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1993 J. Phys. A: Math. Gen. 26 1179

(http://iopscience.iop.org/0305-4470/26/5/035)

J. Phys. A: Math. Gen. 26 (1993) 1179–1191. Printed in the UK

Log-gases, random matrices and the Fisher–Hartwig conjecture

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Received 25 August 1992

Abstract. Some features of the probability $E(n, \mathcal{R})$ of a region $\mathcal{R}$ in certain log-potential systems containing precisely n particles are noted. First, it is shown that a quantity analogous to $E(n, \mathcal{R})$ for a new solvable two-component log-gas can be expressed in terms of the Toeplitz determinant discretization of a Fredholm determinant which occurs in the calculation of $E(n, \mathcal{R})$ for Hermitian random matrices. Second, the first two terms of the asymptotic large-$\mathcal{R}$ expansion of $E(n, \mathcal{R})$ for complex random matrices, when $\mathcal{R}$ is a disk, are derived by using an electrostatic/thermodynamic argument based on an analogy with the two-dimensional one-component plasma. Finally, by using the Fisher–Hartwig 'conjecture' from the theory of Toeplitz determinants, the asymptotics of $E(0, \mathcal{R})$ for a class of one-dimensional lattice systems is shown to obey a sum rule which has been conjectured to be applicable to all fluid systems with exclusively mobile species.

1. Introduction

A quantity which can be used to characterize statistical systems is the distribution of the spacing between nearest-neighbour constituents of the system. The energy excitations of heavy nuclei (see e.g. [1]) and the times of arrival and/or service in a queueing system (see e.g. [2]) are examples of statistical systems which are often characterized in this way. As another example, the spacing between oppositely charged species in two-component log-potential Coulomb systems can be used to specify the phase of the system [3].

For systems in which the constituents can be ordered linearly, the distribution of the spacing between nearest neighbours can be calculated, by differentiation, from the probability that there are no constituents within a prescribed interval. One of the most important calculations of the latter and related probabilities is for the eigenvalue distribution of orthogonal, unitary and symplectic ensembles of random matrices [1].

A fundamental quantity in these random matrix calculations is the Fredholm determinant

$$\Delta(z, t) := \det(\mathbf{1} - z\mathsf{K}) \tag{1.1}$$

where K is the integral operator on the interval $[-t, t]$ with kernel

$$\frac{\sin \pi(x - y)}{\pi(x - y)}. \tag{1.2}$$

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0305-4470/93/051179+13$07.50

For Hermitian random matrices, the determinant (1.1) is related to the probability $E(n, 2t)$ that exactly n eigenvalues lie in the interval $[-t, t]$ by the formula [1]

$$E(n;2t) = \frac{(-1)^n}{n!}\frac{\partial^n}{\partial z^n}\Delta(z,t)\bigg|_{z=1}. \tag{1.3}$$

For arbitrary values of z, the determinant (1.1) is of mathematical interest since it satisfies a nonlinear equation of the Painlevé type [4–7]. This property has been used to calculate the large-t asymptotic expansion of $E(n;2t)$ [8]. In section 2 of this paper we will give a physical interpretation to the Toeplitz determinant discretization of the Fredholm determinant (1.1) for $-1 < z < 0$. This complements the physical interpretation of the same Toeplitz determinant discretization with $z = 1$ given recently in [9]. Explicitly, we will calculate the general (n_1, n_2)-particle distribution function for an asymmetric two-component lattice gas in which the species interact via the logarithmic potential. From this, we can show that the probability a prescribed number of lattice points is free of the most dilute of the two-components is given in terms of the Toeplitz determinant discretization of (1.1).

The quantity analogous to $E(n;2t), E(n;\alpha)$ say, for random complex matrices has recently attracted attention [10–12]. Here we require the probability of exactly n eigenvalues in a disk of radius α in the complex eigenvalue plane. The large-α asymptotic expansion of $E(n;\alpha)$ is given in [12]. In section 3 of this paper we will use a well known [13] analogy between the probability distribution function for the eigenvalues of random complex matrices, and the Boltzmann factor of the two-dimensional one-component plasma at a special value of the coupling, to rederive the leading terms of this expansion. The derivation, which is based on an electrostatic/thermodynamic argument, gives an asymptotic expansion which should remain valid for the plasma system at all couplings.

The plasma systems studied in sections 2 and 3 have an immobile neutralizing background charge density. This feature is responsible for the leading behaviours

$$E(0;2t) \sim e^{-c_1 t^2} \qquad \text{and} \qquad E(0;\alpha) \sim e^{-c_2\alpha^4} \tag{1.4}$$

where in both cases the exponent is proportional to the square of the 'volume' of the particle-free region. For fluid systems with exclusively mobile species, the leading behaviours analogous to (1.4) are expected to have the exponent directly proportional to the volume of the particle-free region [9]. More precisely, consider a one-dimensional lattice gas of M sites with lattice spacing τ, and suppose that the grand partition function Ξ has the large-M behaviour

$$\Xi \sim e^{M\tau\beta P + \omega\log M + O(1)} \tag{1.5}$$

where $\tau\beta P$ denotes the dimensionless pressure. Then the conjecture of [9] states that for large-p,

$$E(0;p) \sim e^{-p\tau\beta P + \omega\log p + O(1)}. \tag{1.6}$$

The aim in section 4 is to verify (1.6) for a class of fluid systems with, in general, n-body potentials. These fluid systems are defined by a special Toeplitz determinant structure for their Boltzmann factor. The conjecture (1.6) is verified by using the so-called Fisher–Hartwig 'conjecture' (formula) [14–16], which gives terms up to and including O(1) in the asymptotic expansion of Toeplitz determinants with discontinuous generating functions. Furthermore, it is found that the terms O(1) in (1.5) and (1.6) agree; a property we conjecture to hold true in general.

2. Physical interpretation of the Toeplitz determinant discretization of $\Delta(z,t)$

2.1. A solvable asymmetric log-gas

Our first objective is to compute the correlation functions for an asymmetric two-component log-gas confined to a one-dimensional lattice. The correlations will then be used to calculate $E_{-}(0;p)$—the probability that an interval of p lattice sites is free of the negatively charged particles. This probability involves the Toeplitz determinant discretization of $\Delta(z,t)$.

Suppose the positively charged particles have density ρ_+, and the negatively charged particles density ρ_-, where $\rho_- < \rho_+$. Charge neutrality is achieved by introducing a uniform background charge of density η such that

$$\rho_+ - \rho_- = \eta. \tag{2.1}$$

Let the charges be restricted to one of two interlacing sublattices which lie along the X-axis: $\{\tau n\}_{n=-M/2+1,\dots,M/2}$ for the positive charges and $\{\tau(m-\phi)\}_{m=-M/2+1,\dots,M/2}$ for the negative charges (for convenience M is taken to be even). Also, impose periodic boundary conditions in the direction of the lattice, period τM.

To facilitate the exact calculation, we have found it necessary to first place the system a finite distance ε from a metal wall and to use the grand canonical ensemble in which the density ρ_+ is controlled by the fugacity ξ_+ and the density ρ_- is controlled by the fugacity ξ_-. With the metal occupying the region $y \geqslant \varepsilon$ in the XY plane, the pair potential experienced by a particle of charge q at $(x,0)$ due to a particle of charge q' at $(x',0)$ is given by

$$\phi(x,x') = -qq' \log\left|\frac{\sin \pi(x-x')/L}{\sin \pi(x-x'+2\mathrm{i}\varepsilon)/L}\right| \tag{2.2}$$

where $L = \tau M$, and there is a self-energy

$$\phi_s(x) = \tfrac{1}{2}q^2 \log|\sin(2\pi\mathrm{i}\varepsilon/L)|. \tag{2.3}$$

In addition to the particles, we require a uniform background of charge density $-q\eta$. Supposing that there are N_+ positive and N_- negative charges, a short calculation using (2.2) gives that the energy due to the particle–background and background–background interaction is

$$-2\pi\eta q^2\varepsilon(N_+ - N_-) + \pi(\eta q)^2\varepsilon L. \tag{2.4}$$

From (2.2)–(2.4) we can write down the Boltzmann factor for this system. At the special value of the coupling $q^2/kT = 2$ the Boltzmann factor can be written as a Cauchy double alternant determinant. The corresponding grand partition function $\Xi_2(a,b)$, generalized to include position-dependent fugacities $\zeta_+ \mapsto \zeta_+ a(n)$, $\zeta_- \mapsto \zeta_- b(m)$, can then be recognized as in expansion of a particular block Toeplitz determinant (details of these steps are given in [17], where a similar model in a two-dimensional domain is considered). The final result is

$$\Xi_2(a,b) = \mathrm{e}^{-2\pi\varepsilon\eta^2/L}\det\left(\mathbf{1}_{2M} + \begin{bmatrix} \mathsf{K}_1(a) & \mathsf{K}_2(a) \\ \mathsf{K}_3(b) & \mathsf{K}_4(b) \end{bmatrix}\right. \tag{2.5a}$$

where

$$\mathsf{K}_1(a) = \frac{\pi \mathrm{i}}{L}\tilde{\zeta}_+ \left[\frac{a(j)}{\sin \pi(j - j' + 2\mathrm{i}\varepsilon/\tau)/M}\right]_{j,j'=1,\ldots,M} \tag{2.5b}$$

$$\mathsf{K}_2(a) = \frac{\pi \mathrm{i}}{L}\tilde{\zeta}_+ \left[\frac{a(j)}{\sin \pi(j - j' + \phi)/M}\right]_{j,j'=1,\ldots,M} \tag{2.5c}$$

$$\mathsf{K}_3(b) = -\frac{\pi \mathrm{i}}{L}\tilde{\zeta}_- \left[\frac{b(j)}{\sin \pi(j - j' - \phi)/M}\right]_{j,j'=1,\ldots,M} \tag{2.5d}$$

$$\mathsf{K}_4(b) = -\frac{\pi \mathrm{i}}{L}\tilde{\zeta}_- \left[\frac{b(j)}{\sin \pi(j - j' - 2\mathrm{i}\varepsilon/\tau)/M}\right]_{j,j'=1,\ldots,M} \tag{2.5e}$$

$\mathbf{1}_n$ denotes the identity matrix of order n and

$$\tilde{\zeta}_+ = \mathrm{e}^{4\pi\varepsilon\eta}\zeta_+ \qquad \tilde{\zeta}_- = \mathrm{e}^{-4\pi\varepsilon\eta}\zeta_- . \tag{2.5f}$$

We note in passing that by rearranging the rows and columns in (2.5a) we can obtain a block anti-cyclic matrix. With $a = b = 1$ this matrix can be diagonalized to give an explicit factorization of the grand partition function:

$$\Xi_2 = \mathrm{e}^{-2\pi\varepsilon\eta^2 L} \prod_{k=1}^{M} \left[\left(1 + \frac{\pi\tilde{\zeta}_+}{\tau \sinh 2\pi\varepsilon/\tau}\mathrm{e}^{-4\pi(\varepsilon/\tau)(k-(M+1)/2)/M}\right)\right.$$
$$\left. \times \left(1 + \frac{\pi\tilde{\zeta}_-}{\tau \sinh 2\pi\varepsilon/\tau}\mathrm{e}^{4\pi(\varepsilon/\tau)(k-(M+1)/2)/M}\right) + \frac{(\pi/\tau)^2\tilde{\zeta}_+\tilde{\zeta}_-}{\sin^2 \pi\phi}\right]. \tag{2.6}$$

The distribution of the zeros of (2.6) for $\zeta_+ = \zeta_-$ has recently been analysed by Smith [18].

2.2. *The correlation functions*

By extending the reasoning given in [17] and [19], it follows from (2.5) that the (j_1, j_2)-particle (dimensionless) distribution function for j_1 positively charged particles at $n_1, \ldots, n_{j_1}$ and j_2 positively charged particles at $m_1, \ldots, m_{j_2}$ is given by

$$\rho(n_1, \ldots, n_{j_1}; m_1, \ldots, m_{j_2})$$
$$= \det \begin{bmatrix} [G_{++}(n_j - n_{j'})]_{j,j'=1,\ldots,j_1} & [G_{+-}(n_j - m_{j'})]_{\substack{j=1,\ldots,j_1 \\ j'=1,\ldots,j_2}} \\ [G_{-+}(m_j - n_{j'})]_{\substack{j=1,\ldots,j_2 \\ j'=1,\ldots,j_1}} & [G_{--}(m_j - m_{j'})]_{j,j'=1,\ldots,j_2} \end{bmatrix} \tag{2.7}$$

where, in the thermodynamic limit $M \to \infty$, $G_{ss'}$ is specified by the set of four equations (for $s_1, s_3 = +, -$)

$$G_{s_1 s_3}(n_1 - n_3) + \tilde{\zeta}_{s_1}\frac{\mathrm{i}^{s_1}}{\tau} \sum_{n_2=-\infty}^{\infty} \frac{G_{s_1 s_3}(n_2 - n_3)}{n_1 - n_2 + 2\mathrm{i}(\varepsilon/\tau)\mathrm{sgn}(s_1)}$$
$$+ \tilde{\zeta}_{s_1}\frac{\mathrm{i}^{s_1}}{\tau} \sum_{n_2=-\infty}^{\infty} \frac{G_{(-s_1)s_3}(n_2 - n_3)}{n_1 - n_2 + \mathrm{sgn}(s_1)\phi}$$
$$= \tilde{\zeta}_{s_1}\frac{\mathrm{i}^{s_1}}{\tau}\left(\frac{\delta_{-s_1,s_3}}{n_1 - n_3 + \mathrm{sgn}(s_1)\phi} + \frac{\delta_{s_1,s_3}}{n_1 - n_3 + 2\mathrm{i}(\varepsilon/\tau)\mathrm{sgn}(s_1)}\right). \tag{2.8}$$

The equations (2.8) can be solved by using Fourier series, as detailed in [17]. Doing this, and taking the limit $\varepsilon \to \infty$ so as to remove the metal wall, we obtain

$$G_{++}(m) = \delta_{m,0} - \lambda_1 I(m) \qquad G_{+-}(m) = -\lambda_1 I(m+\phi)$$
$$G_{-+}(m) = \lambda_2 I(-(m+\phi)) \qquad G_{--}(m) = \lambda_2 I(-m) \tag{2.9a}$$

where

$$\lambda_1 = \frac{1-\tau\rho_+}{1-\tau\eta} \qquad \lambda_2 = \frac{\tau\rho_-}{1-\tau\eta} \tag{2.9b}$$

and

$$I(m) = \int_{\eta\tau}^{1} \mathrm{e}^{-2\pi i m t}\mathrm{d}t. \tag{2.9c}$$

The exact result (2.7), (2.9) complements the exact evaluation of the distribution functions given by Cornu and Jancovici [20] for the continuous two-dimensional domain version of this model.

2.3. *Probability of an interval free of the negative charges*

Let $h_-(p)$ denote the probability that the negative charges are excluded from an interval of p lattice sites. Then for any fluid system defined on a one-dimensional lattice [9]

$$h_-(p) = \sum_{\ell=0}^{p} \frac{(-1)^\ell}{\ell!} \sum_{m_1=1}^{p} \cdots \sum_{m_\ell=1}^{p} \rho_-(m_1,\ldots,m_\ell) \tag{2.10}$$

where $\rho_-(m_1,\ldots,m_\ell)$ denotes the dimensionless distribution function for ℓ particles of negative charge at $m_1,\ldots,m_\ell$. For the present model, from (2.7),

$$\rho_-(m_1,\ldots,m_\ell) = \det[G_{--}(m_j - m_{j'})]_{j,j'=1,\ldots,\ell} \tag{2.11}$$

and (2.10) can be recognized as an expanded form of a Toeplitz determinant. Thus

$$h_-(p) = \det[\delta_{j,k} - G_{--}(j-k)]_{j,k=1,\ldots,p} \tag{2.12}$$

which, after some straightforward rearranging using (2.9a), gives the desired relationship with the discretization of the Fredholm determinant (1.1):

$$h_-(p) = (1-\lambda_2)^p \det\left[\delta_{j,k} + \frac{\lambda_2}{1-\lambda_2}\frac{\sin\pi\eta\tau(j-k)}{\pi(j-k)}\right]_{j,k=1,\ldots,p}. \tag{2.13}$$

3. Asymptotics of $E(n;\alpha)$ for random complex matrices

3.1. The Coulomb gas analogy

Consider a two-dimensional one-component plasma consisting of N mobile positively charged particles (strength q), with positions specified by the complex coordinate $z_j = x_j + \mathrm{i}y_j, j = 1,\ldots,N$. Assume a neutralizing background, in the shape of a disk of radius $\sqrt{N}$ centred at the origin, with charge density $-q/\pi$. The Boltzmann factor for the system is, up to a multiplicative constant (see e.g. [21]),

$$\prod_{\ell=1}^{N} \mathrm{e}^{-\Gamma|z_\ell|^2/2} \prod_{1\leqslant j<k\leqslant N} |z_k - z_j|^\Gamma \tag{3.1}$$

where

$$\Gamma := q^2/kT.$$

With $\Gamma = 2$, (3.1) is identical (up to normalization) to the probability distribution function for the eigenvalues of random complex matrices [13]. In this special case, quantities such as $E(n;\alpha)$—the probability that a randomly chosen point in the complex eigenvalue plane has no eigenvalues within a radius α—can be calculated exactly [12]. From these exact results the asymptotic expansion of $E(0;\alpha)$ and $E(n;\alpha)/E(0;\alpha)$ for large-α can be obtained [12].

It is the objective of this section to reproduce the leading two terms of these expansions using an electrostatic/thermodynamic argument. Since this argument is applicable for all values of Γ, predictions for the behaviour of the asymptotic expansions as functions of Γ are also obtained.

3.2. The electrostatic/thermodynamic argument

Let $D_\alpha(C_\alpha)$ denote the disk (circle) of radius α centred at the origin in the XY plane, which forms the hole in the plasma. The physical basis of our argument is that in the macroscopic hole size limit $\alpha \to \infty$, the plasma behaves like a perfect conductor. Thus the total charge $-q(\alpha^2 - n)$ inside the hole, due to the uniform background and n mobile charges (n is assumed fixed), will be exactly cancelled by an induced surface charge density, of total charge $q(\alpha^2 - n)$, which forms on the boundary of the hole. Furthermore, due to the rotational symmetry of the disk-shaped hole, the induced surface charge will be uniform, and thus have constant charge density $q\sigma = q(\alpha^2 - n)/(2\pi\alpha)$.

Suppose initially that there are no particles in the hole (i.e. $n = 0$). According to a heuristic formula of Dyson [22], $E(0;\alpha)$ is related to the electrostatic energy $q^2 V_1(\alpha)$ of the hole-induced surface charge system, and its entropy

$$V_2(\alpha) := \int_{C_\alpha} \sigma \log\sigma \,\mathrm{d}s \tag{3.2a}$$

$$= 2\pi\alpha\sigma\log\sigma \tag{3.2b}$$

by the formula

$$E(0;\alpha) \sim \exp(-\Gamma V_1(\alpha) - (1 - \Gamma/4)V_2(\alpha)). \tag{3.3}$$

(Note the factor $(1-\Gamma/4)$ replaces $(1-\Gamma/2)$ in [22] since here the plasma system is two-dimensional.)

The electrostatic energy of the hole-induced surface charge system consists of the background–background energy

$$U_1 := -\frac{q^2}{2}\left(\frac{1}{\pi}\right)^2 \int_{D_\alpha}\int_{D_\alpha} \log|\boldsymbol{r}_1-\boldsymbol{r}_2|\,\mathrm{d}\boldsymbol{r}_1\,\mathrm{d}\boldsymbol{r}_2 \tag{3.4a}$$

the background-induced surface charge energy

$$U_2 := q^2\left(\frac{1}{\pi}\right)\left(\frac{\alpha}{2\pi}\right)\int_0^{2\pi}\alpha\,\mathrm{d}\theta_2\int_{D_\alpha}\log|\boldsymbol{r}_1-\alpha\mathrm{e}^{\mathrm{i}\theta_2}|\,\mathrm{d}\boldsymbol{r}_1 \tag{3.4b}$$

and the surface-charge–surface-charge energy

$$U_3 := \frac{q^2}{2}\left(\frac{\alpha}{2\pi}\right)^2\int_0^{2\pi}\int_0^{2\pi}\log|\alpha\mathrm{e}^{\mathrm{i}\theta_1}-\alpha\mathrm{e}^{\mathrm{i}\theta_2}|\alpha\,\mathrm{d}\theta_1\,\alpha\,\mathrm{d}\theta_2 \tag{3.4c}$$

so that

$$q^2V_1(\alpha) = U_1+U_2+U_3. \tag{3.4d}$$

Evaluating the integrals in (3.4*a*)–(3.4*c*) gives

$$V_1(\alpha) = \alpha^4/8. \tag{3.5}$$

Substituting (3.5) and (3.2*b*) (with $\sigma=\alpha/2\pi$) in (3.3) we obtain the asymptotic expansion

$$E(0;\alpha) \sim \exp(-\Gamma\alpha^4/8-(1-\Gamma/4)\alpha^2\log\alpha). \tag{3.6}$$

For $\Gamma=2$, this agrees with the first two terms of the expansion obtained rigorously from the exact expression for $E(0;\alpha)$ [10, 12].

To study the asymptotics of $E(n;\alpha)/E(0;\alpha)$ we introduce an ansatz which, considering that there are now n mobile charges in the hole, is a natural generalization of (3.3):

$$\frac{E(n;\alpha)}{E(0;\alpha)} \sim \exp\{-\Gamma[V_1(n,\alpha)-V_1(0,\alpha)]-(1-\Gamma/4)[V_2(n,\alpha)-V_2(0,\alpha)]\}$$
$$\times\int_{R^2\ldots}\int_{R^2}\mathrm{e}^{-\Gamma E(\boldsymbol{r}_1,\ldots,\boldsymbol{r}_n)}\,\mathrm{d}\boldsymbol{r}_1\ldots\mathrm{d}\boldsymbol{r}_n \tag{3.7}$$

where $V_1(n,\alpha)$ is the electrostatic energy of the hole-induced surface charge (the latter depends on n) system, $V_2(n,\alpha)$ is the entropy of the induced surface charge and $q^2E(\boldsymbol{r}_1,\ldots,\boldsymbol{r}_n)$ is the electrostatic energy of the particle–background (E_1), particle-induced surface charge (E_2) and particle–particle (E_3) interaction.

If we replace the prefactors $(\alpha/2\pi)$ and $(\alpha/2\pi)^2$ in (3.4*b*) and (3.4*c*) by $(\alpha^2-n)/(2\pi\alpha)$ and $[(\alpha^2-n)/(2\pi\alpha)]^2$ respectively, then

$$q^2V_1(n,\alpha) = U_1+U_2+U_3 \tag{3.8}$$

while from (3.2*b*) we obtain

$$V_2(n,\alpha) \sim -(\alpha^2 - n)\log\alpha. \tag{3.9}$$

Furthermore, with the n particles at $\boldsymbol{r}_1,\ldots,\boldsymbol{r}_n$ within the disk D_α,

$$E_1 = q^2\frac{1}{\pi}\sum_{j=1}^{n}\int_{D_\alpha}\log|\boldsymbol{r}-\boldsymbol{r}_j|\,\mathrm{d}\boldsymbol{r} \tag{3.10a}$$

$$E_2 = -q^2(\alpha^2-n)/(2\pi\alpha)\sum_{j=1}^{n}\int_0^{2\pi}\log|\boldsymbol{r}_j-\alpha\mathrm{e}^{\mathrm{i}\theta}|\alpha\,\mathrm{d}\theta \tag{3.10b}$$

$$E_3 = -q^2\sum_{1\leqslant j<k\leqslant n}\log|\boldsymbol{r}_j-\boldsymbol{r}_k|. \tag{3.10c}$$

Evaluating (3.8), (3.10*a*) and (3.10*b*) and substituting the resulting expressions together with (3.10*c*) in (3.7) we obtain

$$\frac{E(n;\alpha)}{E(0;\alpha)} \sim C_n(\Gamma)\frac{\mathrm{e}^{(\Gamma/2)\alpha^2 n}}{\alpha^{\Gamma n^2/2-\Gamma(1-\Gamma/4)n}} \tag{3.11a}$$

where

$$C_n(\Gamma) = \int_{R^2}\cdots\int_{R^2}\mathrm{e}^{-(\Gamma/2)(r_1^2+\cdots r_n^2)}\prod_{1\leqslant j<k\leqslant n}|\boldsymbol{r}_k-\boldsymbol{r}_j|^\Gamma\,\mathrm{d}\boldsymbol{r}_1\ldots\mathrm{d}\boldsymbol{r}_n. \tag{3.11b}$$

With $\Gamma = 2$ [14]

$$C_n(2) = \prod_{j=0}^{n-1} j! \tag{3.12}$$

and (3.11*a*) is in precise agreement with the leading factor of the exact asymptotic expansion given in [12, equation (30)].

4. Asymptotics of $E(0;p)$ for random complex matrices

4.1. *The grand partition function*

Our objective in this and the next subsection is to use the Fisher–Hartwig formula [14–16] to verify (1.6) for a class of one-dimensional single-species fluid systems, in which the particles are restricted to a linear lattice $\{\tau n\}_{n=-M/2+1,\ldots,M/2}$ (for convenience M is chosen to be even). Suppose there are N particles with coordinates $n_1,n_2,\ldots,n_N$, where $-M/2+1\leqslant n_j\leqslant M/2$. Then we define the fluid system by a special determinant structure for its Boltzmann factor:

$$\mathrm{e}^{-\beta E_N} := \det[a(n_j-n_k)]_{j,k=1,\ldots,N} \tag{4.1}$$

where $a(n)$ is completely arbitrary apart from the requirements that (4.1) be greater than or equal to zero for each N and

$$f(x) := 1 + \zeta \sum_{n=-\infty}^{\infty} a(n) \mathrm{e}^{2\pi \mathrm{i} n x} \tag{4.2}$$

be non-zero and piecewise smooth for all $\zeta > 0$. We note that (4.1) is symmetrical in the particle coordinates and translationally invariant.

In general the potential corresponding to (4.1) will have N body interactions. However, in the special case that

$$a(n) = \frac{\mathrm{i}}{\tau n + 2\mathrm{i}\varepsilon} \tag{4.3}$$

use of the Cauchy double alternant determinant identity shows that

$$\det[a(n_j - n_k)]_{j,k=1,\ldots,N} = \left(\frac{1}{2\varepsilon}\right)^N \prod_{1 \leqslant j < k \leqslant N} \frac{|\tau n_k - \tau n_j|^2}{|\tau n_j - (\tau n_k + 2\mathrm{i}\varepsilon)|^2}. \tag{4.4}$$

The right-hand side of (4.4) is the Boltzmann factor of the one-component log-gas at a distance ε from a metal wall [23, 24]. With each τn_j regarded as a continuous variable x_j, the function (4.4) also occurs as the eigenvalue distribution function in Yukawa's theory of perturbed random unitary Hamiltonians [25].

Because of the special structure (4.1), the grand partition function

$$\Xi_M := \sum_{j=0}^{M} \frac{\zeta^j}{j!} \sum_{n_1=-M/2+1}^{M/2} \cdots \sum_{n_j=-M/2+1}^{M/2} \mathrm{e}^{-\beta E_N} \tag{4.5}$$

is precisely the series expansion in ζ of the Toeplitz determinant

$$\Xi_M = \det[\delta_{j,k} + \zeta a(j-k)]_{j,k=-M/2+1,\ldots,M/2} \tag{4.6a}$$

$$= \det\left[\int_0^1 f(x) \mathrm{e}^{-2\pi \mathrm{i}(j-k)}\,\mathrm{d}x\right]_{j,k=-M/2+1,\ldots,M/2}. \tag{4.6b}$$

The large-M expansion of the Toeplitz determinant is intimately related to properties of the generating function $f(x)$ as defined by (4.2).

Suppose $a(n)$ is such that f is non-zero and piecewise smooth, with discontinuities at $t_1, \ldots, t_R$ in the interval $[0, 1]$. Then we can write

$$f(x) = b(x) \prod_{r=1}^{R} t_{\beta_r}(x - x_r) \tag{4.7}$$

where $b(x)$ is piecewise smooth and continuous at $t_1, \ldots, t_R$, and

$$t_\beta(x) := \begin{cases} \mathrm{e}^{-\pi \mathrm{i}\beta(1/2 - x)} & 0 \leqslant x < 1 \\ t_\beta(x+1) & -1 < x < 0 \end{cases} \tag{4.8}$$

for some $\beta_1, \ldots, \beta_r \in \mathbb{C}$. According to the Fisher–Hartwig formula, the Toeplitz determinant (4.6) with generating function (4.7) has the large-M asymptotic expansion

$$\log \Xi_M \sim M \int_0^1 \log(b(x))\, \mathrm{d}x - \log M \sum_{r=1}^{R} \beta_r^2 + E(b; \beta_1, \ldots, \beta_R). \tag{4.9}$$

The constant $E(b; \beta_1, \ldots, \beta_r)$ has been calculated explicitly by Basor [26] (see also [15] and [16]). We are particularly interested in one of its functional properties:

$$E(b; \beta_1, \ldots, \beta_R) = E(1/b; -\beta_1, \ldots, -\beta_R). \tag{4.10}$$

4.2. The hole probability

From (2.10) we know that the hole probability $E(0; p)$ can be calculated from the n-particle distribution function. Furthermore, when the distribution function has a determinant structure the formula (2.10) can be further simplified to give $E(0; p)$ as a single Toeplitz determinant (recall (2.11) and (2.12)). These properties are features of the present model. By introducing position-dependent fugacities in (4.5), it follows (cf (2.7)) that

$$\rho(m_1, \ldots, m_n) = \det[G(m_j - m_k)]_{j,k=1,\ldots,n} \tag{4.11a}$$

where

$$G(m_j - m_k) = \delta_{j,k} - \langle m_j | (\mathbf{1}_M + \zeta \mathbf{A}_M)^{-1} | m_k \rangle \tag{4.11b}$$

$$\mathbf{A}_M = [a(j-k)]_{j,k=-M/2+1,\ldots,M/2}. \tag{4.11c}$$

The notation $\langle j | \mathbf{X} | k \rangle$ denotes the element in row j and column k of the matrix $\mathbf{X}$.

It follows from (4.11b) that, in the limit $M \to \infty$, m fixed, $G(m)$ satisfies the equation

$$G(m_1 - m_3) + \zeta \sum_{m_2=-\infty}^{\infty} a(m_1 - m_2) G(m_2 - m_3) = \zeta a(m_1 - m_3) \tag{4.12}$$

which is straightforward to solve using Fourier series. We find

$$G(m) = \int_0^1 \frac{f(x) - 1}{f(x)} \mathrm{e}^{-2\pi i m x}\, \mathrm{d}x \tag{4.13}$$

where $f(x)$ is defined by (4.2). The analogue of (2.12) then gives

$$E(0, p) = \det\left[\int_0^1 \frac{1}{f(x)} \mathrm{e}^{-2\pi i (j-k)}\right]_{j,k=1,\ldots,p}. \tag{4.14}$$

We observe that the generating function in (4.14) is precisely the reciprocal of the generating function in (4.6b). Hence the decomposition of the former into Fisher–Hartwig form replaces $b(x)$ in (4.7) by $1/b(x)$ and β_r in (4.7) by $-\beta_r$ for each

$r = 1, \ldots, R$. From (4.9) and the functional property (4.10), the large-p expansion of (4.14) is thus

$$\log E(0; p) \sim -p \int_0^1 \log(b(x))\,\mathrm{d}x - \log p \sum_{r=1}^{R} \beta_r^2 + E(b; \beta_1, \ldots, \beta_R). \tag{4.15}$$

Comparison of (4.15) with (4.9) shows that the conjecture (1.6) is valid for this class of fluid system. Furthermore, the constant terms of the RHS of (4.9) and (4.15) are identical. This has also been a feature of the other fluid systems, with exclusively mobile species, for which we have been able to calculate the expansion of Ξ_M, $E(0; p)$ and Ξ_R, $E(0; \alpha)$ [27]. We thus conjecture that the terms O(1) in the expansions (1.5) and (1.6) are equal for general fluid systems of any dimension, provided all components of the system are mobile.

4.3. A sum rule for the density profile

For continuous fluid systems the contact theorem says that the density ρ_s at the boundary of the container is related to the bulk pressure P by

$$\rho_s = \beta P. \tag{4.16}$$

For the present class of lattice fluid systems, it is possible to relate the density ρ_l at the leftmost lattice site to the bulk pressure.

To see this, from (4.9) the bulk pressure is given by

$$\tau \beta P = \int_0^1 \log b(x)\,\mathrm{d}x \tag{4.17}$$

while from (4.11)

$$\tau \rho_l = 1 - \lim_{M \to \infty} R_M \tag{4.18}$$

where

$$R_M = \langle -M/2 + 1 | (\mathbf{1}_M + \zeta \mathbf{A}_M)^{-1} | -M/2 + 1 \rangle. \tag{4.19}$$

Now, with Ξ_M given by (4.6a), Cramer's rule (see e.g. [28, p 218]) gives that

$$R_M = \Xi_M / \Xi_{M+1} \tag{4.20}$$

so from (4.9)

$$\lim_{M \to \infty} R_M = \exp\left(- \int_0^1 \log b(x)\,\mathrm{d}x \right). \tag{4.21}$$

Substituting (4.21) in (4.18) and comparison with (4.17) gives the sum rule

$$\tau \rho_l = 1 - \mathrm{e}^{-\tau \beta P}. \tag{4.22}$$

In the continuum limit $\tau \to 0$, (4.22) reduces to the contact theorem (4.16).

Another sum rule for this system relates the coefficient of $\log M$ in (4.9) to the asymptotic decay of the density profile at large distances from the edge of the system [29]. To derive this sum rule, we note from (4.9) that

$$\langle N\rangle \sim \zeta\frac{\partial\tau\beta P}{\partial\zeta}M + \zeta\frac{\partial\omega}{\partial\zeta}\log M \tag{4.23}$$

where

$$\tau\beta P = \int_0^1 \log(b(x))\,\mathrm{d}x \tag{4.24}$$

and

$$\omega = -\sum_{r=1}^{R}\beta_r^2. \tag{4.25}$$

But physically, we can decompose the average number of particles in the system as

$$\langle N\rangle = N_{\mathrm{b}} + 2N_{\mathrm{s}} \tag{4.26}$$

where N_{b} denotes the number of particles in the bulk and N_{s} denotes the excess number of particles in the neighbourhood of either boundary. The latter quantity is given in terms of the dimensionless density $\rho(\ell)$ (i.e. average number of particle on lattice site ℓ) and dimensionless bulk density $\tau\rho_{\mathrm{b}}$ by

$$N_{\mathrm{s}} = \sum_{\ell=-M/2+1}^{0}(\rho(\ell) - \tau\rho_{\mathrm{b}}). \tag{4.27}$$

Comparing (4.23) and (4.26), and using (4.27), we have that for large-M

$$\zeta\frac{\partial\omega}{\partial\zeta}\log M \sim \sum_{\ell=-M/2+1}^{0}(\rho(\ell) - \tau\rho_{\mathrm{b}}) \tag{4.28}$$

and thus for large-ℓ (but $\ell < M/2$),

$$\rho(-\tfrac{1}{2}M + \ell) - \tau\rho_{\mathrm{b}} \sim \zeta\frac{\partial\omega}{\partial\zeta}\frac{1}{\ell}. \tag{4.29}$$

From (4.11a) and (4.25), the prediction (4.29) can be written as the following conjecture for the behaviour of the diagonal elements of the inverse of a certain class of Toeplitz matrices. Let the generating function of the Toeplitz matrix $(\mathbf{1}_M + \zeta\mathbf{A}_M)$ be of the Fisher–Hartwig type (4.7), and suppose the elements of the matrix are labelled by the pair (j,k) with $-\frac{1}{2}M + 1 \leqslant j,k \leqslant \frac{1}{2}M$ (M even). Then for M and ℓ large but with $\ell < \frac{1}{2}M$,

$$\langle -\tfrac{1}{2}M + \ell|(\mathbf{1}_M + \zeta\mathbf{A}_M)^{-1}| - \tfrac{1}{2}M + \ell\rangle - \langle 0|(\mathbf{1}_M + \zeta\mathbf{A}_M)^{-1}|0\rangle$$
$$\sim \zeta\frac{\partial}{\partial\zeta}\left(\sum_{r=1}^{R}\beta_r^2\right)\frac{1}{\ell}. \tag{4.30}$$

Acknowledgments

Some of this work was done while I was a visitor at the Institute for Theoretical Dynamics, UC Davis. I thank Craig Tracy for the occasion and stimulating interaction. I also thank Harold Widom for the opportunity to visit UC Santa Cruz, and for useful discussions.

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