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Entropy of Open Lattice Systems

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We investigate the behavior of the Gibbs-Shannon entropy of the stationary nonequilibrium measure describing a one-dimensional lattice gas, of L sites, with symmetric exclusion dynamics and in contact with particle reservoirs at different densities. In the hydrodynamic scaling limit, $L \to \infty$, the leading order ($O(L)$) behavior of this entropy has been shown by Bahadoran to be that of a product measure corresponding to strict local equilibrium; we compute the first correction, which is $O(1)$. The computation uses a formal expansion of the entropy in terms of truncated correlation functions; for this system the k^{th} such correlation is shown to be $O(L^{-k+1})$. This entropy correction depends only on the scaled truncated pair correlation, which describes the covariance of the density field. It coincides, in the large L limit, with the corresponding correction obtained from a Gaussian measure with the same covariance.

KEY WORDS: Entropy, exclusion process, hydrodynamic scaling

1. INTRODUCTION

The properties of nonequilibrium stationary states (NESS) of open systems, i.e., ones in contact with infinite reservoirs at different chemical potentials and/or temperatures, is a subject of great interest.[1–15] The simplest nontrivial example of such a system is the one-dimensional simple symmetric exclusion processes (SSEP) on the finite lattice $\Lambda_L = \{1, 2, \ldots, L\}$, with particle reservoirs coupled to sites 1 and L; we take these reservoirs to have densities ρ_a and ρ_b, respectively, with $\rho_a > \rho_b$. The 2^L possible configurations of the system are described by the

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L-tuple $\underline{\tau}_L = (\tau_1, ..., \tau_L)$, with $\tau_i = 1$ if site i is occupied and $\tau_i = 0$ if the site is empty. The stationary measure $\bar{\mu}_L(\underline{\tau}_L)$ of the system is explicitly known in terms of products of noncommuting matrices.[4,10] Using this representation it is possible to obtain considerable information about the truncated correlation functions at k distinct sites, $\langle \tau_{i_1} \cdots \tau_{i_k} \rangle^T_{\bar{\mu}_L}$. In particular these are $O(L^{-k+1})$, in the sense that

$$\lim_{L\to\infty} L^{k-1} \langle \tau_{\lfloor x_1 L \rfloor} \cdots \tau_{\lfloor x_k L \rfloor} \rangle^T_{\bar{\mu}_L} = F_k(x_1, \ldots, x_k), \tag{1.1}$$

for certain continuous functions $F_1(x_1)$, $F_2(x_1, x_2)$, etc; here $\lfloor \xi \rfloor$ is the greatest integer not exceeding ξ. These correlations are thus very long range and contribute, despite their vanishing pointwise as $L \to \infty$, to the fluctuations (and larger deviations) about the typical density profile $\bar{\rho}(x) = F_1(x) = \lim_{L\to\infty} \langle \tau_{\lfloor xL \rfloor} \rangle$ in the hydrodynamic scaling limit, $L \to \infty$, $i/L \to x \in [0, 1]$, where $i = 1, \ldots, L$ labels the lattice sites.[10]

In this hydrodynamic limit the typical density profile $\bar{\rho}(x)$ is the stationary solution of the macroscopic hydrodynamic equation with boundary conditions $\bar{\rho}(0) = \rho_a$, $\bar{\rho}(1) = \rho_b$. For the SSEP this is the simple diffusion equation and so

$$\bar{\rho}(x) = \rho_a(1 - x) + \rho_b x. \tag{1.2}$$

The fluctuations about the typical profile $\bar{\rho}(x)$ are given by a Gaussian field whose covariance is determined by the truncated pair correlation function.[3,10] The result agrees with that obtained from fluctuating hydrodynamics.[16]

In this paper we study the relation between the functions F_k and the $L \to \infty$ limit of the Gibbs-Shannon entropy of the stationary measure $\bar{\mu}_L$, defined for any measure μ_L by

$$S(\mu_L) = -\sum_{\underline{\tau}_L} \mu_L(\underline{\tau}_L) \log \mu_L(\underline{\tau}_L). \tag{1.3}$$

In this limit $S(\bar{\mu}_L)$ is $O(L)$ and only F_1 is relevant to leading order (this is a result of Bahadoran)[17] and our goal here is to show that only F_1 and F_2 are relevant for the first correction, which is $O(1)$.

Our motivation for studying $S(\bar{\mu}_L)$ is its potential connection with deviations from the typical profile $\bar{\rho}(x)$.[18] The expectation of such a connection comes from our experience with equilibrium systems, for which the probability of such deviations is determined by the induced change in the entropy.

In fact, the open SSEP with NESS measure $\bar{\mu}_L$ is, in the hydrodynamic scaling limit, very closely related to such a (local) equilibrium system. To make this more precise, let us define the product measure with expected density n_i at site i by

$$\nu_L^{(n)}(\underline{\tau}_L) = \prod_{i=1}^{L} [n_i \tau_i + (1 - n_i)(1 - \tau_i)], \tag{1.4}$$

and for any macroscopic density profile $\rho(x)$ write (with some abuse of notation) $\nu_L^{(\rho)} = \nu_L^{(n)}$ with $n_i = \rho(i/(L+1))$ (the specific definition of n_i arises from the convention that the system has total length $L+1$, with the boundary reservoirs located on sites $i = 0$ and $i = L+1$). Then the restriction of the NESS measure $\bar{\mu}_L$ to the variables τ_i for i lying in an interval $[\lfloor xL \rfloor, \lfloor xL \rfloor + m]$, where m is independent of L, is indistinguishable, for $L \to \infty$, from the corresponding restriction of the local equilibrium product measure $\nu_L^{(\bar{\rho})}$ (see (1.2)).

For this product measure $\nu_L^{(\bar{\rho})}$ the probability of observing a density profile $\rho(x)$ is given, for large L, by

$$\text{Prob}\left(\{\rho(x)\}|\nu_L^{(\bar{\rho})}\right) \sim e^{-L\mathcal{F}_{\text{eq}}(\{\rho(x)\})}, \tag{1.5}$$

where the free energy or large deviation functional (LDF) $\mathcal{F}_{\text{eq}}$ can be written as

$$-\mathcal{F}_{\text{eq}}(\{\rho(x)\}) = \int_0^1 \big\{[s(\rho(x)) + \lambda(\bar{\rho}(x))\rho(x)] - [s(\bar{\rho}(x)) + \lambda(\bar{\rho}(x))\bar{\rho}(x)]\big\}\, dx. \tag{1.6}$$

Here $s(r) = -(r \log r + (1-r)\log(1-r))$ is the entropy per unit length (or site) of the product measure with constant density r, and

$$\lambda(r) = -\frac{\partial s}{\partial r}(r) = \log\left(\frac{r}{1-r}\right) \tag{1.7}$$

is the chemical potential which yields this density. The connection between the LDF $\mathcal{F}_{\text{eq}}$ and entropy given in (1.6) extends to more general (non product) local equilibrium measures.[19,20]

Given this connection between entropy and large deviations in equilibrium systems, it is natural to ask whether there exists a similar relation between $S(\bar{\mu}_L)$ and the large deviation functional in the NESS of the SSEP, for which $\text{Prob}(\{\rho(x)\}|\bar{\mu}_L)$ is qualitatively different from (1.5).[6,7,9,10] Using results of Kosygina,[21] Bahadoran showed, for a large class of systems including the open SSEP, that

$$\lim_{L\to\infty} \frac{1}{L} S(\bar{\mu}_L) = \lim_{L\to\infty} \frac{1}{L} S\left(\nu_L^{(\bar{\rho})}\right). \tag{1.8}$$

In other words, the Gibbs-Shannon entropy is, to leading order, exactly the same as that of the product measure with density $\bar{\rho}(x)$, i.e., $\nu_L^{(\bar{\rho})}$. It thus does not reflect at all the very different nature of the large deviation functional for the NESS in comparison with that of equilibrium systems.

Information about the probabilities of untypical configurations in the NESS of the SSEP is encoded in the truncated correlation functions, or equivalently in the F_k's of (1.1). These also contribute to the entropy $S(\bar{\mu}_L)$ beyond the leading

order. This is what we investigate in the present note. We find that the difference

$$R_L \equiv S(\bar{\mu}_L) - S\big(\nu_L^{(\bar{\rho})}\big) \tag{1.9}$$

approaches a constant value R as $L \to \infty$; Bahadoran's theorem only says that it grows slower than L. Furthermore R depends only on the pair correlation function F_2, indicating that only configurations which contribute to the Gaussian fluctuations about $\bar{\rho}(x)$ contribute to the entropy at this order. This permits us to obtain an explicit expression for R as the $L \to \infty$ limit of $\hat{R}_L$, the corresponding difference in entropies for a Gaussian measure on variables $\xi_i \in \mathbb{R}, i = 1, \ldots, L$, having the same covariance matrix as $\bar{\mu}_L$. We present analytic arguments in favor of this expression, and also check it numerically via exact computations on systems of different sizes. It appears in fact that our results extend to more general systems having long range truncated correlation functions of the form (1.1), as we discuss in Sec. 2.1.

The outline of the rest of this paper is as follows. In Sec. 2 we describe the SSEP and the corresponding Gaussian model, and in Sec. 2.1 the possible extension to other models, in particular, the weakly asymmetric exclusion process (WASEP). In Sec. 3 we report on numerical computations of the entropy difference $R_L - \hat{R}_L$ for different system sizes and densities, in both the SSEP and the WASEP. In Sec. 4 we compute rigorously the $L \to \infty$ limit of $\hat{R}_L$ for the Gaussian model. In Sec. 5 we establish a relation between an arbitrary measure $\mu(\underline{\tau}_\Lambda)$, where $\underline{\tau}_\Lambda = (\tau_i)_{i\in\Lambda}$ with Λ any finite set of points, and the truncated correlations $\langle \prod_{i\in\Lambda'} \tau_i \rangle^T_{\mu_\Lambda}$ for $\Lambda' \subset \Lambda$; we develop from this an expression for the entropy in terms of the truncated correlations. We use this in Sec. 6 to argue that the difference $\lim_{L\to\infty} R_L$ exists and has value $R = \lim_{L\to\infty} \hat{R}_L$.

2. THE MODELS AND THE RESULTS

We begin with a full description of the SSEP. In this model 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. 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 L at rate δ and removed at rate β. This corresponds[10] to the system being in contact with infinite left and right reservoirs having respective densities

$$\rho_a = \frac{\alpha}{\gamma + \alpha}, \qquad \rho_b = \frac{\delta}{\beta + \delta}\ . \tag{2.1}$$

We also introduce the parameters

$$a = \frac{1}{\gamma + \alpha}, \qquad b = \frac{1}{\beta + \delta}. \tag{2.2}$$

We give in Appendix A a proof of the scaling form (1.1) for this model. The first three truncated correlations are, for $i < j < l$,

$$\langle \tau_i \rangle_{\bar{\mu}_L} = \frac{\rho_a(L + b - i) + \rho_b(i + a - 1)}{L + a + b - 1}, \tag{2.3}$$

$$\langle \tau_i \tau_j \rangle^T_{\bar{\mu}_L} = -\frac{(\rho_a - \rho_b)^2 (i + a - 1)(L + b - j)}{(L + a + b - 1)^2 (L + a + b - 2)}, \tag{2.4}$$

$$\langle \tau_i \tau_j \tau_l \rangle^T_{\bar{\mu}_L} = -2\frac{(\rho_a - \rho_b)^3 (i + a - 1)(L + 1 + b - a - 2j)(L + b - l)}{(L + a + b - 3)(L + a + b - 2)(L + a + b - 1)^3}. \tag{2.5}$$

Thus (1.1) holds for $k = 1, 2, 3$, where for $x < y < z$,

$$F_1(x) = \rho_a(1 - x) + \rho_b x, \tag{2.6}$$

$$F_2(x, y) = -(\rho_a - \rho_b)^2 x(1 - y), \tag{2.7}$$

$$F_3(x, y, z) = -2(\rho_a - \rho_b)^3 x(1 - 2y)(1 - z). \tag{2.8}$$

We remark that if $a = b = 1$ then $\langle \tau_i \rangle_{\bar{\mu}_L} = \bar{\rho}(i/(L + 1))$ and the entropy difference R_L of (1.9) must be negative, since $\nu_L^{(\bar{\rho})}$ maximizes the entropy $S(\mu)$ among all measures μ satisfying $\langle \tau_i \rangle_\mu = \bar{\rho}(i/(L + 1))$. Because our expression (4.16) for $\lim_{L\to\infty} R_L$ is independent of a and b, this limit must be negative or zero.

In the remainder of the paper we argue that, in the SSEP, the next order correction to the result of Bahadoran will be equal to the correction for a Gaussian system with the same covariance. Specifically, let $\hat{\nu}_L$ and $\hat{\mu}_L$ be Gaussian measures on L variables with mean zero and respective covariance matrices J_L and K_L given by

$$(J_L)_{ii} = \langle \tau_i \rangle_{\bar{\mu}_L}(1 - \langle \tau_i \rangle_{\bar{\mu}_L}), \qquad (J_L)_{ij} = 0, \quad i \neq j; \tag{2.9}$$

$$(K_L)_{ii} = \langle \tau_i \rangle_{\bar{\mu}_L}(1 - \langle \tau_i \rangle_{\bar{\mu}_L}), \qquad (K_L)_{ij} = \langle \tau_i \tau_j \rangle^T_{\bar{\mu}_L}, \quad i \neq j. \tag{2.10}$$

We note from (2.3) that $\langle \tau_i \rangle_{\bar{\mu}_L}$ and $1 - \langle \tau_i \rangle_{\bar{\mu}_L}$ do not vanish. The entropies of these Gaussian measures are given by

$$S(\hat{\nu}_L) = \frac{L}{2}(1 + \log 2\pi) + \frac{1}{2} \log \det J_L, \tag{2.11}$$

$$S(\hat{\mu}_L) = \frac{L}{2}(1 + \log 2\pi) + \frac{1}{2} \log \det K_L, \tag{2.12}$$

so that

$$\hat{R}_L \equiv S(\hat{\mu}_L) - S(\hat{\nu}_L) = \frac{1}{2} \log \frac{\det K_L}{\det J_L}. \tag{2.13}$$

The $L \to \infty$ limit of (2.13),

$$R = \lim_{L\to\infty} \hat{R}_L = \lim_{L\to\infty} \frac{1}{2} \log \frac{\det K_L}{\det J_L}, \tag{2.14}$$

exists; see Sec. 4. Further, we claim that this limit gives also the lowest order correction to the result (1.8) of Bahadoran (see (1.9)):

$$\lim_{L\to\infty} R_L = \lim_{L\to\infty} \left[S(\bar{\mu}_L) - S(\nu_L^{(\bar{\rho})}) \right] = R. \tag{2.15}$$

2.1. Other Models

It is natural to ask to what extent these results hold for other lattice gas models. As will become clear in Sec. 6, the key element in our analysis for the SSEP is the scaling behavior (1.1) of the truncated correlation functions. (We also use some technical facts about the way the limit in (1.1) is achieved and the size of the limiting functions F_k.) We expect (2.15) to hold for models having this same scaling behavior and satisfying an additional condition discussed in Remark 4.1.

Unfortunately, less is known about the correlation functions for other lattice gas models than for the SSEP; in particular, we know of no other model of an open NESS for which (1.1) has been established with nonzero F_k, $k \geq 2$ (for zero range processes the NESS is a product measure, i.e., $F_k = 0$ for $k \geq 2$). We expect, however, that this scaling will hold in the weakly asymmetric simple exclusion process (WASEP); see Ref. 22, where expressions corresponding to (2.6) and (2.7) are given for this model. In the WASEP the boundary dynamics are those of the SSEP, but the bulk dynamics are modified so that a particle attempts to hop to its right at rate 1 and to its left at rate $\exp(-\lambda/L)$; λ is a parameter which interpolates between the symmetric process ($\lambda = 0$) and the totally asymmetric process ($\lambda = \pm\infty$). The typical profile $\bar{\rho}(x)$ is the solution of the viscous Burgers equation. We include numerical results for the WASEP in the next section.

The truncated correlation functions are also expected to satisfy (1.1) in the KMP model.[1] This is an open system in which the variable $\xi_i \in \mathbb{R}_+$ at site i, $i = 1, \ldots, L$, represents an energy at that site, and ρ_a and ρ_b are replaced by temperatures T_a and T_b. For this system,[1]

$$F_1^{\mathrm{KMP}}(x) = \lim_{L\to\infty} \langle \xi_{\lfloor xL \rfloor} \rangle = T_a(1-x) + T_b x, \tag{2.16}$$

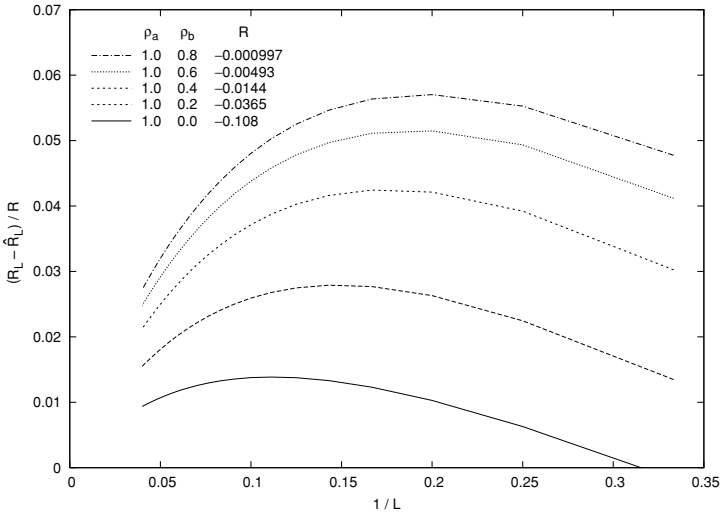

Fig. 1. Differences of corrections to entropies in the SSEP and Gaussian models for $\rho_a = 1$ and several choices of ρ_b. The data are consistent with the vanishing of $R_L - \hat{R}_L$ as $L \to \infty$.

while for $x < y$,[23]

$$F_2^{\mathrm{KMP}}(x, y) = \lim_{L\to\infty} L\left\langle \xi_{\lfloor xL \rfloor} \xi_{\lfloor yL \rfloor} \right\rangle = (T_a - T_b)^2 x(1 - y). \tag{2.17}$$

One can also imagine that for more general diffusive systems, such as those described by the macroscopic fluctuation theory,[7,9] the long range part of the truncated correlation functions scales as in (1.1).

3. NUMERICAL RESULTS

We have investigated (2.15) numerically for the SSEP, at several different values of the boundary densities ρ_a, ρ_b, and for the WASEP, at $\rho_a = 1$, $\rho_b = 0$, for several different values of λ. For all computations we have taken $a = b = 1$ (see (2.2)). We were able to consider systems up to size $L = 25$. In each case we computed the measure $\bar{\mu}_L$ explicitly and from this $S(\bar{\mu}_L)$, $S(\nu_L^{(\rho)})$, $S(\hat{\mu}_L)$, and $S(\hat{\nu}_L)$, and thus, from (1.9) and (2.13), R_L and $\hat{R}_L$. For the SSEP we could also compute the limiting value R, defined in (2.14), to a high degree of accuracy, using (2.4).

Figures 1 and 2 present our results for the SSEP. In order to show results for several parameter values on the same figure, we plot the normalized difference

$$\frac{R_L - \hat{R}_L}{R} \tag{3.1}$$

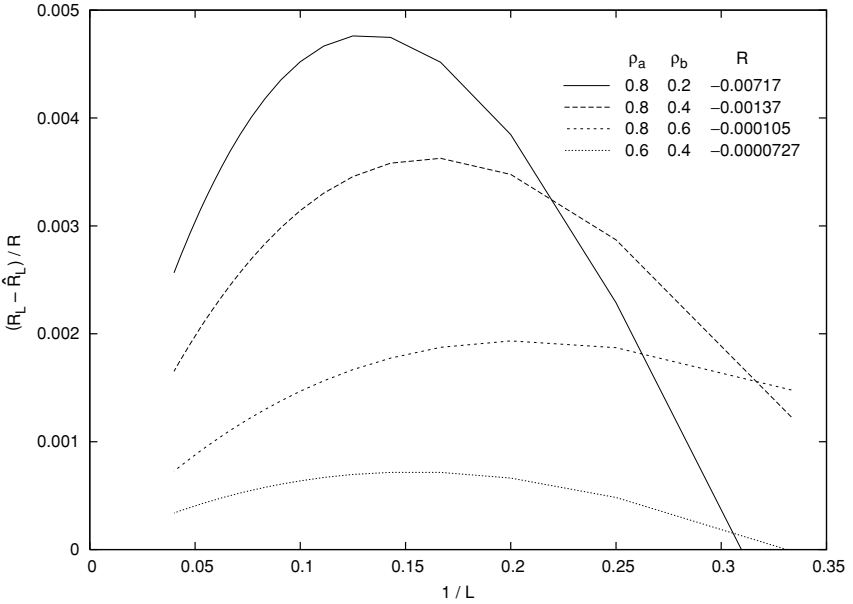

Fig. 2. Same as Figure 1 for other choices of ρ_a and ρ_b.

as a function of $1/L$. The table within each figure gives the values of ρ_a and ρ_b for each curve, as well as the corresponding value of R. Confirmation of (2.15) corresponds in each case to $\lim_{1/L\to 0}(R_L - \hat{R}_L)/R = 0$. This certainly appears to hold, but the maximum system size we have been able to achieve is perhaps too small for the evidence to be completely convincing.

Figure 3 gives similar plots for the WASEP, at different values of λ, with $\rho_a = 1$, $\rho_b = 0$. Here we have no closed form for the two-point correlation function, so that an accurate computation of R is more difficult than for the SSEP; we therefore plot the unnormalized difference $R_L - \hat{R}_L$ against $1/L$. The behavior for small L is quite irregular, particularly for negative values of λ, but the large-L behavior again provides some confirmation that $\lim_{1/L\to 0}(R_L - \hat{R}_L) = 0$, i.e., that (2.15) holds for this model.

4. THE GAUSSIAN LIMIT

In this section we evaluate the limit R of (2.14). Let us write

$$\frac{\det K_L}{\det J_L} = \det\left[J_L^{-1/2}\, K_L\, J_L^{-1/2}\right] = \det(I + U_L), \tag{4.1}$$

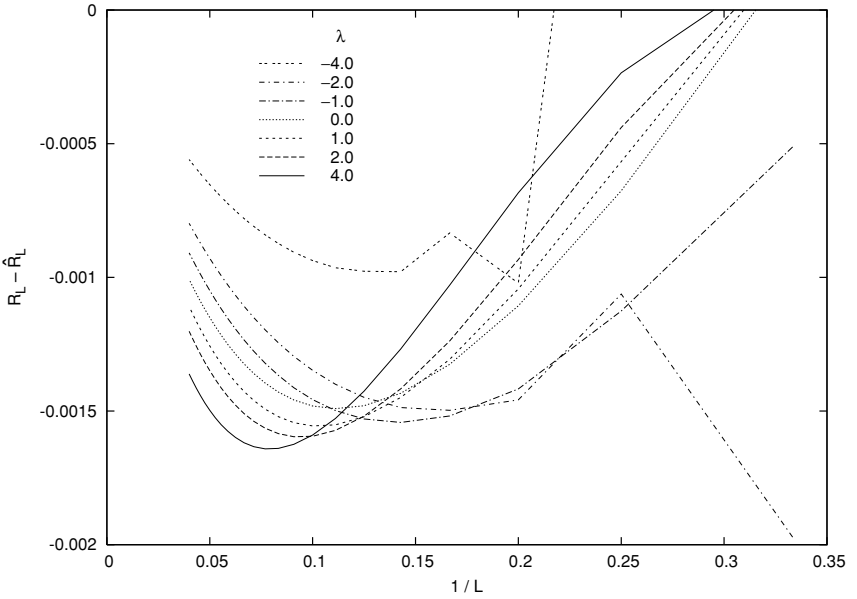

Fig. 3. Same as Figures 1 and 2 for the WASEP.

where

$$U_L = J_L^{-1/2}[K_L - J_L]J_L^{-1/2}, \tag{4.2}$$

so that $(U_L)_{ii} = 0$, $i = 1, \ldots, L$, and

$$(U_L)_{ij} = \frac{\langle \tau_i \tau_j \rangle^T}{\sqrt{\langle \tau_i \rangle (1 - \langle \tau_i \rangle) \langle \tau_j \rangle (1 - \langle \tau_j \rangle)}}, \qquad 1 \le i \ne j \le L. \tag{4.3}$$

In order to pass to a continuum limit it is convenient to relate U to the integral operator H_L on $L^2([0, 1])$ with kernel

$$h_L(x, y) = L(U_L)_{ij}, \quad \text{for } \frac{i-1}{L} < x \le \frac{i}{L}, \ \frac{j-1}{L} < y \le \frac{j}{L}, \tag{4.4}$$

that is, $(H_L\phi)(x) = \int_0^1 h_L(x, y)\phi(y)\,dy$ for $\phi \in L^2([0, 1])$. Since H_L has rank (at most) L, all but L of the eigenvalues of $I + H_L$ are equal to 1, so that the determinant $\det(I + H_L)$ is certainly well defined. Then

$$\det(I + U_L) = \det(I + H_L), \tag{4.5}$$

since if we define

$$\psi_{L,i}(x) = \begin{cases} \sqrt{L}, & \text{if } (i-1)/L < x \le i/L, \\ 0, & \text{otherwise,} \end{cases} \tag{4.6}$$

then the $\psi_{L,i}$ for $i = 1, \ldots, L$ form an orthonormal set in $L^2([0, 1])$ which spans the range of H_L and satisfies $H_L \psi_{L,i} = \sum_j (U_L)_{ji} \psi_{L,j}$.

Now (1.1) implies that for $x \neq y$, $\lim_{L\to\infty} h_L(x, y) = h(x, y)$, where

$$h(x, y) = \frac{F_2(x, y)}{\sqrt{F_1(x)(1 - F_1(x))F_1(y)(1 - F_1(y))}}. \tag{4.7}$$

Let H be the integral operator on $L^2([0, 1])$ with kernel h. It can be shown that H is of trace class (we define this precisely below), so that $\det(I + H)$ is well defined.[24] However, it is not true that $\lim_{L\to\infty} \det(I + H_L) = \det(I + H)$; essentially, this is because the diagonal elements of H_L are zero rather than being given by the obvious extension of (4.3), and as a consequence H_L does not converge to H in trace norm. To evaluate the limit correctly it is helpful to introduce the *regularized determinant*;[24] one needs then only convergence of H_L to H in a weaker sense.

We now discuss the general theory of the regularized determinant in the (relatively simple) context in which we will use it. Let A be a compact integral operator on $L^2([0, 1])$ with symmetric kernel $a(x, y) = a(y, x)$, so that $(A\phi)(x) = \int_0^1 a(x, y)\phi(y)\, dy$; A is self-adjoint and hence diagonalizable: $A\phi_n = \lambda_n \phi_n$ for some orthonormal basis ϕ_n. A is of *trace class* if $\|A\|_1 \equiv \sum_n |\lambda_n| < \infty$ and of *Hilbert-Schmidt class* if $\|A\|_2 \equiv \sum_n |\lambda_n|^2 < \infty$; we also have

$$\|A\|_2 \equiv \int_0^1 \int_0^1 |a(x, y)|^2\, dx\, dy. \tag{4.8}$$

If A is of trace class then both the trace $\operatorname{Tr} A = \sum_n \lambda_n$ and the Fredholm determinant $\det(I + A) = \prod(1 + \lambda_n)$ are well defined and satisfy $\log \det(I + A) = \operatorname{Tr} \log(I + A)$. If A is of Hilbert-Schmidt class then $\det(I + A)$ may not be defined but $\tilde{A} = e^{-A}(I + A) - I$ is of trace class and the regularized determinant $\det_2(I + A)$ is defined by

$$\det_2(I + A) = \det(I + \tilde{A}). \tag{4.9}$$

We note several properties of $\det_2$ which we will need below: (i) if A is of trace class then

$$\det_2(I + A) = \det(I + A)e^{-\operatorname{Tr} A}; \tag{4.10}$$

(ii) if A is Hilbert-Schmidt and $k \geq 2$ then A^k is of trace class, with

$$\operatorname{Tr} A^k = \int_0^1 dx_1 \cdots \int_0^1 dx_k\, h(x_1, x_2) \cdots h(x_{k-1}, x_k) h(x_k, x_1), \tag{4.11}$$

and $\operatorname{Tr} A^k$ is continuous in the Hilbert-Schmidt norm, i.e.,

$$\lim_{n\to\infty} \operatorname{Tr} A_n^k = \operatorname{Tr} A^k \quad \text{if} \quad \lim_{n\to\infty} \|A_n - A\|_2 = 0; \tag{4.12}$$

(iii) $\det_2(I + A)$ is continuous in the Hilbert-Schmidt norm, i.e.,

$$\lim_{n\to\infty} \det_2(I + A_n) = \det_2(I + A) \quad \text{if} \quad \lim_{n\to\infty} \|A_n - A\|_2 = 0; \tag{4.13}$$

and (iv) if the operator norm of A satisfies $\|A\| < 1$ then

$$\log \det_2(I + A) = \sum_{n=2}^{\infty} \frac{(-1)^{n+1}}{n} \operatorname{Tr} A^n. \tag{4.14}$$

In order to apply these ideas we note that it follows from (2.3), (2.4), (2.6), and (2.7) that the kernel $h(x, y)$ is square integrable and that

$$\lim_{L\to\infty} \|H_L - H\|_2 = \lim_{L\to\infty} \int_0^1 \int_0^1 |h_L(x, y) - h(x, y)|^2 \, dx \, dy = 0. \tag{4.15}$$

Now from (4.10) and the fact that $\operatorname{Tr} H_L = 0$ it follows that $\det(I + H_L) = \det_2(I + H_L)$, and hence from (4.1), (4.13), and (4.15), $\lim_{L\to\infty} \det(I + U_L) = \det_2(I + H)$. Thus from (2.14) and (4.1),

$$R = \lim_{L\to\infty} [S(\hat{\mu}_L) - S(\hat{\nu}_L)] = \frac{1}{2} \log \det_2(I + H). \tag{4.16}$$

Remark 4.1: (a) It follows from (2.6) and (2.7) that $|h(x, y| \leq 1$, with strict equality possible only for $x = y$ and $\rho_a = 1 - \rho_b = 1$; this implies that the operator norm of H is less than one, so that from (4.14) we have the expansion

$$R = \sum_{n=2}^{\infty} \frac{(-1)^{n+1}}{2n} \operatorname{Tr} H^n. \tag{4.17}$$

The convergence of the expansion (4.17) is the additional condition for the validity of (2.15) referred to in Sec. 2.1.

(b) The operators $-H_L$ may be shown to be positive semi-definite, and hence $-H$ is also; from $\int_0^1 (-h(x, x))\, dx < \infty$ and the continuity of $h(x, y)$ it then follows that H is of trace class.[24] Thus in fact $\det_2(I + H)$ is given by (4.10).

5. TRUNCATED CORRELATIONS AND ENTROPY

In this section we derive an expression for the probability of a configuration, and an expansion for the entropy, in terms of truncated correlation functions. The results hold in a more general setting than the specific models we are considering here. Thus let Λ be any finite set and μ_Λ be a measure on the configurations $\underline{\tau}_\Lambda$ on Λ: $\underline{\tau}_\Lambda = (\tau_i)_{i\in\Lambda}$, $\tau_i = 0, 1$. In particular, Λ might be a subset of a larger set, say $\Lambda \subset \mathbb{Z}^d$, and μ the restriction of some measure on the configurations on this larger set to the configurations on Λ. For any set $A = \{i_1, \ldots, i_k\} \subset \Lambda$ we will write μ_A for the marginal of μ_Λ on configurations defined on A and ν_A

for the product measure on the configurations on A which has the same one-site probabilities as does μ_Λ: for a configuration $\underline{\tau}_A = (\tau_{i_1}, \ldots, \tau_{i_k})$ with $\tau_i = 0, 1$, and with $t_i = \langle \tau_i \rangle_{\mu_\Lambda}$,

$$\nu_A(\underline{\tau}_A) = \prod_{i \in A} t_i^{\tau_i}(1 - t_i)^{1-\tau_i} = \prod_{i \in A}[\tau_i t_i + (1 - \tau_i)(1 - t_i)]. \tag{5.1}$$

5.1. Probabilities and Truncated Correlations

For the subset $A = \{i_1, \ldots, i_k\} \subset \Lambda$ we denote the truncated correlation function $\langle \tau_{i_1} \cdots \tau_{i_k} \rangle^T_{\mu_\Lambda}$ on the sites of A by t_A; if $A = \{i\}$ we usually write t_i rather than $t_{\{i\}}$, in accord with (5.1). Recall that t_A is defined recursively by writing the (untruncated) correlation function on the sites of A as a sum, over all partitions of A into disjoint subsets, of the products of the truncated functions for the subsets: letting $\mathcal{P}(A)$ denote the set of all partitions of A into disjoint subsets we have[25]

$$\langle \tau_{i_1} \cdots \tau_{i_k} \rangle_{\mu_\Lambda} = \sum_{\pi \in \mathcal{P}(A)} \prod_{B \in \pi} t_B, \tag{5.2}$$

where π labels a particular partition.

For use in the next subsection it is convenient to rewrite the measure μ_Λ by factoring out the product measure ν_Λ:

$$\mu_\Lambda(\underline{\tau}_\Lambda) = \nu_\Lambda(\underline{\tau}_\Lambda)(1 + x_\Lambda(\underline{\tau}_\Lambda)), \tag{5.3}$$

where

$$x_\Lambda(\underline{\tau}_\Lambda) = \sum_{\pi \in \tilde{\mathcal{P}}(\Lambda)} \prod_{i \in C_\pi} g_i(\tau_i) \prod_{B \in \pi} t_B. \tag{5.4}$$

Here $\tilde{\mathcal{P}}(A)$, $A \subset \Lambda$, denotes the set of nonempty families $\pi = \{B_1, \ldots, B_{k(\pi)}\}$ of pairwise disjoint subsets of A in which each set B_i contains at least two points, with $C_\pi = \cup_i B_i$ for $\pi \in \tilde{\mathcal{P}}(A)$, and

$$g_i(\tau_i) = t_i^{-\tau_i}[-(1 - t_i)]^{-(1-\tau_i)} = (-1)^{1-\tau_i} \frac{1}{\nu_{\{i\}}(\tau_i)}. \tag{5.5}$$

To verify this formula one multiplies both sides of (5.3) by some product $\tau_{i_1} \ldots \tau_{i_k}$ and sums over $\underline{\tau}_\Lambda$; the result is just (5.2).

Remark 5.1: An alternate way of viewing (5.3) is to introduce *truncated measures* $\hat{\mu}_A$ defined by a recursion analogous to that for the truncated correlation functions:

$$\mu_A(\underline{\tau}_A) = \sum_{\pi \in \mathcal{P}(A)} \prod_{B \in \pi} \hat{\mu}_B(\underline{\tau}_B). \tag{5.6}$$

Disentangling (5.6), on sees that $\hat{\mu}_A$ is a linear combination of measures on the configurations on A, but for $|A| > 1$ with some negative coefficients; that is, $\hat{\mu}_A$ is

a signed measure. There is a surprisingly simple relation between these truncated measures and the truncated correlation functions: we claim that

$$\hat{\mu}_{\{i\}}(\tau_i) = \mu_{\{i\}}(\tau_i), \tag{5.7}$$

and if $|B| \geq 2$,

$$\hat{\mu}_B(\underline{\tau}_B) = (-1)^{|B|} \prod_{i \in B} (-1)^{\tau_i} t_B = \left[\prod_{i \in B} (2\tau_i - 1) \right] t_B; \tag{5.8}$$

i.e., $\hat{\mu}_B(\underline{\tau}_B)$ is equal to either t_B or $-t_B$, depending only on whether $\sum_{i \in B}(1 - \tau_i)$ is even or odd. Equation (5.7) is an immediate consequence of the definition (5.6). Equation (5.8) may be verified by substituting (5.7) and (5.8) into the right hand side of (5.6), multiplying the result by some product $\prod_{i \in C} \tau_i$, where $C \subset A$, and summing over all $\underline{\tau}_A$; the result is just (5.2). If we now substitute (5.7) and (5.8) into (5.6) we obtain (5.3).

5.2. Expansion of the Entropy

In this subsection we obtain a series expansion for the entropy difference $S(\mu_\Lambda) - S(\nu_\Lambda)$. Other graphical expansions for the entropy have been obtained, for example in.[26,27] From (5.3) and the definition (1.3) we have

$$\begin{aligned} S(\mu_\Lambda) &= -\sum_{\underline{\tau}_\Lambda} \nu_\Lambda(\underline{\tau}_\Lambda)(1 + x_\Lambda(\underline{\tau}_\Lambda)) \log[\nu_\Lambda(\underline{\tau}_\Lambda)(1 + x_\Lambda(\underline{\tau}_\Lambda))] \\ &= -\sum_{\underline{\tau}_\Lambda} \nu_\Lambda(\underline{\tau}_\Lambda) \Big[\log \nu_\Lambda(\underline{\tau}_\Lambda) + x_\Lambda(\underline{\tau}_\Lambda) \log \nu_\Lambda(\underline{\tau}_\Lambda) \\ &\qquad + (1 + x_\Lambda(\underline{\tau}_\Lambda)) \log(1 + x_\Lambda(\underline{\tau}_\Lambda)) \Big]. \end{aligned} \tag{5.9}$$

With the expansion

$$(1 + x) \log(1 + x) = x + \sum_{n=2}^{\infty} \frac{(-1)^n}{n(n-1)} x^n, \tag{5.10}$$

and the identities

$$\sum_{\underline{\tau}_\Lambda} \nu_\Lambda(\underline{\tau}_\Lambda) x_\Lambda(\underline{\tau}_\Lambda) = 0, \qquad \sum_{\underline{\tau}_\Lambda} \nu_\Lambda(\underline{\tau}_\Lambda) x_\Lambda(\underline{\tau}_\Lambda) \log \nu_\Lambda(\underline{\tau}_\Lambda) = 0, \tag{5.11}$$

which follow from (5.3) and the equations $\langle 1 \rangle_{\mu_\Lambda} = \langle 1 \rangle_{\nu_\Lambda} = 1$ and $\langle \tau_i \rangle_{\mu_\Lambda} = \langle \tau_i \rangle_{\nu_\Lambda} = t_i$, respectively, (5.9) yields

$$S(\mu_\Lambda) - S(\nu_\Lambda) = \sum_{\underline{\tau}_\Lambda} \nu_\Lambda(\underline{\tau}_\Lambda) \sum_{n=2}^{\infty} \frac{(-1)^{n+1}}{n(n-1)} x_\Lambda(\underline{\tau}_\Lambda)^n. \tag{5.12}$$

This expansion requires that $|x_\Lambda(\underline{\tau}_\Lambda)| < 1$ for all $\underline{\tau}_\Lambda$; for the SSEP we have checked this condition numerically for $L = 1, \ldots, 23$ at several values of ρ_a, ρ_b.

We next insert the definition (5.4) of x_Λ into (5.12) and expand $x_\Lambda(\underline{\tau}_\Lambda)^n$:

$$S(\mu_\Lambda) - S(\nu_\Lambda) = \sum_{\underline{\tau}_\Lambda} \nu_\Lambda(\underline{\tau}_\Lambda) \sum_{n=2}^{\infty} \frac{(-1)^{n+1}}{n(n-1)} \sum_{\pi_1,\ldots\pi_n} \prod_{j=1}^{n} \Big[\prod_{i\in C_{\pi_j}} g_i(\tau_i) \prod_{B\in\pi_j} t_B \Big] \tag{5.13}$$

This expression can be reorganized as an (infinite) linear combination of monomials M in the variables t_B. The coefficient of the monomial M is

$$\sum_{n=2}^{\infty} \frac{(-1)^{n+1}}{n(n-1)} c_n(M) \sum_{\underline{\tau}_\Lambda} \nu_\Lambda(\underline{\tau}_\Lambda) \prod_{i\in\Lambda} g_i(\tau_i)^{m_i(M)}, \tag{5.14}$$

where $c_n(M)$ is the number of n-tuples $(\pi_1, \ldots, \pi_n)$ such that M is given by the product $\prod_{j=1}^{n} \prod_{B\in\pi_j} t_B$, and $m_i(M)$ is the number of factors t_B in the monomial M such that $i \in B$.

We can carry out the sum over $\underline{\tau}_\Lambda$ in (5.14), using (with $m_i = m_i(M)$)

$$h_i(M) \equiv \sum_{\tau_i=0,1} t_i^{\tau_i}(1-t_i)^{1-\tau_i} g_i(\tau_i)^{m_i} = \left[\frac{1}{t_i^{m_i-1}} + \frac{(-1)^{m_i}}{(1-t_i)^{m_i-1}} \right]. \tag{5.15}$$

Since $h_i(M) = 1$ if $m_i(M) = 0$, (5.13) and (5.14) yield

$$S(\mu_\Lambda) - S(\nu_\Lambda) = \sum_{M} d(M)\, M \prod_{i\in D_M} h_i(M), \tag{5.16}$$

where D_M is the set of indices i such that $m_i(M) > 0$ and

$$d(M) = \sum_{n=2}^{\infty} \frac{(-1)^{n+1}}{n(n-1)} c_n(M). \tag{5.17}$$

Since $h_i(M) = 0$ if $m_i(M) = 1$, we may restrict the sum in (5.16) to monomials M for which $m_i(M) \geq 2$ for $i \in D_M$.

We obtain a graphical representation for (5.16) by associating to each monomial M a graph G_M; G_M has a vertex for each factor t_B in M, and vertices corresponding to factors t_B, t_C are joined by an edge if and only if $B \cap C \neq \emptyset$. We will show in Appendix B that $d(M) = 0$ unless G_M is connected; from this observation together with the remarks above it follows that the sum in (5.16) can be restricted to the set $\mathcal{M}$ of all monomials for which $m_i(M) \geq 2$ for all $i \in D_M$ and for which G_M is connected. We also show in Appendix B that if G_M is a cycle with $k \geq 3$ vertices then $d(M) = (-1)^{k+1}$. Note finally that if G_M consists of two vertices joined by an edge then the requirement that $m_i(M) \geq 2$ for $i \in D_M$ implies that $M = t_B^2$ for some B, so that $c_n(M) = \delta_{n,2}$ and $d(M) = -1/2$ from (5.17).

6. ENTROPY FOR THE SSEP

We now apply the expansion (5.16) to the special case of the SSEP, taking μ_Λ to be the NESS measure $\bar{\mu}_L$ on Λ_L and thus ν_Λ to be the product measure $\nu_L^{(\bar{\rho})}$, which we will here write as $\bar{\nu}_L$. We will use (1.1) to identify the order, as $L \to \infty$, of the terms in the series; we then show that in this limit the leading order terms in this series sum to R. We do not, however, give estimates which would completely justify the neglect of the higher order terms.

Let us denote the order in L of a monomial $M \in \mathcal{M}$ by $-j_M$, that is, we suppose that M is $O(L^{-j_M})$ as $L \to \infty$. From (1.1) we know that t_B is of order $L^{-(|B|-1)}$, so that if M has k factors (not necessarily distinct), $M = t_{B_1} \cdots t_{B_k}$, then $j_M = \sum_{i=1}^{k} (|B_i| - 1)$. Since $|B_l| \geq 2$ for each l, $k \leq (1/2) \sum |B_l|$. But then, because $m_i \geq 2$ for $i \in D_M$,

$$j_M = \sum_{l=1}^{k} |B_l| - k \geq \frac{1}{2} \sum_{l=1}^{k} |B_l| \geq |D_M|; \tag{6.1}$$

note that $|D_M|$ is the total number of sites which belong to some B_i. Equality holds in (6.1) if and only if

$$|B_l| = 2 \text{ for each factor } t_{B_l} \text{ of } M, \text{ and } m_i(M) = 2 \text{ for each } i \in D_M. \tag{6.2}$$

The terms satisfying condition (6.2) give the leading order contribution to $S(\bar{\mu}_L) - S(\bar{\nu}_L)$, as we now discuss.

Let $\mathcal{M}_1 \subset \mathcal{M}$ be the monomials for which $j_M = |D_M|$, that is, those which satisfy (6.2), and let $\mathcal{M}_2 = \mathcal{M} \setminus \mathcal{M}_1$. Then we write (5.16) in the form

$$S(\bar{\mu}_L) - S(\bar{\nu}_L) = \sum_{k=2}^{L} \sum_{\substack{A \subset \{1,\ldots,L\} \\ |A|=k}} (s_{L,1}(A) + s_{L,2}(A)), \tag{6.3}$$

where

$$s_{L,j}(A) = \sum_{\substack{M \in \mathcal{M}_j \\ D_M = A}} d(M)\, M \prod_{i \in D_M} h_i(M), \qquad j = 1, 2, \tag{6.4}$$

so that when $j = 1$, each summand in (6.4) is of order $L^{-|A|}$, while when $j = 2$, each term is of higher order.

We first consider the sum of the $s_{L,1}(A)$. For $M \in \mathcal{M}_1$, (5.15) and (6.2) imply that $h_i(M) = 1/[t_i(1 - t_i)]$. Moreover, (6.2) and the requirement that G_M be connected imply that G_M is a cycle or, if $|D_M| = 2$, a single edge connecting two vertices, and for these graphs we know the value of $d(M)$, as discussed at the

end of Sec. 5. This leads to

$$s_{L,1}(A) = \frac{(-1)^{|A|+1}}{2} \sum_{\sigma} \prod_{i \in A} \frac{t_{\{i,\sigma(i)\}}}{t_i(1-t_i)}, \tag{6.5}$$

where the sum is over all cyclic permutations σ of A. Here the overall factor of 1/2 arises for $|A| = 2$ from $d(M) = -1/2$ and for $|A| \geq 3$ from the fact that the permutations from a cycle and from the reverse cycle give rise to the same monomial. Thus

$$\begin{aligned} \sum_{|A|=k} s_{L,1}(A) &= \frac{(-1)^{k+1}}{2k} \sum_{1 \leq i_1 \neq i_2 \neq \cdots \neq i_k \leq L} (U_L)_{i_1 i_2} (U_L)_{i_2 i_3} \cdots (U_L)_{i_{k-1} i_k} (U_L)_{i_k i_1} \\ &= \frac{(-1)^{k+1}}{2k} \big[\operatorname{Tr} H_L^k + O(L^{-1}) \big], \end{aligned} \tag{6.6}$$

where H_L was defined in (4.4) and the $O(L^{-1})$ error arises from the fact that the sum omits terms in which some of the indices i_j coincide.

It follows from (6.6), (4.12) and (4.15) that for $k \geq 2$,

$$\lim_{L \to \infty} \sum_{|A|=k} s_{L,1}(A) = \frac{(-1)^{k+1}}{2k} \operatorname{Tr} H^k. \tag{6.7}$$

It is also true that

$$\lim_{L \to \infty} \sum_{k=2}^{\infty} \sum_{|A|=k} s_{L,1}(A) = \sum_{k=2}^{\infty} \frac{(-1)^{k+1}}{2k} \operatorname{Tr} H^k = R \tag{6.8}$$

(see (4.17)); this will follow from (6.7) and the Lebesgue dominated convergence theorem if we show that $|\sum_{|A|=k} s_{L,1}(A)| \leq e_k$ for some convergent series $\sum_k e_k$. Now since $U_{ij} \leq 0$ for all i, j and hence the $O(L^{-1})$ term in (6.6) has the opposite sign to $\operatorname{Tr} H_L^k$, and since for any $\epsilon > 0$, $|h_L(x,y)| \leq |h(x,y)| + \epsilon = |h(x,y) - \epsilon|$ for sufficiently large L, we have from (4.11) that for such L,

$$\Big| \sum_{|A|=k} s_{L,1}(A) \Big| \leq \frac{1}{2k} \Big| \operatorname{Tr} H_L^k \Big| \leq \frac{1}{2k} \Big| \operatorname{Tr}(H - \epsilon C)^k \Big|, \tag{6.9}$$

where C is the integral operator with kernel $c(x,y) \equiv 1$. If we take ϵ sufficiently small that $\|H - \epsilon C\| < 1$ then (6.9) furnishes the needed bound.

We now consider the contribution to (6.4) of the terms $s_{L,2}(A)$, each of which is $O(L^{-j})$ with $j > |A|$. Since there are order L^k sets A with $|A| = k$, we have formally that

$$\lim_{L \to \infty} \sum_{|A|=k} s_{L,2}(A) = 0. \tag{6.10}$$

We will assume that (6.10) holds and can in fact be extended to

$$\lim_{L\to\infty} \sum_{k=2}^{L} \sum_{|A|=k} s_{L,2}(A) = 0. \tag{6.11}$$

From (6.3), (6.8), and (6.11) we have

$$\lim_{L\to\infty} [S(\bar{\mu}_L) - S(\bar{\nu}_L)] = R, \tag{6.12}$$

which verifies (2.15).

7. CONCLUSION

In this paper we have seen how the truncated pair correlation function which describes the Gaussian fluctuations of the density profile in the non-equilibrium steady state of the simple exclusion process also determines the leading correction, which is of order 1, to the entropy $S(\mu)$. One could also ask how the higher order truncated correlation functions, which are related to higher order terms in the expansion of the LDF around $\bar{\rho}$, contribute to further corrections to the entropy. Going beyond the simple exclusion process (and the WASEP and KMP model), in which local equilibrium corresponds to a product measure, it would be interesting to consider more general non-equilibrium steady states in which, in addition to the weak long range part of the correlation of the form (1.1), there is an $O(1)$ short range part. The simplest extension of our result would be that the leading order term would again be given by that of the local equilibrium and that the leading correction would again be that coming from the non local part of the truncated pair correlation. Another interesting extension would be to cases in which the leading order of the entropy is still obtained from a local equilibrium product measure but the long range part of the correlation obeys another scaling or in which the fluctuations of the density are not Gaussian (as in the asymmetric simple exclusion process; see Ref. 28).

For isolated systems at equilibrium, that is, in the microcanonical ensemble, all microscopic configurations have equal probability, and so $S(\mu) = -\log \mu = \log |\Omega|$, where $|\Omega|$ is the number of configurations, or the phase space volume, available to the system. When one moves to the canonical ensemble, still at equilibrium, the probabilities of configurations visited by the system fluctuate: the Gibbs-Shannon entropy $S(\mu)$ is just the expectation of the logarithm of these probabilities. The variance of this logarithm is, up to a trivial temperature factor, the variance of the energy; it is an extensive quantity whose value per unit volume (or lattice site) $V(\mu)$ is related to the specific heat. One expects further that, in equilibrium systems, the quantity $[-\log \mu - S(\mu)]/\sqrt{L V(\mu)}$ will in the $L \to \infty$ limit approach a standard normal random variable; this is an exercise for

one-dimensional systems in Ref. 29. It is easily verified that the same holds for the local equilibrium measure $\bar{\nu}_L$ considered here.

A natural question now is: in what respect is the distribution of this logarithm in nonequilibrium steady states, such as the NESS of the SSEP, different from or similar to the distribution in equilibrium systems? For example, are there characteristics of this distribution which can be related to physically measurable macroscopic quantities?

Although we do not know yet whether such questions have general answers, we have measured for small system sizes the quantity $V(\bar{\mu}_L)$:

$$V(\bar{\mu}_L) = \frac{1}{L}\left\langle [-\log \bar{\mu}_L(\tau_L) - S(\bar{\mu}_L)]^2 \right\rangle_{\bar{\mu}_L}. \tag{7.1}$$

Our results are plotted in Fig. 4 for $\rho_a = 1$ and $\rho_b = 0$; $V(\bar{\mu}_L)$ appears to approach a fixed value in the large L limit. For comparison we have also plotted there the corresponding quantity $V^*(\bar{\mu}_L)$ defined by

$$V^*(\bar{\mu}_L) = \frac{1}{L}\left\langle [-\log \bar{\nu}_L(\tau_L) - S(\bar{\nu}_L)]^2 \right\rangle_{\bar{\mu}_L}. \tag{7.2}$$

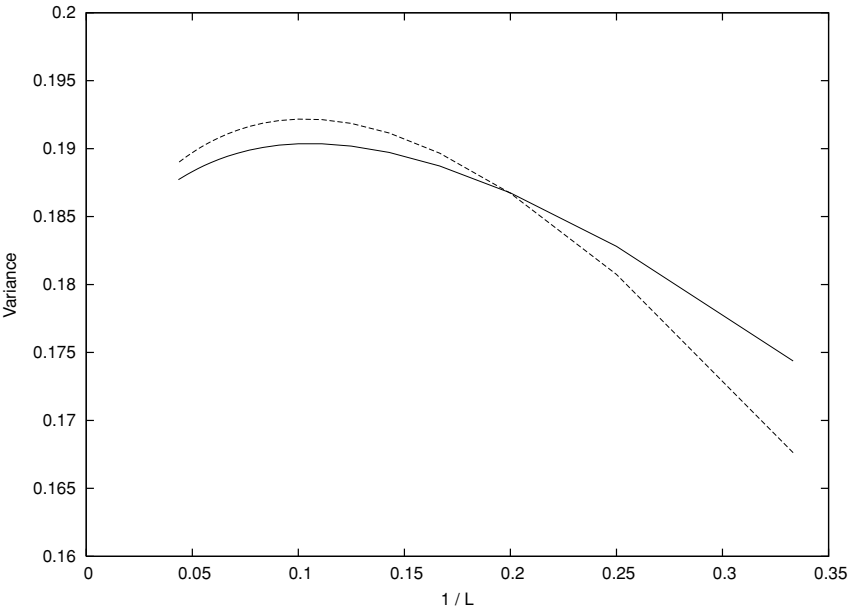

Fig. 4. Variances $V(\bar{\mu}_L)$ (solid line) and $V^*(\bar{\mu}_L)$ (dashed line), evaluated for small systems for the SSEP with $\rho_a = 1$ and $\rho_b = 0$, plotted against $1/L$. Equation (7.3) predicts a large L convergence to 0.179956.

In fact, by repeating the arguments of Secs. 5 and 6 one can show that the limiting values of these two quantities coincide and are given by

$$\lim_{L\to\infty} V(\bar{\mu}_L) = \int_0^1 dx\, F_1(x)(1-F_1(x)) \left(\log \frac{F_1(x)}{1-F_1(x)}\right)^2 + 2\int_0^1 dx \int_x^1 dy\, F_2(x,y) \left(\log \frac{F_1(x)}{1-F_1(x)}\right)\left(\log \frac{F_1(y)}{1-F_1(y)}\right). \quad (7.3)$$

The first term in (7.3) is the corresponding quantity for the local equilibrium system:

$$\lim_{L\to\infty} V(\bar{\nu}_L) = \lim_{L\to\infty} \frac{1}{L}\left\langle [-\log \bar{\nu}_L(\tau_L) - S(\bar{\nu}_L)]^2 \right\rangle_{\bar{\nu}_L} = \int_0^1 dx\, F_1(x)(1-F_1(x)) \left(\log \frac{F_1(x)}{1-F_1(x)}\right)^2. \quad (7.4)$$

The difference between (7.3) and (7.4) shows that in contrast to the entropy itself, for which local equilibrium gives correctly the leading order in L,[17] the two point correlations affect the leading order of the variance $LV(\bar{\mu}_L)$. For $\rho_a = 1$ and $\rho_b = 0$ the expression (7.3) takes the value $\pi^2/9 - 11/12 \approx 0.179956$, and the expression (7.4) the value $(\pi^2 - 6)/18 \approx 0.214978$.

APPENDIX A: CORRELATION FUNCTIONS IN THE SSEP

Correlation functions in the SSEP may be obtained via the *matrix method*.[4] One introduces matrices D and E and vectors $|V\rangle$ and $\langle W|$ which satisfy

$$DE - ED = D + E, \quad (A.1)$$

$$(\beta D - \delta E)|V\rangle = |V\rangle, \quad (A.2)$$

$$\langle W|(\alpha E - \gamma D) = \langle W|, \quad (A.3)$$

where α, β, γ, and δ were defined in Sec. 2. Then

$$\bar{\mu}_L(\tau_1, \ldots, \tau_L) = \frac{\langle W|(\tau_1 D + (1-\tau_1)E)\cdots(\tau_L D + (1-\tau_L)E)|V\rangle}{\langle W|(D+E)^L|V\rangle}, \quad (A.4)$$

and so (in this section we write $\langle\cdot\rangle_{\bar{\mu}_L} \equiv \langle\cdot\rangle_L$)

$$\langle \tau_{i_1} \cdots \tau_{i_k} \rangle_L = \frac{\langle W|(D+E)^{i_1-1} D (D+E)^{i_2-i_1-1} D \cdots D (D+E)^{L-i_k}|V\rangle}{\langle W|(D+E)^L|V\rangle}. \quad (A.5)$$

The normalization factor in (A.5) has been evaluated in Ref. 10:

$$\langle W|(D+E)^L|V\rangle = \frac{\Gamma(a+b+L)}{\Gamma(a+b)(\rho_a-\rho_b)^L}\langle W|V\rangle. \tag{A.6}$$

Now one obtains a recursion relation for the correlation functions: starting from the formula (A.5) for $\langle \tau_{i_1}\cdots\tau_{i_k}\tau_{i_{k+1}}\rangle_L$, one first commutes the rightmost factor of D to the extreme right in the product, using $[D, D+E] = D+E$, then writes $D|V\rangle = (\beta+\delta)^{-1}\big(|V\rangle + \delta(D+E)|V\rangle\big)$ (which is equivalent to (A.2)); the result is

$$\begin{aligned}\langle \tau_{i_1}\cdots\tau_{i_k}\tau_{i_{k+1}}\rangle_L = {} & \frac{(\rho_a-\rho_b)(L+b-i_{k+1})}{L+a+b-1}\langle \tau_{i_1}\cdots\tau_{i_k}\rangle_{L-1} \\ & + \rho_b\langle \tau_{i_1}\cdots\tau_{i_k}\rangle_L. \end{aligned}\tag{A.7}$$

Taking $k = 0$, 1, and 2 one recovers (2.3), (2.4), and (2.5); (A.7) may now be written in the form

$$\langle \tau_{i_1}\cdots\tau_{i_k}\tau_{i_{k+1}}\rangle_L = (\langle \tau_{i_{k+1}}\rangle_L - \rho_b)\big(\Delta\langle \tau_{i_1}\cdots\tau_{i_k}\rangle\big)_L + \langle \tau_{i_{k+1}}\rangle_L\langle \tau_{i_1}\cdots\tau_{i_k}\rangle_L, \tag{A.8}$$

where for any sequence $c_1, c_2, c_3, \ldots$ we write

$$(\Delta c)_L = c_{L-1} - c_L, \qquad L \geq 2. \tag{A.9}$$

The truncated correlation functions $t_{A,L} \equiv \langle \tau_{i_1}\cdots\tau_{i_k}\rangle_L^T$, where $A = \{i_1, \ldots, i_k\}$ with $k \geq 1$, are defined recursively by

$$\langle \tau_{i_1}\cdots\tau_{i_k}\rangle_L = \sum_{\pi\in\mathcal{P}(A)}\prod_{B\in\pi} t_{B,L}, \tag{A.10}$$

(see (5.2)). We claim that for $k \geq 1$ these functions satisfy the recursion

$$t_{A\cup\{i_{k+1}\},L} = (\langle \tau_{i_{k+1}}\rangle_L - \rho_b)\sum_{\pi\in\mathcal{P}(A)}\prod_{B\in\pi}(\Delta t_B)_L, \tag{A.11}$$

which, together with $t_{\{i\},L} = \langle \tau_i\rangle_L$, determines all the $t_{A,L}$. We will verify (A.11) below, after we have shown that it implies (1.1).

It follows from (A.11) that for $A = \{i_1, \ldots, i_k\}$, $t_{A,L} = v_L^k(\underline{i})$, where $\underline{i} = (i_1, \ldots, i_k)$ and $v_L^k(\underline{i})$ is a rational function of L and $i_1, \ldots, i_k$ which is a polynomial of degree 1 in each of the i_j. For $\underline{x} = (x_1, \ldots, x_k) \in \mathbb{R}^k$ let us define $u_L^k(\underline{x}) = v_L^k(L\underline{x})$; u is again rational and a polynomial of degree 1 in each x_j, so that we will obtain (1.1) if we show that $u_L^k = O(L^{-k+1})$. We show this by induction on k; for $k = 1$ it is an immediate consequence of (2.3). But if $u_L^k = O(L^{-k+1})$ for $k < k_0$ then from

$$(\Delta v^k)_L(L\underline{x}) = (\Delta u^k)_L(\underline{x}) + \big[u_{L-1}^k([1+(L-1)^{-1}]\underline{x}) - u_{L-1}^k(\underline{x})\big] \tag{A.12}$$

it follows that $(\Delta v^k)_L(L\underline{x}) = O(L^{-k})$ if $k < k_0$, and $u_L^k = O(L^{-k+1})$ for $k = k_0$ follows by evaluating (A.11) at $\underline{i} = L\underline{x}$.

Remark A.1: The recursion (A.11) implies a similar recursion for the F_k. Recall that the operator $\sum_{i=1}^{k} x_i \partial/\partial x_i$ acts on a monomial of degree d in $x_1, \ldots, x_k$ as multiplication by d, so that the operator $D_k = k - 1 + \sum_{i=1}^{k} x_i \partial/\partial x_i$ multiplies such a monomial by $k + d - 1$. Then

$$F_{k+1}(x_1, \ldots, x_k, x_{k+1}) = (F_1(x_{k+1}) - \rho_b) \sum_{\pi \in \mathcal{P}(\{1,\ldots,k\})} \prod_{B \in \pi} [D_{|B|} F_{|B|}]((x_i)_{i \in B}). \tag{A.13}$$

This follows by writing $t_{A,L} = \sum_d L^{-(k+d-1)} P_d + \text{h.o.t.}$, where P_d is homogeneous of degree d in $i_1, \ldots, i_k$ and h.o.t. denotes terms which are $O(L^{-k})$ after the substitutions $i_j = Lx_j$, $j = 1, \ldots, L$. We will not use this formula and so omit further details, but we do note that an easy consequence is that, for $k \geq 2$, F_k depends on α, β, γ, and δ only through an overall factor of $(\rho_a - \rho_b)^k$.

Proof of the recursion (A.11): To verify (A.11) we need a formula for the action of Δ on a product (see (A.9)). Suppose that $c^{(1)}, \ldots, c^{(k)}$ are sequences (i.e., $c^{(i)} = (c_L^{(i)})_{L=1}^{\infty}$) and that we multiply such sequences componentwise, so that $(c^{(1)} \cdots c^{(k)})_L = c_L^{(1)} \cdots c_L^{(k)}$. Then trivially

$$(1 + \Delta)\big(c^{(1)} \cdots c^{(k)}\big) = \big[(1 + \Delta)c^{(1)}\big] \cdots \big[(1 + \Delta)c^{(k)}\big], \tag{A.14}$$

and so with $X = \{1, 2, \ldots, k\}$,

$$\Delta(c^{(1)} \cdots c^{(k)}) = \sum_{\emptyset \neq Y \subset X} \prod_{i \in Y} \Delta c^{(i)} \prod_{j \in X \setminus Y} c^{(j)}. \tag{A.15}$$

For example,

$$\Delta\big(c^{(1)}c^{(2)}\big) = \Delta c^{(1)}c^{(2)} + c^{(1)}\Delta c^{(2)} + \Delta c^{(1)}\Delta c^{(2)}, \tag{A.16}$$

$$\begin{aligned}\Delta\big(c^{(1)}c^{(2)}c^{(3)}\big) = {} & \Delta c^{(1)}c^{(2)}c^{(3)} + c^{(1)}\Delta c^{(2)}c^{(3)} + c^{(1)}c^{(2)}\Delta c^{(3)} \\ & + \Delta c^{(1)}\Delta c^{(2)}c^{(3)} + \Delta c^{(1)}c^{(2)}\Delta c^{(3)} + c^{(1)}\Delta c^{(2)}\Delta c^{(3)} \\ & + \Delta c^{(1)}\Delta c^{(2)}\Delta c^{(3)}.\end{aligned} \tag{A.17}$$

We now verify (A.11); the case $k = 1$ is precisely (A.8) for $k = 1$, and we proceed by induction on k. We use (A.10) to write $\langle \tau_{i_1} \cdots \tau_{i_k} \tau_{i_{k+1}} \rangle_L$, the left hand side of (A.8), in terms of truncated correlations, separating the terms in which i_{k+1} is grouped with some element of a partition of A from those in which $\{i_{k+1}\}$ is an element of the partition of $A \cup \{i_{k+1}\}$:

$$\sum_{\pi \in \mathcal{P}(A)} \sum_{B \in \pi} t_{B \cup \{i_{k+1}\}, L} \prod_{\substack{C \in \pi \\ C \neq B}} t_{C,L} + t_{\{i_{k+1}\},L} \sum_{\pi \in \mathcal{P}(A)} \prod_{B \in \pi} t_{B,L}. \tag{A.18}$$

On the other hand, with (A.10) the right hand side of (A.8) becomes

$$(\langle\tau_{i_{k+1}}\rangle_L - \rho_b) \sum_{\pi\in\mathcal{P}(A)} \Big(\Delta \prod_{B\in\pi} t_B\Big)_L + \langle\tau_{i_{k+1}}\rangle_L \sum_{\pi\in\mathcal{P}(A)} \prod_{B\in\pi} t_{B,L}. \tag{A.19}$$

Since (A.18) and (A.19) are the two sides of (A.8) we may equate these expressions to obtain

$$\sum_{\pi\in\mathcal{P}(A)} \sum_{B\in\pi} t_{B\cup\{i_{k+1}\},L} \prod_{\substack{C\in\pi\\ C\neq B}} t_{C,L} = (\langle\tau_{i_{k+1}}\rangle_L - \rho_b) \sum_{\pi\in\mathcal{P}(A)} \Big(\Delta \prod_{B\in\pi} t_B\Big)_L. \tag{A.20}$$

On the right hand side of (A.20) we use (A.15) to write

$$\sum_{\pi\in\mathcal{P}(A)} \Big(\Delta \prod_{B\in\pi} t_B\Big)_L = \sum_{\pi\in\mathcal{P}(A)} \sum_{\emptyset\neq\sigma\subset\pi} \prod_{C\in\sigma} (\Delta t_C)_L \prod_{C\in\pi\setminus\sigma} t_{C,L}. \tag{A.21}$$

On the left side of (A.20) the term with $\pi = \{A\}$ is just $t_{A\cup\{i_{k+1}\},L}$; we take the remaining terms to the other side of the equation and in these terms use the induction assumption to write

$$t_{B\cup\{i_{k+1}\},L} = (\langle\tau_{i_{k+1}}\rangle_L - \rho_b) \sum_{\sigma\in\mathcal{P}(B)} \prod_{C\in\sigma} (\Delta t_C)_L. \tag{A.22}$$

After these manipulations, (A.20) becomes

$$\begin{aligned} t_{A\cup\{i_{k+1}\},L} = (\langle\tau_{i_{k+1}}\rangle_L - \rho_b)\Big[&\sum_{\pi\in\mathcal{P}(A)} \sum_{\emptyset\neq\sigma\subset\pi} \prod_{C\in\sigma} (\Delta t_C)_L \prod_{C\in\pi\setminus\sigma} t_{C,L} \\ &- \sum_{\substack{\pi\in\mathcal{P}(A)\\ \pi\neq\{A\}}} \sum_{B\in\pi} \sum_{\sigma\in\mathcal{P}(B)} \prod_{C\in\sigma} (\Delta t_C)_L \prod_{\substack{C\in\pi\\ C\neq B}} t_{C,L}\Big]. \end{aligned} \tag{A.23}$$

We now reorganize this expression. In the first sum we separate the term $\pi = \{A\}$, which is simply $(\Delta t_A)_L$ (since necessarily $\sigma = \{A\}$ also); in the remaining terms of this sum we relabel π as π', with $\pi' \neq \{A\}$. Now every term in the second sum is labeled by a partition π, a distinguished set $B \in \pi$, and a further partition σ of B; this data clearly gives rise to a new partition π' of A, $\pi' = (\pi \cup \sigma) \setminus \{B\}$, and a distinguished subset σ of π'; note that $\sigma \neq \emptyset$ since σ is a partition of B and $\sigma \neq \pi'$ since $\pi \neq \{A\}$ and hence $|\pi| \geq 2$. Thus

$$\begin{aligned} t_{A\cup\{i_{k+1}\},L} = (\langle\tau_{i_{k+1}}\rangle_L - \rho_b)\Big[&(\Delta t_A)_L \\ &+ \sum_{\substack{\pi'\in\mathcal{P}(A)\\ \pi'\neq\{A\}}} \Big(\sum_{\emptyset\neq\sigma\subset\pi'} \prod_{C\in\sigma} (\Delta t_C)_L \prod_{C\in\pi'\setminus\sigma} t_{C,L} \\ &- \sum_{\emptyset\neq\sigma\not\subseteq\pi'} \prod_{C\in\sigma} (\Delta t_C)_L \prod_{C\in\pi'\setminus\sigma} t_{C,L}\Big)\Big]. \end{aligned} \tag{A.24}$$

In the sum over π' only the terms with $\sigma = \pi'$ survive, leading to (A.11):

$$t_{A\cup\{i_{k+1}\},L} = (\langle\tau_{i_{k+1}}\rangle_L - \rho_b) \sum_{\pi'\in\mathcal{P}(A)} \prod_{B\in\pi'} (\Delta t_B)_L. \tag{A.25}$$

APPENDIX B: THE COEFFICIENTS $d(M)$

In this appendix we derive the two properties of the combinatorial factors $d(M)$ (see (5.17)) which are needed in Sec. 6: that $d(M) = 0$ if G_M is not connected, and that $d(M) = (-1)^{k+1}$ if G_M is a cycle on k vertices. Our approach is to relate $d(M)$ to the number of colorings of the graph G_M. The condition that only monomials M for which $m_i(M) \geq 2$ for all $i \in D_M$ occur in (5.16) implies that every component of G_M contains at least two vertices, and we assume that all graphs considered in what follows satisfy this condition.

For any graph G we let $\bar{c}_n(G)$ be the number of n-colorings of G, where an *n-coloring* of G is an assignment of colors to the vertices of G, using exactly n colors, in such a way that adjacent vertices are given distinct colors. For example, if G is a cycle on four vertices then $\bar{c}_4(G) = 24$, $\bar{c}_3(G) = 12$, and $\bar{c}_2(G) = 2$. Note that the condition that every component of G have at least two vertices implies that $\bar{c}_1(G) = 0$. We also define

$$\bar{d}(G) = \sum_{n=2}^{\infty} \frac{(-1)^{n+1}}{n(n-1)} \bar{c}_n(G). \tag{B.1}$$

Suppose now that M is a monomial occurring in (5.16), say $M = \prod_B t_B^{k_B}$ with the t_B distinct; the graph G_M has $\sum_B k_B$ vertices, and we will denote the k_B vertices corresponding to B by $v_{B,1}, \ldots, v_{B,k_B}$. Recall that $c_n(M)$ is the number of n-tuples $\underline{\pi} = (\pi_1, \ldots, \pi_n)$, with $\pi_i \in \tilde{\mathcal{P}}(D_M)$, such that $M = \prod_{j=1}^n \prod_{C\in\pi_j} t_C$. An n-coloring of G_M immediately yields such a $\underline{\pi}$, by taking π_i to be the set of all B such that some $v_{B,j}$ is assigned color i. Each $\underline{\pi}$ arises in this way from $\prod_B k_B!$ distinct colorings, since for each B we may permute the colors assigned to the $v_{B,j}$ without changing $\underline{\pi}$. Thus $\bar{c}_n(G_M) = c_n(M) \prod_B k_B!$, and

$$\bar{d}(G_M) = d(M) \prod_B k_B! \,. \tag{B.2}$$

We next derive a recursion relation for $\bar{d}(G)$. We first select some vertex v of G, and let N_v be the set of vertices of G which are adjacent to v. Every n-coloring of G induces a partition λ of N_v, where two vertices are in the same set of the partition iff they have the same color; note that vertices in N_v which are adjacent cannot lie in the same element of λ. Conversely, given any partition λ of N_v satisfying this latter restriction we define the graph G_λ by (i) removing from G the vertex v and all edges adjacent to it, (ii) collapsing all vertices belonging to a

single subset $B \in \lambda$ into a single vertex w_B in G_λ (which may give a multi-graph; if so, we replace any multiple edges by a single edge), and (iii) joining each pair w_B, $w_{B'}$ of new vertices produced in this way by an edge. Then every n-coloring of G is obtained by choosing λ and then either (a) choosing one of the n colors to assign to v and using the remaining colors for some $(n-1)$-coloring of G_λ, or (b) choosing an n-coloring of G_λ, then choosing one of the $n - |\lambda|$ colors not used on the new vertices w_B to assign to v. This leads to the recursion

$$\bar{c}_n(G) = \sum_\lambda [n\bar{c}_{n-1}(G_\lambda) + (n - |\lambda|)\bar{c}_n(G_\lambda)]. \tag{B.3}$$

Then if no G_λ is 1-colorable, so that $\bar{c}_{n-1}(G_\lambda) = 0$ if $n = 2$,

$$\begin{aligned}
\bar{d}(G) &= \sum_{n=2}^{\infty} \frac{(-1)^{n+1}}{n(n-1)}\, \bar{c}_n(G) \\
&= \sum_\lambda \Big[\sum_{n=2}^{\infty} \frac{(-1)^{n+1}}{(n-1)(n-2)} (n-2)\bar{c}_{n-1}(G_\lambda) \\
&\quad + \sum_{n=2}^{\infty} \frac{(-1)^{n+1}}{n(n-1)} (n - |\lambda|)\bar{c}_n(G_\lambda) \Big] \\
&= \sum_\lambda \sum_{n=2}^{\infty} \frac{(-1)^{n+1}}{n(n-1)} [n - |\lambda| - (n-1)]\bar{c}_n(G_\lambda) \\
&= \sum_\lambda (1 - |\lambda|)\bar{d}(G_\lambda).
\end{aligned} \tag{B.4}$$

This is the desired recursion.

As a first consequence of (B.4) we show that if G is a disconnected graph in which every component has at least two vertices, then $\bar{d}(G) = 0$. We argue by induction on the number n of vertices of G; certainly $n \geq 4$. If $n = 4$ then G has two components, each a single edge joining two vertices, and an application of (B.4) shows that $\bar{d}(G) = 0$ (there will be only one partition λ, with $|\lambda| = 1$, in the sum). We now argue by induction on n; if we apply (B.4) with any vertex v of G, every $\bar{d}(G_\lambda)$ on the right hand side will vanish by the induction assumption unless the "new" component of G_λ has a single vertex, in which case $|\lambda| = 1$; thus $\bar{d}(G) = 0$.

As a second application we compute $\bar{d}(G)$ for G a cycle. First note that if G is a graph with 2 vertices joined by an edge then $\bar{d}(G) = -1$, by a simple direct calculation. If G is a cycle with $k \geq 3$ vertices and v is any vertex of G then N_v contains two vertices, say $N_v = \{w_1, w_2\}$, and the sum in (B.4) has one term $\lambda = \lambda_0 \equiv \{\{w_1\}, \{w_2\}\}$ and, if $k \geq 4$ so that w_1 and w_2 are not adjacent, also

one with $\lambda = \{N_v\}$. The latter term, even if present, does not contribute since $|\lambda| = 1$, so $\bar{d}(G) = -\bar{d}(G_{\lambda_0})$. But G_{λ_0} is a cycle with $k-1$ vertices or, if $k = 3$, the two-vertex graph considered above; thus $\bar{d}(G) = (-1)^{k+1}$ by induction on k.

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