that (5.5) and (5.6) can be solved. Now it follows from (5.3) that

$$\mathscr{G}(\{\rho\}, \{F\}) = \mathscr{G}_0(\{r\}, (F(x_0), F(x_1),..., F(x_n))), \tag{5.7}$$

where $\{r\} = (r_1,..., r_n)$ and for $\{H\} = (H_0,..., H_n)$ a sequence satisfying

$$\rho_0 = H_0 \geqslant H_1 \geqslant \cdots \geqslant H_n = \rho_1, \tag{5.8}$$

we have defined

$$\mathscr{G}_0(\{r\}, \{H\}) = \sum_{i=1}^{n} y_i \log\left(-\frac{1}{y_i} \int_{H_{i-1}}^{H_i} \frac{dz}{\psi_i(z)}\right) - \log(\rho_0 - \rho_1). \tag{5.9}$$

Equation (2.7) suggests that we consider the problem of maximizing $\mathcal{G}_0$. Since $\mathcal{G}_0$ is continuously differentiable in $\{H\}$ on the interior of the compact domain (5.8) and equal to $-\infty$ on its boundary, it achieves a maximum at some interior point $\{H^*\}$ at which

$$\frac{\partial \mathcal{G}_0}{\partial H_i}(\{r\},\{H^*\}) \equiv \frac{1}{A_{i+1}\psi_{i+1}(H_i^*)} - \frac{1}{A_i\psi_i(H_i^*)} = 0, \tag{5.10}$$

for $i = 1,..., n-1$, where

$$A_i = \frac{1}{y_i}\int_{H_{i-1}^*}^{H_i^*} \frac{dz}{\psi_i(z)}. \tag{5.11}$$

Since (5.10) and (5.11) correspond to (5.5) and (5.6), we obtain a solution of the latter equations, and hence a solution F_ρ of (2.3) and (2.4), by taking $F_\rho(x_i) = H_i^*$. Note that the argument above could be used to construct a solution of (2.3) and (2.4) from any point $\{H\}$ at which

$$\frac{\partial \mathcal{G}_0}{\partial H_i}(\{r\},\{H\}) = 0, \qquad i = 1,..., n-1; \tag{5.12}$$

since the solution is unique (see Section 5.1), $\{H^*\}$ is the only point satisfying (5.12).

It is now easy to verify (2.7) for $\rho(x)$. For if $F(x)$ is any continuously differentiable monotone function with $F(0) = \rho_0$ and $F(1) = \rho_1$, then from Jensen's inequality applied on each interval $[x_{i-1}, x_i]$,

$$\begin{aligned}\mathcal{G}(\{\rho\},\{F\}) &\leqslant \sum_{i=1}^{n} y_i \log\left(-\frac{1}{y_i}\int_{F(x_{i-1})}^{F(x_i)} \frac{dz}{\psi_i(z)}\right) - \log(\rho_0 - \rho_1)\\ &\leqslant \sup_H \mathcal{G}_0(\{r\},\{H\})\\ &= \mathcal{G}_0(\{r\},\{H^*\}) = \mathcal{G}(\{\rho\},\{F_\rho\}) = \mathcal{F}(\{\rho\}).\end{aligned} \tag{5.13}$$

We now discuss briefly the extension of these results to arbitrary profiles. A general proof of existence of a solution of (2.3) and (2.4) may be given which is independent of the arguments above: if $\rho(x)$ is continuous then Theorem XII.5.1 of ref. 35 implies immediately the existence of a solution F_ρ of (2.3) and (2.4), and for measurable $\rho(x)$ only slight modifications of the proof in ref. 35 are necessary. The uniqueness theorem for the initial value problem for (2.3) implies that the derivative of the solution must be everywhere nonzero, so that the solution is monotonic. Equation (2.7) may be verified for arbitrary $\rho(x)$ by a limiting argument from the same result (proved above) for piecewise constant densities; the key idea is to show that F_ρ and F'_ρ are, in the uniform norm, continuous functions of ρ in the L^1 norm.

5.3. Convexity of $\mathscr{F}(\{\rho\})$

Finally we show that $\mathscr{F}(\{\rho\})$ is strictly convex. Recall that F_ρ is the solution of (2.3) and (2.4) corresponding to the profile ρ. From (2.6),

$$\left.\frac{\delta \mathscr{G}}{\delta F(x)}\right|_{\{\rho\},\{F_\rho\}} = 0, \tag{5.14}$$

we have

$$\left.\frac{\delta^2 \mathscr{G}}{\delta \rho(y)\,\delta F(x)}\right|_{\{\rho\},\{F_\rho\}} + \int_0^1 \left.\frac{\delta^2 \mathscr{G}}{\delta F(u)\,\delta F(x)}\right|_{\{\rho\},\{F_\rho\}} \frac{\delta F_\rho(u)}{\delta \rho(y)}(\{\rho\})\,du = 0, \tag{5.15}$$

and therefore

$$\begin{aligned}\frac{\delta^2 \mathscr{F}}{\delta \rho(x)\,\delta \rho(y)}(\{\rho\}) &= \frac{\delta}{\delta \rho(x)}\left(\left.\frac{\delta \mathscr{G}}{\delta \rho(y)}\right|_{\{\rho\},\{F_\rho\}}\right)\\ &= \left.\frac{\delta^2 \mathscr{G}}{\delta \rho(x)\,\delta \rho(y)}\right|_{\{\rho\},\{F_\rho\}} - \int_0^1\int_0^1 \left.\frac{\delta^2 \mathscr{G}}{\delta F(u)\,\delta F(w)}\right|_{\{\rho\},\{F_\rho\}}\\ &\quad\times \frac{\delta F_\rho(u)}{\delta \rho(x)}(\{\rho\})\,\frac{\delta F_\rho(w)}{\delta \rho(y)}(\{\rho\})\,du\,dw.\end{aligned} \tag{5.16}$$

Since $\mathscr{G}(\{\rho\},\{F\})$ has a maximum at F_ρ the second term in this expression is positive semidefinite. The first term is positive definite:

$$\left.\frac{\delta^2 \mathscr{G}}{\delta \rho(x)\,\delta \rho(y)}\right|_{\{\rho\},\{F_\rho\}} = \frac{\delta(x-y)}{\rho(x)(1-\rho(x))}. \tag{5.17}$$

6. OPTIMAL PROFILES

The convexity of $\mathscr{F}(\{\rho\})$ established above implies the existence of a unique global minimum, corresponding to the optimal or most likely profile $\bar{\rho}(x)$. From (2.8) it follows that $\bar{\rho}(x)$ must satisfy

$$\log\left[\frac{\bar{\rho}(x)(1-F(x))}{(1-\bar{\rho}(x))\,F(x)}\right] = 0, \tag{6.1}$$

where $F(x)$ is the solution of (2.3) and (2.4) corresponding to $\bar{\rho}(x)$. Equation (6.1) leads immediately to

$$F(x) = \bar{\rho}(x), \tag{6.2}$$

and with (2.3) this implies that $F''(x) = 0$; the boundary conditions (2.4) then yield

$$F(x) = \bar{\rho}(x) = \rho_0 + (\rho_1 - \rho_0)\, x, \tag{6.3}$$

verifying that the optimal profile is as given in (2.9).

We may also ask for the most likely profile $\rho(x)$ under a constraint of the form

$$\int_0^1 \psi(x)\, \rho(x)\, dx = K, \tag{6.4}$$

with fixed weighting function $\psi(x)$ and constant K. From (2.8) one sees that $\rho(x)$ must satisfy

$$\frac{\rho(x)(1-F(x))}{(1-\rho(x))\, F(x)} = \exp[c\psi(x)] \tag{6.5}$$

for some constant c, where again $F(x)$ is the solution of (2.3) and (2.4) corresponding to $\rho(x)$.

In particular, we may impose the constraint of a fixed mean density ρ^* by taking $\psi(x) \equiv 1$, $K = \rho^*$. Then from (6.5),

$$\frac{\rho(x)(1-F(x))}{(1-\rho(x))\, F(x)} = e^c, \tag{6.6}$$

and we find from (2.3) that F must satisfy

$$\frac{F''(x)}{F'^2(x)} = \frac{e^c - 1}{1 + (e^c - 1)\, F(x)}. \tag{6.7}$$

The solutions of (6.7) have the form $F(x) = A + B\exp(-\theta x)$, which with the boundary conditions (2.4) leads to

$$F(x) = \frac{(\rho_1 - \rho_0 e^{-\theta}) - (\rho_1 - \rho_0)\, e^{-\theta x}}{(1 - e^{-\theta})}; \tag{6.8}$$

from (2.3) one then finds an exponential profile

$$\rho(x) = \frac{[(1-\rho_0)\, e^{-\theta} - (1-\rho_1)][(\rho_1 - \rho_0 e^{-\theta})\, e^{\theta x} - (\rho_1 - \rho_0)]}{(1-e^{-\theta})(\rho_1 - \rho_0)}. \tag{6.9}$$

Here θ is a free constant which must be chosen to satisfy the constraint of mean density ρ^*. If $\rho^* = (\rho_0 + \rho_1)/2$, the expected (and typical) total density in the stationary state, then $\theta = 0$ and (6.9) reproduces the optimal profile $\bar{\rho}(x)$.

Remarks. (a) Unless $\theta = 0$ or $\rho_0 = 1$,

$$\rho(0) \equiv \lim_{x \searrow 0} \rho(x) \neq \rho_0. \tag{6.10}$$

Thus when we constrain the total number of particles to be different from its most likely value, the optimal profile is discontinuous at $x = 0$ (unless $\rho_0 = 1$). Similar conclusions hold at $x = 1$, where a discontinuity occurs unless $\theta = 0$ or $\rho_1 = 0$, and, by symmetry, in the case $\rho_0 < \rho_1$.

(b) In the limit $\rho_1 \nearrow \rho_0$, one should scale $\theta \sim \rho_0 - \rho_1$ in order to obtain a meaningful answer. The resulting optimal profile is constant, with an arbitrary density $\rho_0 + \theta \rho_0 (1 - \rho_0)/(\rho_0 - \rho_1)$.

(c) If θ is chosen such that

$$e^{-\theta} = \frac{1 - \rho_1 + \rho_1 \lambda}{1 - \rho_0 + \rho_0 \lambda}, \tag{6.11}$$

one can recover (4.7) and (4.8); (4.7) by calculating $\int_0^1 \rho(x)\, dx$ from (6.9), and (4.8) from (2.2), (6.8) and (6.9).

Finally, we may also impose simultaneously several constraints of the form (6.4). For example, we can decompose the system as the union of disjoint boxes and then fix the mean density in some of these, imposing no constraints in the remainder. Then (6.1) will hold in the unconstrained boxes, so that $F(x) = \rho(x)$ will be linear there, and (6.6) will hold in the constrained boxes (with a box-dependent constant c), so that F and ρ will be exponential there; the specified mean densities in the constrained boxes and the requirement of continuity of F and F' at the box boundaries then completely determine F and hence ρ, which will, in general, be discontinuous at the boundaries.

Suppose, for example, that we require that the density vanish for $0<x<x_0$, with no additional constraint. Then

$$F(x)=\begin{cases}1-(1-\rho_0)\,e^{Bx}, & \text{if} \quad x\leqslant x_0,\\ \rho_1-(1-\rho_0)\,Be^{Bx_0}(x-1), & \text{if} \quad x>x_0,\end{cases} \tag{6.12}$$

and continuity of F at $x=x_0$ requires that B satisfy

$$\frac{1-\rho_1}{1-\rho_0}=[1+B(1-x_0)]\,e^{Bx_0}. \tag{6.13}$$

From (2.2) we find that $\mathscr{F}(\{\rho\})$, which in this case is simply the probability that $\rho(x)$ vanish for $0<x<x_0$, is given by

$$\mathscr{F}(\{\rho\})=-\log\left(\frac{\rho_0-\rho_1}{B}\right)+(1-x_0)\log\left(\frac{1-\rho_1}{1+B(1-x_0)}\right). \tag{6.14}$$

If now we take $\rho_0\to 1$ with ρ_1 and x_0 fixed, (6.13) implies that $B\simeq -x_0^{-1}\log(1-\rho_0)$ and therefore

$$\mathscr{F}(\{\rho\})\simeq x_0\log(-\log(1-\rho_0)). \tag{6.15}$$

Thus the probability of finding zero density in the box $x<x_0$ when $\rho_0=1$ is super-exponentially small.

7. SMALL FLUCTUATIONS IN THE PROFILE

We have already given in (4.10) the formula for the probability of small fluctuations in the total number of particles in the system. In this section we compute, directly from the large deviation functional $\mathscr{F}(\{\rho\})$, the covariance of small fluctuations in the profile around the stationary profile $\bar{\rho}(x)=(1-x)\,\rho_0+x\rho_1$ (2.9). We show also that the result agrees with with a direct computation of the correlation functions from the microscopic measure describing the SNS (note that the possibility that these two computations might disagree had been conjectured in ref. 12).

7.1. Small Fluctuations from Large Deviations

For a small fluctuation of the density profile around its optimum $\bar{\rho}(x)$,

$$\rho(x)=\bar{\rho}(x)+\epsilon(x), \qquad \epsilon(x)\ll 1, \tag{7.1}$$

there will be a corresponding variation of $F(x)$,

$$F(x) = \bar{\rho}(x) + \phi(x). \tag{7.2}$$

From (2.4) we have $\phi(0) = \phi(1) = 0$, and from (2.3) $\phi(x)$ will satisfy, to first order in $\epsilon(x)$,

$$\epsilon(x) = \phi(x) + \frac{\bar{\rho}(x)(1-\bar{\rho}(x))}{\bar{\rho}'(x)^2}\,\phi''(x). \tag{7.3}$$

From (2.2), again to lowest (quadratic) order in $\epsilon(x)$,

$$\mathscr{F}(\{\rho\}) = -\frac{1}{2}\int_0^1 dx \left\{ \frac{\phi'(x)^2}{\bar{\rho}'^2} - \frac{\bar{\rho}(x)(1-\bar{\rho}(x))}{\bar{\rho}'^4}\,\phi''(x)^2 \right\}. \tag{7.4}$$

One can rewrite (7.3) as

$$\epsilon(x) = \int_0^1 dy\, C(x, y)\,\phi''(y), \tag{7.5}$$

with $C(x, y)$ given by

$$C(x, y) = -(1-x)\, y\theta(x-y) - x(1-y)\,\theta(y-x) + \frac{\bar{\rho}(x)(1-\bar{\rho}(x))}{\bar{\rho}'^2}\,\delta(y-x), \tag{7.6}$$

where $\theta(x)$ is the Heaviside function, or with a more compact notation,

$$C(x, y) = \Delta^{-1}(x, y) + \frac{\bar{\rho}(x)(1-\bar{\rho}(x))}{\bar{\rho}'^2}\,\delta(x-y). \tag{7.7}$$

Here Δ is the second derivative operator with Dirichlet boundary conditions at $x = 0$ and $x = 1$. The expression (7.4) can then be written as

$$\begin{aligned} \mathscr{F}(\{\rho\}) &= \frac{1}{2\bar{\rho}'^2}\int_0^1 dx \int_0^1 dy\, \phi''(x)\, C(x, y)\, \phi''(y) \\ &= -\frac{1}{2\bar{\rho}'^2}\int_0^1 dx \int_0^1 dy\, \epsilon(x)\, C^{-1}(x, y)\, \epsilon(y), \end{aligned} \tag{7.8}$$

where we have used (7.5). This formula expresses the fact that, for large N, density fluctuations are approximately Gaussian with covariance matrix

$\bar{\rho}'^2 C(x, y)/N$. Using the explicit expression (7.6) of C, this leads to the formula for the correlations $\langle \epsilon(x)\, \epsilon(y) \rangle$:

$$\begin{aligned}\langle \epsilon(x)\, \epsilon(y) \rangle &= \frac{\bar{\rho}'^2 C(x, y)}{N} \\ &= \frac{1}{N} \{ -\bar{\rho}'^2 [(1-x)\, y\theta(x-y) + (1-y)\, x\theta(y-x)] \\ &\quad + \bar{\rho}(x)(1-\bar{\rho}(x))\, \delta(x-y) \}. \end{aligned} \tag{7.9}$$

This result was obtained earlier by Spohn,[3] and shown there to agree with the results from fluctuating hydrodynamics.

7.2. Microscopic Correlation Functions

One may also compute correlations directly from from the algebra (3.3)–(3.5) and the normalization factor (3.11). By recursions over i and j one finds for $1 \leqslant i \leqslant N$ that

$$\begin{aligned}&\langle W|\, (D+E)^{i-1} D (D+E)^{N-i}\, |V\rangle \\ &\quad = \rho_0 \langle W|\, (D+E)^N\, |V\rangle - (a+i-1) \langle W|\, (D+E)^{N-1}\, |V\rangle, \end{aligned} \tag{7.10}$$

and for $1 \leqslant j < i \leqslant N$ that

$$\begin{aligned}&\langle W|\, (D+E)^{j-1} D (D+E)^{i-j-1} D (D+E)^{N-i}\, |V\rangle \\ &\quad = \rho_0^2 \langle W|\, (D+E)^N\, |V\rangle - \rho_0 (2a+i+j-2) \langle W|\, (D+E)^{N-1}\, |V\rangle \\ &\qquad + (a+j-1)(a+i-2) \langle W|\, (D+E)^{N-2}\, |V\rangle. \end{aligned} \tag{7.11}$$

Using (3.11), one obtains from (7.10) the average profile

$$\langle \tau_i \rangle = \rho_0 + \frac{a+i-1}{a+b+N-1} (\rho_1 - \rho_0), \tag{7.12}$$

and from (7.11) the truncated (microscopic) correlation function: for $j < i$,

$$\langle \tau_j \tau_i \rangle - \langle \tau_j \rangle \langle \tau_i \rangle = -(\rho_1 - \rho_0)^2 \frac{(a+j-1)(b+N-i)}{(a+b+N-1)^2\, (a+b+N-2)}. \tag{7.13}$$

Equations (7.12) and (7.13) agree with the corresponding formulas in ref. 3, where for rates satisfying $\alpha + \beta = a = \gamma + \delta = b = 1$, random walk methods were used to calculate the one particle and pair correlation for this system.

In the large N limit, (7.12) yields the linear profile (2.9), and by summing (7.13) over i and j, one recovers (2.14). Moreover, we may recover (7.9): if we divide the system into boxes of size Δx (with $1 \ll \Delta x^{-1} \ll N$) and write, for x and y multiples of Δx,

$$\epsilon(x) \simeq \frac{1}{N\Delta x} \sum_{i=Nx}^{N(x+\Delta x)} \tau_i - \rho(x), \qquad \epsilon(y) \simeq \frac{1}{N\Delta x} \sum_{i=Ny}^{N(y+\Delta x)} \tau_i - \rho(y), \tag{7.14}$$

then

$$\langle \epsilon(x)\, \epsilon(y) \rangle - \langle \epsilon(x) \rangle \langle \epsilon(y) \rangle$$
$$\simeq \frac{1}{N^2 \Delta x^2} \left\{ \delta_{x,y} \sum_{i=Nx}^{N(x+\Delta x)} (\langle \tau_i \rangle - \langle \tau_j \rangle^2) + \sum_{j=Nx}^{N(x+\Delta x)} \sum_{i=Ny}^{N(y+\Delta x)} (\langle \tau_j \tau_i \rangle - \langle \tau_j \rangle \langle \tau_i \rangle) \right\}, \tag{7.15}$$

and this, with (7.12) and (7.13), yields (7.9).

8. EXAMPLES

Although in general the calculation of the large deviation function $\mathscr{F}(\{\rho\})$ for a given profile $\rho(x)$ is not easy, since it requires the solution of the nonlinear second order differential equation (2.3), there are nevertheless some cases for which it can be done. Piecewise constant profiles were discussed in Section 5.2; in particular, for a profile of constant density r the large deviation functional is given by (2.12), and this function can be found explicitly when $r = 0$ or 1 (in which case $F(x)$ is exponential) or $r = 1/2$ (when $F(x)$ is sinusoidal). $\mathscr{F}(\{\rho\})$ can also be found explicitly in some cases for the optimal profiles under constraint, discussed in Section 6.

One may also construct examples by specifying $F(x)$ and obtaining $\rho(x)$ from (2.3) and $\mathscr{F}(\{\rho\})$ from (2.2). One must check in each case that $0 \leqslant \rho(x) \leqslant 1$, since this is not guaranteed by (2.3). In the remainder of this section we give two examples of this type which address the question: for what profiles $\rho(x)$ is $\mathscr{F}(\{\rho\})$ infinite? If $1 > \rho_0 > \rho_1 > 0$ then $\mathscr{F}(\{\rho\}) < \infty$; this follows from (2.2) and the fact that, by the uniqueness theorem for the initial value problem for (2.3) (see remark at the end of Section 5.2), $F'(x)$ cannot vanish. Suppose then that $\rho_0 = 1$ (analysis of the case $\rho_1 = 0$ is similar). The examples below suggest that $\mathscr{F}(\{\rho\}) = \infty$ when $\lim_{x \to 0} \rho(x) = 0$ and this limit is approached faster than any power of x. This is also supported by the example at the end of Section 6, which shows that $\mathscr{F}(\{\rho\}) = \infty$ if $\rho_0 = 1$ and $\rho(x)$ vanishes identically on an arbitrarily small interval $0 < x < x_0$. However, we have not formulated any sharp conjecture.

In both examples we take $\rho_0 = 1$. For the first, define

$$F(x) = 1-(1-\rho_1)\, e^{c(1-1/x^n)}, \tag{8.1}$$

with c a positive constant. Note that F is monotone decreasing and satisfies the boundary conditions (2.4). Then

$$F'(x) = -\frac{nc}{x^{n+1}}\,(1-F(x)), \tag{8.2}$$

$$F''(x) = -\left(\frac{nc}{x^{n+1}}\right)^2\left(1-\frac{n+1}{cn}\,x^n\right)(1-F(x)), \tag{8.3}$$

and hence from (2.3),

$$\rho(x) = \frac{n+1}{cn}\,x^n F(x). \tag{8.4}$$

Thus $\rho(x)$ vanishes like x^n at $x=0$, while $\lim_{x\to 1}\rho(x) = \rho_1(n+1)/cn$. Certainly we may choose c (e.g., $c=(n+1)/n$) to ensure that $0 \leqslant \rho(x) \leqslant 1$ for all x (note that by choosing c sufficiently small we see that (2.3) for an admissible F does not guarantee $0 \leqslant \rho(x) \leqslant 1$). If we then write (2.2) in the form

$$\mathscr{F}(\{\rho\}) = \int_0^1 dx\left\{\rho(x)\log\frac{\rho(x)(1-F(x))}{(1-\rho(x))\,F(x)} + \log\frac{(1-\rho(x))}{(1-\rho_1)} + \log\frac{-F'(x)}{(1-F(x))}\right\} \tag{8.5}$$

then (8.1), (8.2), and (8.4) show that $\mathscr{F}(\{\rho\}) < \infty$.

Finally, we again take $\rho_0 = 1$ and $c > 0$ and define

$$F(x) = 1-(1-\rho_1)\, e^{c(e-e^{1/x})}. \tag{8.6}$$

Then

$$F'(x) = -\frac{ce^{1/x}}{x^2}\,(1-F(x)), \tag{8.7}$$

$$F''(x) = -\left(\frac{ce^{1/x}}{x^2}\right)^2\left(1-\frac{2x+1}{c}\,e^{-1/x}\right)(1-F(x)), \tag{8.8}$$

and

$$\rho(x)=\frac{2x+1}{c}e^{-1/x}F(x). \tag{8.9}$$

Now $\rho(x)$ vanishes faster than any power of x at $x=0$. Again we may choose c (e.g., $c=3$) so that $0\leqslant\rho(x)\leqslant 1$ for all x; if we then write (2.2) as in (8.5) we see from (8.6), (8.7), and (8.9) that although the first two terms are finite, the last contributes $\int_0^1 dx/x$, so that $\mathcal{F}(\{\rho\})=\infty$.

9. CONCLUSION

In the present work, we have seen that the large deviation functional $\mathcal{F}(\{\rho\})$ of the density profile $\rho(x)$ can be calculated for the SSEP, starting from the known weights of the microscopic configurations. We find that the large deviation function is in general finite, although there are counter-examples (see (2.12) and Section 8).

The simplest way we found to write our results is a parametric form (2.2)–(2.4) in which both the large deviation function and the density profile are expressed in terms of a monotonic function $F(x)$ varying between ρ_0 and ρ_1, the densities of the two reservoirs at the two ends of the system.

An interesting question posed by the present work is how the additivity property of the free energy of equilibrium systems is modified in the nonequilibrium case. We first note that if a system of N sites, in contact with left and right reservoirs at chemical potentials corresponding to densities ρ_a and ρ_b, is described by a macroscopic coordinate x satisfying $a\leqslant x\leqslant b$ (rather than $0\leqslant x\leqslant 1$), then the probability P of observing a profile $\rho(x)$, $a\leqslant x\leqslant b$, satisfies

$$\log P\simeq -\frac{N}{b-a}\mathcal{F}_{[a,b]}(\{\rho\};\rho_a,\rho_b), \tag{9.1}$$

where

$$\mathcal{F}_{[a,b]}(\{\rho\};\rho_a,\rho_b)\equiv\int_a^b dx\left\{\rho(x)\log\left(\frac{\rho(x)}{F(x)}\right)+(1-\rho(x))\log\left(\frac{1-\rho(x)}{1-F(x)}\right)\right.$$
$$\left.+\log\left(\frac{(b-a)\,F'(x)}{\rho_b-\rho_a}\right)\right\}, \tag{9.2}$$

and $F(x)$ is related to $\rho(x)$ on the interval $a<x<b$ by (2.3) with the boundary conditions

$$F(a)=\rho_a, \qquad F(b)=\rho_b. \tag{9.3}$$

(Note that $F'(x)$ has the same sign as $\rho_b-\rho_a$, so that the argument of the log is positive in the last term of (9.2).)

Now consider two systems, of Nu and $N(1-u)$ sites respectively (with $0<u<1$), with the left system in contact with left and right reservoirs at chemical potentials corresponding to densities ρ_0 and ρ_m and the right system with reservoirs corresponding to densities ρ_m and ρ_1 (with no other relation between them, in particular with no particles jumping directly from one system to the other). If $\rho(x)$ is a profile on $0<x<1$ and $\rho^{(1)}(x)$ and $\rho^{(2)}(x)$ are its restrictions to the intervals $0<x<u$ and $u<x<1$, then we would like to relate the probability P_N of observing $\rho(x)$ to the probabilities $P_N^{(1)}$ and $P_N^{(2)}$ of observing $\rho^{(1)}(x)$ and $\rho^{(2)}(x)$ in the two subsystems. If $\mathscr{F}$ were truly local we would have $P_N \simeq P_N^{(1)} P_N^{(2)}$. The most naive generalization of this idea here would be that $P_N \simeq \sup_{\rho_m} (P_N^{(1)} P_N^{(2)})$ or, since from (9.1) $\log P_N^{(1)} \simeq -N\mathscr{F}_{[0,u]}(\{\rho^{(1)}\};\ \rho_0, \rho_m)$ and $\log P_N^{(2)} \simeq -N\mathscr{F}_{[u,1]}(\{\rho^{(2)}\};\ \rho_m, \rho_1)$, equivalently that $\mathscr{F}_{[0,1]}(\{\rho\}; \rho_0, \rho_1)=\inf_{\rho_m} [\mathscr{F}_{[0,u]}(\{\rho^{(1)}\}; \rho_0, \rho_m)+\mathscr{F}_{[u,1]}(\{\rho^{(2)}\}; \rho_m, \rho_1)]$. One can check, however, that this is not true.

Instead, we observe that if we define a "modified free energy" $\mathscr{H}$ by

$$\mathscr{H}_{[a,b]}(\{\rho\}; \rho_a, \rho_b)=\mathscr{F}_{[a,b]}(\{\rho\}; \rho_a, \rho_b)+(b-a)\log\left(\frac{\rho_a-\rho_b}{b-a}\right), \tag{9.4}$$

then we obtain from (2.7) the "additivity" property

$$\mathscr{H}_{[0,1]}(\{\rho\}; \rho_0, \rho_1)=\sup_{\rho_m} \{\mathscr{H}_{[0,u]}(\{\rho^{(1)}\}; \rho_0, \rho_m)+\mathscr{H}_{[u,1]}(\{\rho^{(2)}\}; \rho_m, \rho_1)\}. \tag{9.5}$$

The occurrence in (9.5) of the supremum rather than infimum is a consequence of (2.2), but we do not understand its physical basis at this time.

It is perhaps surprising that the additivity property (9.5) suffices to determine the large deviation functional completely. For suppose we divide our system as above, but into n rather than 2 subsystems, with division points $0=x_0<x_1<\cdots<x_n=1$, and denote the corresponding reservoir densities by $\rho_0=F_0>F_1>\cdots>F_{n-1}>F_n=\rho_1$. Then iterating (9.5) we find that

$$\mathscr{F}_{[0,1]}(\{\rho\}; \rho_0, \rho_1)$$
$$=\sup_{F_1,\dots,F_{n-1}} \sum_{j=1}^{n} \left\{\mathscr{F}_{[x_{j-1},x_j]}(\{\rho\}; F_{j-1}, F_j)+y_j\log\left(\frac{F_{j-1}-F_j}{(\rho_0-\rho_1)\,y_j}\right)\right\}, \tag{9.6}$$

where $y_j = x_j - x_{j-1}$. When n is large and all y_j are small,

$$F_j - F_{j-1} \simeq y_j F'(x_j); \tag{9.7}$$

moreover, since $F_j \simeq F_{j-1}$, that is, the two reservoirs at the ends of the interval $[x_{j-1}, x_j]$ have essentially the same chemical potentials, we can expect each this subsystem to be in equilibrium, so that from (2.10),

$$\mathscr{F}_{[x_{j-1}, x_j]}(\{\rho\}; F_{j-1}, F_j)$$
$$\simeq y_j \left[\rho(x_j) \log\left(\frac{\rho(x_j)}{F(x_j)}\right) + (1-\rho(x_j)) \log\left(\frac{1-\rho(x_j)}{1-F(x_j)}\right)\right]. \tag{9.8}$$

By substituting (9.7) and (9.8) into (9.6) and taking the limit $n \to \infty$ with $y_j \to 0$ for all j, we obtain our basic result (2.7).

Clearly it would be of great interest to give a direct derivation of the additivity property (9.5), and to know if this property is limited to the SSEP or whether similar relations hold for more general systems.

APPENDIX A: DERIVATION OF (3.7) AND (3.9)

A.1. A First Consequence of (3.3)

Let us first prove that if D and E are operators satisfying (3.3),

$$DE - ED = D + E, \tag{A.1}$$

then

$$e^{xD+yE} = \left(\frac{(x-y)\, e^y}{xe^y - ye^x}\right)^E \left(\frac{(x-y)\, e^x}{xe^y - ye^x}\right)^D. \tag{A.2}$$

Equation (A.2) and similar equations below are to be interpreted in terms of formal power series in x and y.

One can easily check from (A.1) that for all $p \geqslant 0$

$$DE^p = (E+1)^p\, D + E(E+1)^p - E^{p+1}, \tag{A.3}$$

which means that for "arbitrary functions" $f(E)$, one has

$$Df(E) = f(E+1)\, D + E[f(E+1) - f(E)]. \tag{A.4}$$

Then if one tries to write $e^{z(xD+yE)}$ under the form

$$e^{z(xD+yE)} = e^{tE} e^{uD}, \tag{A.5}$$

one gets that

$$\frac{dt}{dz} = x(e^t - 1) + y, \tag{A.6}$$

$$\frac{du}{dz} = xe^t, \tag{A.7}$$

and by integrating over z, one obtains (A.2).

A.2. Other Consequences of (3.3)

Using (A.2), one derives easily the following three identities:

$$e^{xD+yE} = \left(\frac{xe^x - ye^y}{(x-y)\, e^y}\right)^D \left(\frac{xe^x - ye^y}{(x-y)\, e^x}\right)^E, \tag{A.8}$$

$$e^{xD} e^{yE} = \left(\frac{e^y}{e^x + e^y - e^{x+y}}\right)^E \left(\frac{e^x}{e^x + e^y - e^{x+y}}\right)^D, \tag{A.9}$$

$$e^{xE} e^{yD} = \left(\frac{e^x + e^y - 1}{e^x}\right)^D \left(\frac{e^x + e^y - 1}{e^y}\right)^E. \tag{A.10}$$

Then combining (A.8) and (A.9), one can also show that

$$\begin{aligned} e^{xE} e^{yD} = {} & \left(\frac{(\rho_0 - \rho_1)\, e^x}{1 - (1-\rho_0)\, e^x - \rho_1 e^y}\right)^{\rho_0 E - (1-\rho_0)\, D} \\ & \times \left(\frac{(\rho_0 - \rho_1)\, e^y}{1 - (1-\rho_0)\, e^x - \rho_1 e^y}\right)^{(1-\rho_1)\, D - \rho_1 E}, \end{aligned} \tag{A.11}$$

and that

$$\begin{aligned} e^{uE} e^{vD} e^{xD+yE} = {} & \left(\frac{(x-y)\, e^{u+y}}{(x-y)\, e^y + y(e^{v+y} - e^{v+x})}\right)^E \\ & \times \left(\frac{(x-y)\, e^{v+x}}{(x-y)\, e^y + y(e^{v+y} - e^{v+x})}\right)^D. \end{aligned} \tag{A.12}$$

A.3. Derivation of (3.7)

As a consequence of (A.12) we see that if $\{x_n\}$ and $\{y_n\}$ are two sequences and if the sequences $\{u_n\}$ and $\{v_n\}$ are defined by the recursion

$$e^{u_{n+1}E}e^{v_{n+1}D} = e^{u_nE}e^{v_nD}e^{x_{n+1}D+y_{n+1}E}, \tag{A.13}$$

with the initial condition

$$u_0 = v_0 = 0, \tag{A.14}$$

then the general expressions of u_n and v_n are given by

$$e^{v_n} = \left[e^{\sum_{i=1}^n y_i - x_i} + \sum_{i=1}^n \frac{y_i}{x_i - y_i} \left(e^{y_i - x_i} - 1\right) e^{\sum_{j>i} y_j - x_j} \right]^{-1}, \tag{A.15}$$

$$e^{u_n} = e^{\sum_{i=1}^n y_i - x_i} \left[e^{\sum_{i=1}^n y_i - x_i} + \sum_{i=1}^n \frac{y_i}{x_i - y_i} \left(e^{y_i - x_i} - 1\right) e^{\sum_{j>i} y_j - x_j} \right]^{-1}. \tag{A.16}$$

Therefore

$$e^{\mu_1\lambda_1 D + \mu_1 E} \cdots e^{\mu_k\lambda_k D + \mu_k E} = e^{u_nE}e^{v_nD}, \tag{A.17}$$

where u_n and v_n are given by

$$e^{v_n} = \left[e^{\sum_{i=1}^n \mu_i(1-\lambda_i)} + \sum_{i=1}^n \frac{1}{\lambda_i - 1} \left(e^{\mu_i(1-\lambda_i)} - 1\right) e^{\sum_{j>i} \mu_j(1-\lambda_j)} \right]^{-1}, \tag{A.18}$$

$$e^{u_n} = e^{\sum_{i=1}^n \mu_i(1-\lambda_i)} \left[e^{\sum_{i=1}^n \mu_i(1-\lambda_i)} + \sum_{i=1}^n \frac{1}{\lambda_i - 1} \left(e^{\mu_i(1-\lambda_i)} - 1\right) e^{\sum_{j>i} \mu_j(1-\lambda_j)} \right]^{-1}. \tag{A.19}$$

Then using (A.11), one can rewrite (A.17) as

$$e^{\mu_1\lambda_1 D + \mu_1 E} \cdots e^{\mu_k\lambda_k D + \mu_k E} = e^{U_n[-D+\rho_0(D+E)]}e^{V_n[D-\rho_1(D+E)]}, \tag{A.20}$$

where

$$e^{V_n} = \frac{\rho_1 - \rho_0}{g}, \qquad e^{U_n} = e^{V_n + \sum_{i=1}^n \mu_i(1-\lambda_i)}, \tag{A.21}$$

with g given by (3.9). Lastly, with ρ_0, ρ_1, a, and b given by (1.4) and (3.8), the algebraic rules (3.4) and (3.5) can be written as

$$[D-\rho_1(D+E)]\,|V\rangle = b\,|V\rangle, \tag{A.22}$$

$$\langle W|\,[-D+\rho_0(D+E)] = a\langle W|, \tag{A.23}$$

and one obtains (3.7) from (A.20).

APPENDIX B: DERIVATION OF (4.1)–(4.4)

Consider a system of N sites, divided into n boxes, with a fugacity λ_1 on the N_1 first sites on the left, then λ_2 on the next N_2 sites and so on, λ_n on the last N_n sites. Clearly we have

$$N = N_1 + N_2 + \cdots + N_n. \tag{B.1}$$

Let us define Ω by

$$\begin{aligned}\Omega &= \frac{\langle W|\,(\lambda_1 D+E)^{N_1}\cdots(\lambda_n D+E)^{N_n}\,|V\rangle}{\langle W\,|\,V\rangle}\\ &= \sum_{0\leqslant M_i\leqslant N_i} \lambda_1^{M_1}\cdots\lambda_n^{M_n}\,\frac{\Omega_{N_1,\ldots,N_n}(M_1,\ldots,M_n)}{\langle W\,|\,V\rangle},\end{aligned} \tag{B.2}$$

(see (3.6)), and Ω_0 as in (3.11),

$$\Omega_0 = \frac{\langle W|\,(D+E)^N\,|V\rangle}{\langle W\,|\,V\rangle}. \tag{B.3}$$

Here we have suppressed the dependence of Ω_0 on N and of Ω on $N_1,\ldots, N_n$ and $\lambda_1,\ldots, \lambda_n$. Suppose that for large $N_1,\ldots, N_n$, the quantity defined by (B.2) has the following behavior:

$$\Omega \sim e^{Nh(y_1,\, y_2,\ldots,\, y_n;\, \lambda_1,\ldots,\, \lambda_n)} N_1!\cdots N_n!, \tag{B.4}$$

where

$$y_i = \frac{N_i}{N}. \tag{B.5}$$

Clearly one has that the average density r_i of particles in box i, in the ensemble with fugacities $\lambda_1,..., \lambda_n$, is given by

$$r_i\, y_i = \frac{\langle M_i \rangle_{\lambda_1,..., \lambda_n}}{N} = \frac{1}{N} \frac{\partial \log \Omega}{\partial \log \lambda_i} \simeq \frac{\partial h}{\partial \log \lambda_i}. \tag{B.6}$$

If we assume that the distribution of the M_i is strongly peaked near their mean values then

$$\begin{aligned} \Omega \equiv \Omega_0 \sum_{M_1,..., M_n} \lambda_1^{M_1} \cdots \lambda_n^{M_n} P_{N_1,..., N_n}(M_1,..., M_n) \\ \approx \Omega_0 \lambda_1^{r_1 y_1 N} \cdots \lambda_n^{r_n y_n N} P_{N_1,..., N_n}(r_1\, y_1 N,..., r_n\, y_n N), \end{aligned} \tag{B.7}$$

where $P_{N_1,..., N_n}(M_1,..., M_n)$ denotes the probability computed in the ensemble in which $\lambda_i = 1$ for all i. From (B.4) and (B.7),

$$\frac{\log P_{N_1,...N_n}(M_1,..., M_n)}{N} \simeq h(y_1,..., y_n; \lambda_1,..., \lambda_n) - r_1\, y_1 \log \lambda_1 - \cdots - r_n\, y_n \log \lambda_n + K, \tag{B.8}$$

with $M_i = r_i\, y_i$ and K given by (see (3.11))

$$K = -\frac{\log \Omega_0}{N} + \sum_{i=1}^{n} \frac{\log(N_i!)}{N} \simeq \log(\rho_0 - \rho_1) + \sum_{i=1}^{n} y_i \log y_i. \tag{B.9}$$

We thus obtain $P_{N_1,..., N_n}(M_1,..., M_n)$ in a parametric form (B.8): as we vary the λ_i's, the densities r_i in the boxes vary according to (B.6).

Let us now see how we can extract the function h which appears in (B.4) from (3.6)–(3.9). If we consider the generating function (3.6),

$$Z = \sum_{N_1=0}^{\infty} \cdots \sum_{N_n=0}^{\infty} \frac{\mu_1^{N_1}}{N_1!} \cdots \frac{\mu_n^{N_n}}{N_n!} \frac{\langle W | (\lambda_1 D + E)^{N_1} \cdots (\lambda_n D + E)^{N_n} | V \rangle}{\langle W | V \rangle}, \tag{B.10}$$

and use the asymptotic form (B.4), we see that Z becomes singular along a manifold

$$g = 0, \tag{B.11}$$

where

$$g = \max_{y_1,..., y_n \text{ with } y_1 + \cdots + y_n = 1} [h(y_1,..., y_n; \lambda_1,..., \lambda_n) + y_1 \log \mu_1 + \cdots + y_n \log \mu_n]. \tag{B.12}$$

Along this manifold, we have obviously

$$h = -\sum_{i=1}^{n} y_i \log \mu_i, \tag{B.13}$$

so that (B.8) and (B.9) reduce to (4.2). Moreover we see from (B.12) that

$$y_i = \frac{1}{C} \frac{\partial g}{\partial \log \mu_i}, \tag{B.14}$$

where the constant C is a Lagrange multiplier associated to the constraint that $\sum_i y_i = 1$, and this establishes (4.3). Lastly (4.4) follows simply from the fact that along the hypersurface given by (B.11) and (B.12), one has

$$\frac{\partial g}{\partial \log \lambda_i} = \frac{\partial h}{\partial \log \lambda_i}, \tag{B.15}$$

which shows that (4.4) follows from (B.6).

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