Painlevé Functions in Statistical Physics

 $\mathbf{b}\mathbf{y}$

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Abstract

We review recent progress in limit laws for the one-dimensional asymmetric simple exclusion process (ASEP) on the integer lattice. The limit laws are expressed in terms of a certain Painlevé II function. Furthermore, we take this opportunity to give a brief survey of the appearance of Painlevé functions in statistical physics.

2010 Mathematics Subject Classification: 34M55, 60K35, 82B23. Keywords: Painlevé function, ASEP, Bethe Ansatz, KPZ scaling.

"It was a pleasant surprise to me that such special functions actually appeared in concrete problems of theoretical physics \dots "

Mikio Sato [4]

§1. Introduction

The appearance of Painlevé functions in the 2D Ising model is well-known [37, 64]. Equally well-known is that this provided one impetus for M. Sato, T. Miwa and M. Jimbo [48] to develop their theory of *holonomic quantum fields* which connects the theory of isomondromy preserving deformations of linear differential equations with the *n*-point correlation functions of the 2D Ising model.¹

The general consensus in the field of "exactly solvable models" is that correlation functions are expressible in terms of Painlevé functions only in models that are *free fermion models*. More precisely, one expects that for the appearance of functions of the Painlevé type, it is necessary for the underlying model or process to be a determinantal process in the sense of Soshnikov [52]. In addition to the 2D

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This is a contribution to the special issue "The golden jubilee of algebraic analysis".

Communicated by M. Kashiwara. Received December 13, 2009.

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¹A complete account of the SMJ theory can be found in the recent monograph by Palmer [39].

Ising model, some notable examples where Painlevé functions arise in correlation functions include the one-dimensional impenetrable Bose gas [21, 28, 33, 34], the Ising chain in a tranverse field [41], the distribution functions of random matrix theory [1, 5, 16, 22, 28, 56, 57, 58], Hammersley's growth process [7, 8], corner and polynuclear growth models [9, 24, 29, 42, 43] and the totally asymmetric simple exclusion process (TASEP) [12, 29, 44]. Universality theorems in random matrix theory have extended the appearance of Painlevé functions to a wide class of matrix ensembles [13, 17, 18, 19, 51].² In recent developments [3, 45, 46, 47] Painlevé II appears in the long time asymptotics of explicit formulas for the exact height distribution for the KPZ equation [32] with narrow wedge initial condition.

As just noted, one does not expect Painlevé functions to arise in correlation functions in models that are exactly solvable in the sense of Baxter [11] but are not free fermion models, e.g. 6-vertex model, XXZ quantum spin chain, Baxter's 8-vertex model. Having said that, the *universality conjecture* arising in the theory of phase transitions suggests, for instance, that the scaling limit of a large class of ferromagnetic 2D Ising models is the same as that of the Onsager 2D Ising model; and hence, Painlevé functions are conjectured to appear (in the massive scaling limit) in models outside of the class of exactly solvable models. This last statement is substantiated by the developments in [3, 45, 46, 47].

In this paper we review recent progress [59, 60, 61, 62, 63] on the current fluctuations in the asymmetric simple exclusion process (ASEP) on the integer lattice \mathbb{Z} [35, 36]. ASEP is in the class of Bethe Ansatz solvable models [23, 25] but only for certain values of the parameters is ASEP a determinantal process [29, 44, 49]. That ASEP is Bethe Ansatz solvable comes as no surprise *once* one realizes that the generator of ASEP is a similarity (not unitary!) transformation of the XXZ-quantum spin Hamiltonian [2, 50, 65]. Our main results relate the limiting current fluctuations in ASEP for certain initial conditions to the TW distributions F_1 and F_2 of random matrix theory [58, 59]. Both F_1 and F_2 are expressible in terms of the same Hastings–McLeod solution of Painlevé II [20, 26] (see §4.2).

§2. Master equation and Bethe Ansatz solution

Since its introduction in 1970 by F. Spitzer [53], the asymmetric simple exclusion process (ASEP) has attracted considerable attention both in the mathematics and physics literature due to the fact it is one of the simplest lattice models describing

 $^{^{2}}$ It is also worth noting that due to the close connection of random matrix theory to multivariate statistical analysis, these same distribution functions involving Painlevé functions are now routinely used in data analysis [30, 31, 40].

transport far from equilibrium. Recall [35, 36] that the ASEP on the integer lattice \mathbb{Z} is a continuous time Markov process η_t where $\eta_t(x) = 1$ if $x \in \mathbb{Z}$ is occupied at time t, and $\eta_t(x) = 0$ if x is vacant at time t. Particles move on \mathbb{Z} according to two rules: (1) A particle at x waits an exponential time with parameter one, and then chooses y with probability p(x, y); (2) If y is vacant at that time it moves to y, while if y is occupied it remains at x. The adjective "simple" refers to the fact that the allowed jumps are only one step to the right, p(x, x + 1) = p, or one step to the left, p(x, x - 1) = q = 1 - p. The totally asymmetric simple exclusion process (TASEP) allows jumps only to the right (p = 1) or only to the left (p = 0).³ In the mapping from the XXZ quantum spin chain, the anisotropy parameter Δ of the spin chain is related to the hopping probabilities p and q by

$$\Delta = \frac{1}{2\sqrt{pq}} \ge 1,$$

the ferromagnetic regime of the XXZ spin chain.

We begin with a system of N particles and later take the limit $N \to \infty$. A configuration is specified by giving the location of the N particles. We denote by $Y = \{y_1, \ldots, y_N\}$ with $y_1 < \cdots < y_N$ the initial configuration of the process and write $X = \{x_1, \ldots, x_N\} \in \mathbb{Z}^N$. When $x_1 < \cdots < x_N$ then X represents a possible configuration of the system at a later time t. We denote by $P_Y(X;t)$ the probability that the system is in configuration X at time t, given that it was initially in configuration Y.

Given $X = \{x_1, \ldots, x_N\} \in \mathbb{Z}^N$ we set

$$X_i^+ = \{x_1, \dots, x_{i-1}, x_i + 1, x_{i+1}, \dots, x_N\},\$$

$$X_i^- = \{x_1, \dots, x_{i-1}, x_i - 1, x_{i+1}, \dots, x_N\}.$$

The master equation for a function u on $\mathbb{Z}^N \times \mathbb{R}^+$ is

(1)
$$\frac{d}{dt}u(X;t) = \sum_{i=1}^{N} (p \, u(X_i^-;t) + q \, u(X_i^+;t) - u(X;t)),$$

and the boundary conditions are, for i = 1, ..., N - 1,

(2)
$$u(x_1, \dots, x_i, x_i + 1, \dots, x_N; t)$$

= $pu(x_1, \dots, x_i, x_i, \dots, x_N; t) + qu(x_1, \dots, x_i + 1, x_i + 1, \dots, x_N; t).$

The initial condition is

(3)
$$u(X;0) = \delta_Y(X) \quad \text{when } x_1 < \dots < x_N.$$

³It is TASEP that is a determinantal process.

The basic fact is that if u(X;t) satisfies the master equation, the boundary conditions, and the initial condition, then $P_Y(X;t) = u(X;t)$ when $x_1 < \cdots < x_N$. This is, of course, one of Bethe's basic ideas (see, e.g., [10]): incorporate the interaction (in this case the exclusion property) into the boundary conditions (2) of a free particle system (1).

Recall that an *inversion* in a permutation σ is an ordered pair $\{\sigma(i), \sigma(j)\}$ in which i < j and $\sigma(i) > \sigma(j)$. We define [65]

(4)
$$S_{\alpha\beta} = -\frac{p + q\xi_{\alpha}\xi_{\beta} - \xi_{\alpha}}{p + q\xi_{\alpha}\xi_{\beta} - \xi_{\beta}}$$

and then

$$A_{\sigma} = \prod \{ S_{\alpha\beta} : \{\alpha, \beta\} \text{ is an inversion in } \sigma \}.$$

We also set

$$\varepsilon(\xi) = p\,\xi^{-1} + q\,\xi - 1.$$

In the next theorem we shall assume $p \neq 0$, so the A_{σ} are analytic at zero in all the variables. Here and later all differentials $d\xi$ incorporate the factor $(2\pi i)^{-1}$.

Theorem 2.1. We have

(5)
$$P_Y(X;t) = \sum_{\sigma \in \mathcal{S}_N} \int_{\mathcal{C}_r} \cdots \int_{\mathcal{C}_r} A_\sigma \prod_i \xi_{\sigma(i)}^{x_i - y_{\sigma(i)} - 1} e^{\sum_i \varepsilon(\xi_i) t} d\xi_1 \cdots d\xi_N,$$

where C_r is a circle centered at zero with radius r so small that all the poles of the integrand lie outside C_r .

The proof that $P_Y(X;t)$ satisfies (1) is immediate and the fact it satisfies the boundary conditions (2) is exactly the same argument as in the XXZ problem [65]. The difficulty lies in showing (5) satisfies the initial condition (3). Observe that the term in (5) corresponding to the identity permutation does satisfy the initial condition. Thus the proof will be complete once one demonstrates that the remaining n! - 1 terms sum to zero at t = 0. This is indeed the case and the result depends crucially upon the choice of the contours C_r [59]. For the special case of TASEP, p = 1, it follows from (4) and (5) that the right-hand side of (5) can be expressed as an $N \times N$ determinant as first obtained in [49].

We note that unlike the usual applications of Bethe Ansatz, it is not the spectral theory of the operator that is of interest but rather the transition probability $P_Y(X;t)$. Thus there are no Bethe equations in our approach; and hence, no issues concerning the completeness of the Bethe eigenfunctions. Indeed, there is not even an Ansatz in this approach! We remark that this result extends with only minor modifications to the solution $\Psi(x_1, \ldots, x_N; t)$ of the time-dependent Schrödinger

equation with XXZ Hamiltonian where the x_i 's denote the location of the N "up spins" in a sea of "down spins" on \mathbb{Z} .

§3. Marginal distributions and the large N limit

We henceforth assume q > p so there is a net drift of particles to the left. Here we consider two different initial conditions. The first, called *step initial condition*, starts with particles located at $\mathbb{Z}^+ = \{1, 2, ...\}$. The second initial condition is the *step Bernoulli initial condition*: each site in \mathbb{Z}^+ , independently of the others, is initially occupied with probability ρ , $0 < \rho \leq 1$; all other sites are initially unoccupied. In each of these cases it makes sense to speak of the position of the *m*th particle from the left at time t, $x_m(t)$, and its distribution function $\mathbb{P}(x_m(t) \leq x)$. It is elementary to relate $\mathbb{P}(x_m(t) \leq x)$ to the distribution of the total current \mathcal{T} at position x at time t,

$$\mathcal{T}(x,t) :=$$
 number of particles $\leq x$ at time t ;

namely,

$$\mathbb{P}(\mathcal{T}(x,t) \le m) = 1 - \mathbb{P}(x_{m+1}(t) \le x)$$

For this reason we first concentrate on $\mathbb{P}_Y(x_m(t) \leq x)$ and only at the end translate the results into statements concerning \mathcal{T} . (The subscript Y denotes the initial configuration.)

Now for finite Y,

$$\mathbb{P}_Y(x_m(t) = x) = \sum_{x_1 < \dots < x_{m-1} < x < x_{m+1} < \dots < x_N} P_Y(x_1, \dots, x_{m-1}, x, x_{m+1}, \dots, x_N; t).$$

Since the contours C_r in (5) have $r \ll 1$, the sums over x_{m+1}, \ldots, x_N can be interchanged with the integrations in variables $\xi_{\sigma(j)}^{x_j}$, $m+1 \leq j \leq N$, and the geometric series summed. To perform the sums over x_1, \ldots, x_{m-1} , the contours in the $\xi_{\sigma(j)}^{x_j}$ variables, $1 \leq j \leq m-1$, must be deformed out beyond the unit circle and then the sums can be interchanged with the integrations. This deformation beyond the unit circle can be done in such a way as not to encounter any poles of the integrand. However, upon deforming these contours back to C_r (after the geometric series are summed) one does encounter poles; and one finds some remarkable cancellations: only the residues from the poles at $\xi_i = 1$ are nonzero. The result is a sum over all subsets of S of $\{1, \ldots, N\}$ with $|S^c| < m$ whose summands involve |S|-dimensional integrals with contours C_r .⁴ However, this resulting expression for $\mathbb{P}_Y(x_m(t) = x)$ is not so useful for taking the $N \to \infty$ limit.

The next step is to expand the contours to C_R , $R \gg 1$. It is then possible to take the $N \to \infty$ limit in the resulting expressions. The details [59] are involved and they depend crucially upon some algebraic identities which we now state.

§3.1. Three identities

Let

$$f(i,j) := p + q\xi_i\xi_j - \xi_i.$$

Identity #1:

(6)
$$\sum_{\sigma \in S_N} \operatorname{sgn}(\sigma) \frac{\prod_{i < j} f(\sigma(i), \sigma(j))}{(\xi_{\sigma(1)} - 1)(\xi_{\sigma(1)}\xi_{\sigma(2)} - 1) \cdots (\xi_{\sigma(1)}\xi_{\sigma(2)} \cdots \xi_{\sigma(N)} - 1)} = q^{N(N-1)/2} \frac{\prod_{i < j} (\xi_j - \xi_i)}{\prod_j (\xi_j - 1)}.$$

Identity #2: For $N \ge m + 1$,

(7)
$$\sum_{|S|=m} \prod_{\substack{i \in S \\ j \in S^c}} \frac{f(i,j)}{\xi_j - \xi_i} \left(1 - \prod_{j \in S^c} \xi_j \right) = q^m {N-1 \brack m} (1 - \prod_{j=1}^N \xi_j)$$

In (7) the sum runs over all subsets S of $\{1, \ldots, N\}$ with cardinality m, and S^c denotes the complement of S in $\{1, \ldots, N\}$. Here $\begin{bmatrix} N\\m \end{bmatrix}$ is a slightly modified τ -binomial coefficient, $\tau := p/q$,

$$\begin{split} [N] &:= \frac{p^N - q^N}{p - q}, \quad [0] := 1, \\ [N]! &:= [N] \left[N - 1 \right] \cdots [1], \\ [m] &:= \frac{[N]!}{[m]! [N - m]!} = q^{m(N - m)} \begin{bmatrix} N \\ m \end{bmatrix}_{\tau} \end{split}$$

where $\begin{bmatrix} N \\ m \end{bmatrix}_{\tau}$ is the usual τ -binomial coefficient. We define $\begin{bmatrix} N \\ m \end{bmatrix}_{\tau} = 0$ for m < 0. In proving (7) we first proved a simpler identity:

Identity #3:

$$\sum_{|S|=m} \prod_{i \in S \atop j \in S^c} \frac{f(i,j)}{\xi_j - \xi_i} = \begin{bmatrix} N \\ m \end{bmatrix}.$$

We believe that these identities suggest a deeper mathematical structure that is yet to be discovered.

 $^{^{4}}$ This is Theorem 5.1 in [59].

§3.2. Final expression for $\mathbb{P}(x_m(t) \le x)$ for step Bernoulli initial conditions

We denote by \mathbb{P}_{ρ} the probability measure for ASEP with step Bernoulli initial conditions. For $\rho = 1$ the measure is ASEP with step initial condition. Let

$$c_{m,k} := (-1)^m q^{k(k-1)} \tau^{m(m-1)/2} \tau^{-km} \begin{bmatrix} k-1\\ m-1 \end{bmatrix}_{\tau}.$$

Observe that $c_{m,k} = 0$ when m > k.

Theorem 3.1 ([59, 63]). Assume q > p. Then

(8)
$$\mathbb{P}_{\rho}(x_{m}(t) \leq x) = \sum_{k \geq 1} \frac{q^{k(k-1)/2} \tau^{k(k+1)/2}}{k!} c_{m,k} \int_{\mathcal{C}_{R}} \cdots \int_{\mathcal{C}_{R}} \prod_{1 \leq i \neq j \leq m} \frac{\xi_{j} - \xi_{i}}{f(i,j)} \\ \times \prod_{i} \frac{\rho}{\xi_{i} - 1 + \rho(1 - \tau)} \prod_{i=1}^{m} \frac{\xi_{i}^{x} e^{t\varepsilon(\xi_{i})}}{1 - \xi_{i}} d\xi_{i}.$$

The contour C_R , a circle of radius $R \gg 1$ centered at the origin, is chosen so that all (finite) poles of the integrand lie inside the contour.

We remark that for TASEP, p = 0, the above sum reduces to one term; and this term can be shown to be equal to an $m \times m$ determinant.

The final simplification results if we use the identity [60]

$$\det\left(\frac{1}{f(i,j)}\right)_{1\le i,j\le k} = (-1)^k (pq)^{k(k-1)/2} \prod_{i\ne j} \frac{\xi_j - \xi_i}{f(i,j)} \prod_i \frac{1}{(1-\xi_i)(q\xi_i - p)}$$

in (8) and recognize the summand, a k-dimensional integral, as the coefficient of λ^k in the Fredholm expansion of det $(I - \lambda K_{\rho})$ where K_{ρ} acts on functions on C_R by

$$f(\xi) \mapsto \int_{\mathcal{C}_R} K_{\rho}(\xi, \xi') f(\xi') d\xi'$$

where

(9)
$$K_{\rho}(\xi,\xi') = q \frac{\xi^{x} e^{t\varepsilon(\xi)}}{p + q\xi\xi' - \xi} \frac{\rho(\xi - \tau)}{\xi - 1 + \rho(1 - \tau)}, \quad \tau = \frac{p}{q}.$$

Note that when $\rho = 1$, the case of step initial condition, the last factor in $K_{\rho}(\xi, \xi')$ equals one.

Since the coefficient of λ^k in the expansion of $\det(I - \lambda K_{\rho})$ is equal to

$$\frac{(-1)^k}{k!} \int \det(I - \lambda K_{\rho}) \, \frac{d\lambda}{\lambda^{k+1}},$$

this fact together with the τ -binomial theorem gives the final result for $\mathbb{P}_{\rho}(x_m(t) \leq x)$.

Theorem 3.2 ([59, 63]). Let \mathbb{P}_{ρ} denote the probability measure for ASEP with step Bernoulli initial condition with density ρ and $x_m(t)$ denote the position of the mth particle from the left at time t. Then

(10)
$$\mathbb{P}_{\rho}(x_m(t) \le x) = \int_{\mathcal{C}} \frac{\det(I - \lambda K_{\rho})}{\prod_{j=0}^{m-1} (1 - \lambda \tau^j)} \frac{d\lambda}{\lambda}$$

where the contour C is a circle centered at the origin enclosing all the singularities at $\lambda = \tau^{-j}$, $0 \le j \le m-1$ and K_{ρ} is the integral operator whose kernel is given by (9).

§4. Limit theorems

§4.1. KPZ scaling

The scaling limit that is of most interest is the KPZ scaling limit [32, 54]. In the terminology here this scaling limit is

$$m \to \infty$$
, $t \to \infty$ with $\sigma = m/t \le 1$ fixed.

As we shall see, the limiting distribution will depend upon the relative sizes of σ and ρ^2 . For the moment we concentrate on the cases $0 < \sigma < \rho^2$ and $\sigma = \rho^2$ with $0 < \rho \leq 1$. As in any central limit theorem, to obtain a nontrivial limit the x in $\mathbb{P}_{\rho}(x_m(t) \leq x)$ must also be scaled (this too is part of KPZ scaling). In anticipation of the theorem we set

$$x := c_1 t + c_2 t^{1/3} s$$

where the $\frac{1}{3}$ is the famous KPZ universality exponent [32, 38] and

$$c_1 := -1 + 2\sqrt{\sigma}, \quad c_2 := \sigma^{-1/6} (1 - \sqrt{\sigma})^{2/3}.$$

The two distribution functions that arise in the KPZ scaling limit are defined in the next section.

§4.2. Distributions F_1 and F_2

The distributions F_1 and F_2 can be defined by either their Fredholm determinant representations or their representations in terms of a Painlevé II function. Here we take the latter route. Let q denote the solution to the Painlevé II equation

$$q'' = xq + 2q^3$$

satisfying

$$q(x) \sim \operatorname{Ai}(x), \quad x \to \infty,$$

where $\operatorname{Ai}(x)$ is the Airy function. That such a solution exists and is unique was proved by Hastings and McCleod [26].⁵ Then we have

(11)
$$F_2(s) = \exp\left(-\int_s^\infty (x-s)q(x)^2 \, dx\right),$$

(12)
$$F_1(s) = \exp\left(-\frac{1}{2}\int_s^\infty q(x)\,dx\right)F_2(s)^{1/2}.$$

The asymptotics of these distributions as $x \to \infty$ is straightforward given the large x asymptotics of the Airy function; however, the complete asymptotic expansion as $x \to -\infty$ has only recently been given [6]. For high-accuracy numerical evaluation of F_1 and F_2 , it turns out that it is better to start with their Fredholm determinant representations [15].

§4.3. Limit laws

The asymptotic analysis [61, 63] of the Fredholm determinant in the formula for $\mathbb{P}_{\rho}(x_m(t) \leq x)$ in (10) required the development of new methods since the operator K_{ρ} is not of the usual "integrable integral operator" form normally appearing in random matrix theory [14, 27, 57]. The main point is that the kernel K_{ρ} has the same Fredholm determinant as a sum of two kernels; one has large norm but fixed spectrum and its resolvent can be computed exactly, and the other is better behaved [61].

We now state the results of this asymptotic analysis.

Theorem 4.1 ([61, 63]). When $0 \le p < q$, $\gamma := q - p$,

(13)
$$\lim_{t \to \infty} \mathbb{P}_{\rho}\left(\frac{x_m(t/\gamma) - c_1 t}{c_2 t^{1/3}} \le s\right) = F_2(s) \quad \text{when } 0 < \sigma < \rho^2,$$

(14)
$$\lim_{t \to \infty} \mathbb{P}_{\rho} \left(\frac{x_m(t/\gamma) - c_1 t}{c_2 t^{1/3}} \le s \right) = F_1(s)^2 \quad \text{when } \sigma = \rho^2, \ \rho < 1.$$

This theorem implies a limit law for the current fluctuations. Define

$$v = x/t$$
, $a_1 = (1+v)^2/4$, $a_2 = 2^{-4/3}(1-v^2)^{2/3}$.

Theorem 4.2. When $0 \le p < q$, $\gamma := q - p$,

(15)
$$\lim_{t \to \infty} \mathbb{P}_{\rho} \left(\frac{\mathcal{T}(vt, t/\gamma) - a_1 t}{a_2 t^{1/3}} \le s \right) = 1 - F_2(-s) \quad when -1 < v < 2\rho - 1,$$

(16)
$$\lim_{t \to \infty} \mathbb{P}_{\rho} \left(\frac{\mathcal{T}(vt, t/\gamma) - a_1 t}{a_2 t^{1/3}} \le s \right) = 1 - F_1(-s)^2 \quad when \ v = 2\rho - 1, \ \rho < 1.$$

 $^{^5\}mathrm{A}$ modern account of Painlevé transcendents can be found in the monograph by Fokas et al. [20].

Table 1. The mean (μ_{β}) , variance (σ_{β}^2) , skewness (S_{β}) and kurtosis (K_{β}) of F_{β} , $\beta = 1, 2$. The numbers are courtesy of F. Bornemann and M. Prähofer.

β	μ_eta	σ_{eta}^2	S_{eta}	K_{β}
1	-1.206533574582	1.607781034581	0.29346452408	0.1652429384
2	-1.771086807411	0.8131947928329	0.224084203610	0.0934480876

For step initial condition with $0 < \sigma < 1$ the limit laws are (13) and (15) [61, 62]. When $\sigma > \rho^2$ (or $v > 2\rho - 1$) the fluctuations are of order $t^{1/2}$ and the limiting distribution is Gaussian (see [63] for details).

For TASEP, p = 0, with step initial condition the limit law (15) was first proved by Johansson [29]. For TASEP with step Bernoulli initial condition the limit laws (15) and (16) were conjectured by Prähofer and Spohn [44] and proved recently by Ben Arous and Corwin [12]. The fact that these limit laws remain essentially identical (the only change is the factor γ in the time slot) is a very strong statement of KPZ Universality. From the integrable systems perspective, these results are, to the best of the authors' knowledge, the first limit laws of Bethe Ansatz solvable models (outside the class of determinantal models) where the correlation functions are expressible in terms of Painlevé functions.

§5. Conclusions

Today Painlevé functions occur in many areas of theoretical statistical physics. In the case of KPZ fluctuations there are now experiments [38, 55] on stochastically growing interfaces where quantities such as the skewness and the kurtosis of F_{β} (see Table 1), as well as the distribution functions themselves, are compared with experiment. In [55] K. Takeuchi and M. Sano conclude that their measurements "... have shown without fitting that the fluctuations of the cluster local radius asymptotically obey the Tracy–Widom distribution of the GUE random matrices."

Acknowledgements

This work was supported by the National Science Foundation under grants DMS-0906387 (first author) and DMS-0854934 (second author).

Note added in proof. The proof of Theorem 2.1 of [59] contains an error in Lemma 2.2. See the arXiv reference, version 3, for a corrected proof.

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