Refined evaluation of the level-spacing distribution of symplectic ensembles: Moments and implications

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To obtain a more precise value for the variance σ^2 of the joint probability distribution of a symplectic ensemble, we extend previous numerical evaluations of a power series. Our result $\sigma^2 \approx 0.1041$ shows that the excellent approximation using the analytically simple Wigner surmise fractionally overestimates this value. This behavior is important in establishing the trend of a generalization of the surmise to describe the terrace-width distribution on vicinal surfaces. We also obtain precise estimates of the skewness and the kurtosis of the exact distribution, as well as the related moments.

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The study of fluctuation phenomena has proved particularly rewarding because of their universal properties [1–3]. Beginning with the work of Wigner and of Dyson [4], this field—associated with random matrix theory (RMT)—has now attained profound sophistication and has been applied to an astonishingly broad range of physical systems. In particular, formally exact solutions have been developed for the distribution of the nearest-neighbor level spacings of energy eigenstates of systems described by Hamiltonians with orthogonal, unitary, or symplectic symmetry.

As formulated in the Calogero-Sutherland (CS) model [5,6], there is a remarkable correspondence between these energy levels and the positions of fermions in one-dimensional (1D) space that interact with an inverse-square repulsive potential, so that the distribution of the separations between energy eigenvalues also describes the spacings (in the 1D space) between the fermions. This insight has led to further applications of the theory, many of which are described in excellent reviews [1–3]. A noteworthy example that is not covered is the terrace-width distribution (TWD) on a vicinal [7] surface. Steps traverse the surface without crossing, leading to the association of their configurations with the world lines of fermions evolving in 1D space, with the inverse-square repulsions coming from steric and elastic effects. Some of us have explored the implications of this correspondence for several years [8–15].

Of particular interest is the [normalized] probability density (or joint probability distribution [16]) $P^{[\beta]}(s)$. [$P^{[\beta]}(s)ds$ is the probability that the nearest-neighbor spacing lies between s and $s+ds$; s denotes the energy difference between adjacent levels or the distance between adjacent fermions, in either case divided by its average value.] The scale of s is set so that the mean of $P^{[\beta]}(s)$ is unity. For $s \ll 1$, $P^{[\beta]}(s) \propto s^{\beta}$ [17]. According to the CS model,

$$\beta = 1 + \sqrt{1 + 4\tilde{A}}, \tag{1}$$

where the dimensionless parameter $\tilde{A}$ is proportional to the strength of the s^{-2} repulsion between levels (or fermions or steps). The special cases $\beta=1,2,4$ (or $\tilde{A}=-1/4,0,2$) correspond orthogonal, unitary, and symplectic ensembles, respectively. While most RMT studies focus on the first two cases [2,16], the last is the most relevant to vicinal surfaces (though the unitary case of "free fermions" with just entropic repulsions is also germane [9] and much studied). It is well established that the exact solution for a symplectic ensemble can be well approximated by the Wigner surmise

$$P_W^{[4]}(s) = \left(\frac{64}{9\pi}\right)^3 s^4 \exp\left(-\frac{64}{9\pi}s^2\right). \tag{2}$$

From Eq. (1) we see that in principle β can take on arbitrary values. Moreover, the proportionality of $P^{[\beta]}(s)$ to s^{β} at $s \ll 1$ for values of β beyond the special cases has been rigorously established [18,19]. In accounting for experimental data for vicinal surfaces, for which $\tilde{A}$ ranges from 0 to $\sim 10-20$ (cf. Table II of Ref. [12]), we have advocated and described thoroughly [10–15] the use of a generalization (to arbitrary β) of the Wigner surmise of Eq. (2). (For those interested in [more] details about applications to vicinal surfaces, the latest in the series [15] provides a good perspective of the whole endeavor [10–15] while Ref. [14] is based on an overview presentation for theorists.)

The experimental TWD is typically characterized by just its width. Hence, it is important to determine precisely the variance σ^2 of $P^{[4]}$. In the second edition of Mehta's authoritative classic [1], the second moment $(1+\sigma^2)$ is listed [20] as 1.105. This value was disconcerting since we expected [15] the exact variance to be *smaller* than the variance 0.10447 of the Wigner surmise Eq. (2). (In the limit that $\beta \to \infty$, the variance of a Wigner-like expression is 1% too large while for free fermions, $\beta=2$, it is 1% too small, and for $\beta=1$ it is over 4% too small. (Cf. Refs. [1,10,15], especially Table II of Ref. [15].) Hence, we suspected [15] that a numerical imprecision led to a rounding error, so that the exact variance to three decimal places should be 0.104 rather than 0.105. While superficially minor, this difference is important in establishing the overall trend of the generalization of the Wigner surmise relative to the limited exact information available [22].

In order to confirm our hypothesis, we needed to extend the earlier analysis by Dietz and Haake [23] (hereafter DH)

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TABLE I. Tabulation of P_l of Eq. (5), using Eq. (4), up to $l=62$. Numbers in square brackets denote powers of 10.

l	P_l	l	P_l
1	0	32	4.069314164[−6]
2	0	33	−1.208912930[−6]
3	0	34	−4.320684951[−7]
4	11.54478116	35	1.444119216[−7]
5	0	36	3.831511457[−8]
6	−26.04398239	37	−1.542093305[−8]
7	0	38	−2.373910020[−9]
8	29.37643465	39	1.481972070[−9]
9	0	40	−2.106884211[−11]
10	−22.1273823	41	−1.289235835[−10]
11	0	42	3.975772815[−11]
12	12.60254549	43	1.020528743[−11]
13	−0.08972077	44	−8.818304854[−12]
14	−5.767995139	45	−7.384058833[−13]
15	0.142183183	46	1.443470291[−12]
16	2.185535259	47	4.902183361[−14]
17	−0.11136461	48	−2.032183919[−13]
18	−0.696689017	49	−2.990951537[−15]
19	0.057406553	50	2.584509877[−14]
20	0.188941319	51	1.663636643[−16]
21	−2.187532238[−2]	52	−3.036116364[−15]
22	−4.401657003[−2]	53	−7.985564711[−18]
23	6.560453940[−3]	54	3.335453235[−16]
24	8.888154747[−3]	55	2.262609974[−19]
25	−1.609790563[−3]	56	−3.454096248[−17]
26	−1.568617360[−3]	57	2.075792033[−20]
27	3.318113094[−4]	58	3.390775820[−18]
28	2.436873663[−4]	59	−6.081053185[−21]
29	−5.855493089[−5]	60	−3.168731972[−19]
30	−3.348583956[−5]	61	1.020388478[−21]
31	8.975777681[−6]	62	2.828240383[−20]

(see also Ref. [3]), finding eventually that $\sigma^2_{\beta=4}=0.1041$. We communicated these results to Mehta in time for inclusion in his third edition of Ref. [1], which duly lists the second moment as 1.104. In this brief paper, we present the numerical data supporting our claim. In the process of this work, we also obtained the third and fourth moments, allowing us to compute the skewness and kurtosis of $P^{[4]}(s)$.

Following DH we first write as a Taylor's series the probability $E^{[4]}(s)$ that a randomly chosen interval of size s contains no levels,

$$E^{[4]}(s)=\sum_{l=0}^{\infty}E_l s^l, \tag{3}$$

where

TABLE II. Summary of results for moments and related properties of $P(s)$ for symplectic ensemble. For the μ's and the variance, all tabulated digits are significant. For skewness and kurtosis, (1) indicates ±0.001 uncertainty.

Property	Exact	Wigner surmise
μ_2	1.1041	$\frac{45\pi}{128}\doteq 1.10447$
μ_3	1.3241	$\frac{27\pi}{64}\doteq 1.32536$
μ_4	1.7044	$\frac{2835\pi^2}{16384}\doteq 1.70778$
variance	0.1041	0.10447
skewness	0.350(1)	0.35424
kurtosis	3.027(1)	3.03698

$$E_l=\sum_{n=1,2,\ldots}^{l\geq 2n^2-n}\pi^{l-n}\frac{(-1)^{(l+n)/2}}{n!}\sum_{l_1,\ldots,l_n}^{1,2,\ldots}\delta\left(\sum_{i=1}^{n}l_i,\frac{l-n}{2}\right)\times\sum_{t_1}^{0,\ldots,l_1},\ldots,\sum_{t_n}^{0,\ldots,l_n}\det\left(\frac{1}{2l_i-2t_i+2t_j+1}\right)\times\prod_{k}^{1\ldots n}\binom{2l_k+1}{2t_k}\frac{1}{(2l_k+1)!}\left(1-\frac{4t_k}{2l_k+1}\right). \tag{4}$$

Terms with $n\leqslant 5$ are enough to determine the first 62 coefficients P_l, which are given in Table I. This table extends to $l=62$ the list given in DH to $l=42$ [24]. There is a corresponding Taylor expansion) for the probability density $P^{[4]}(s)=(d^2/ds^2)E^{[4]}(s)$,

$$P(s)=\sum_{l=0}^{\infty}P_l s^l,\quad P_l=(l+2)(l+1)E_{l+2}. \tag{5}$$

These Taylor coefficients P_l are tabulated in Table I.

The asymptotic distribution obtained by Dyson [21] is [1,23,25]

$$E_{\text{as}}=2^{9/8}e^B|2\pi s-1|^{-1/8}e^{-(\pi^2/4)s^2+(\pi/2)s}\quad P_{\text{as}}=E''_{\text{as}}(s), \tag{6}$$

where $B=\frac{1}{24}\ln 2+\frac{3}{2}\zeta'(-1)\approx-0.219250583$ Ref. [1]. As our first approximant of the exact $P^{[4]}$, we use the power series with the coefficients from Table I up to some crossover value of s, after which we use P_{as} from Eq. (6). We select this crossover s as that value which produces both normalization and unit mean of the approximant. This value is $s=1.9187$, with negligible change on the scale of ±0.0003. It is then straightforward to estimate μ_2, μ_3, and μ_4, the second, third, and fourth moments, respectively. These are listed in Table II.

DH suggest that an improved approximant can be found by multiplying the asymptotic expression P_{as} by a Padé interpolation expression, which has the particular advantage of removing the obvious singularity in Eq. (6) at $s=\frac{1}{2}\pi$. For the Padé interpolant we used the expression in DH,

$$\text{Padé} = \frac{\sum_{m=1}^{l_{max}/2} \nu_{8m-7} x^{m-1}|x|^{1/8} + \nu_{8m} x^m}{\Delta_0 + \sum_{m=1}^{l_{max}/2} \Delta_{8m-1} x^{m-1}|x|^{-1/8} + \Delta_{8m} x^m}, \quad (7)$$

where $x \equiv 2\pi s - 1$. We began by using the values for ν_m and Δ_m tabulated in DH (for $l_{max}=42$ in the Taylor expansion, and replaced the pure asymptotic expression by the version multiplied by the Padé interpolant above the crossover value of s, consistent with the procedure used by DH [26]. We found no change in the moments to five decimal places (though the optimal crossover value for s rose modestly to 1.9193, so we did not pursue extending DH's tabulated values of ν_m and Δ_m.

As listed in Table II, the variance of $P^{[4]}(s)$ is found to be $\sigma^2 \equiv \mu_2 - 1 = 0.1041$. The third and fourth moments are measured to be $\mu_3 = 1.3241$ and $\mu_4 = 1.7044$, respectively. Our various checks indicate that all these digits are significant. One can also calculate the moments by directly using Eqs. (3) and (5), which gives the same result as the previous case. Because of the subtractions involved, the skewness $(\mu_3 - 3\mu_2 + 2)/\sigma^3$ and the kurtosis $(\mu_4 - 4\mu_3 + 6\mu_2 - 3)/\sigma^4$ are very sensitive to the precision of the moments used to determine them. Accordingly, we computed them "directly" rather than by using the computed moments. In Table II we list their values as 0.35 and 3.027, respectively; these numbers should be viewed as ±0.001. In any case, all these values are lower, albeit marginally, than the corresponding values for the Wigner surmise for $\beta=4$, so that the latter serves not just as an excellent approximation but also as an upper bound for these statistical properties of $P^{[4]}(s)$.

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[1] M. L. Mehta, *Random Matrices*, 2nd ed. (Academic, New York, 1991); 3rd ed. (Elsevier, Amsterdam, 2004).
[2] T. Guhr, A. Müller-Groeling, and H. A. Weidenmüller, Phys. Rep. **299**, 189 (1998).
[3] F. Haake, *Quantum Signatures of Chaos*, 2nd ed. (Springer, Berlin, 1991).
[4] F. J. Dyson, J. Math. Phys. **3**, 140 (1962); F. J. Dyson and M. L. Mehta, *ibid.* **4**, 701 (1963).
[5] F. Calogero, J. Math. Phys. **10**, 2191 (1969); **10**, 2197 (1969).
[6] B. Sutherland, J. Math. Phys. **12**, 246 (1971); Phys. Rev. A **4**, 2019 (1971).
[7] I.e., a surface that is misoriented from (and so in the vicinity of) a high-symmetry (facet) orientation. For reviews, see H.-C. Jeong and E. D. Williams, Surf. Sci. Rep. **34**, 171 (1999); M. Giesen, Prog. Surf. Sci. **68**, 1 (2001).
[8] N. C. Bartelt, T. L. Einstein, and E. D. Williams, Surf. Sci. **240**, L591 (1990).
[9] B. Joós, T. L. Einstein, and N. C. Bartelt, Phys. Rev. B **43**, 8153 (1991).
[10] T. L. Einstein and O. Pierre-Louis, Surf. Sci. **424**, L299 (1999).
[11] M. Giesen and T. L. Einstein, Surf. Sci. **449**, 191 (2000) describes detailed applications of the generalized Wigner surmise to extensive experimental data.
[12] T. L. Einstein, H. L. Richards, S. D. Cohen, and O. Pierre-Louis, Surf. Sci. **493**, 460 (2001), based on an invited review at the International Symposium on Surface and Interface Properties of Different Symmetry Crossing, 2000, Nagoya, Japan, October 2000.
[13] H. L. Richards, S. D. Cohen, T. L. Einstein, and M. Giesen, Surf. Sci. **453**, 59 (2000), has many useful formulas and results for confronting experimental data.
[14] T. L. Einstein, Ann. Henri Poincare **4** (Suppl. 2), S811 (2003), from Proc. TH-2202 [International Conf. on Theoretical Physics], Paris, July 2002, cond-mat/0306347.
[15] Hailu Gebremariam, S. D. Cohen, H. L. Richards, and T. L. Einstein, Phys. Rev. B **69**, 125404 (2004).
[16] K. A. Muttalib, J.-L. Pichard, and A. D. Stone, Phys. Rev. Lett. **59**, 2475 (1987).
[17] In Refs. [10,12–15] the exponent β is denoted ϱ to avoid confusion with the step-free energy per length β and the step stiffness $\tilde{\beta}$.
[18] P. J. Forrester, Nucl. Phys. B **388**, 671 (1992); J. Stat. Phys. **72**, 39 (1993).
[19] Z. N. C. Ha, Nucl. Phys. B **435[FS]**, 604 (1995). F. D. M. Haldane, in *Correlation Effects in Low-Dimensional Electronic Systems*, edited by A. Okiji and N. Kawakami (Springer, Berlin, 1994), 3.
[20] In both editions of Ref. [1], Eq. (16.4.6) gives the second moment of $P(s)$.
[21] F. J. Dyson, Commun. Math. Phys. **47**, 171 (1976).
[22] Of course, for $\beta=4$, the Wigner surmise [Eq. (2)] is an excellent and sufficient approximation for analyzing experimental and simulational data.
[23] B. Dietz and F. Haake, Z. Phys. B: Condens. Matter **80**, 153 (1990).
[24] Our values (including the sign) for P_{40} and P_{42} differ from those in DH, for unknown reasons.
[25] According to Ref. [1] [see Eq. (12.6.17)] there is an additional term in E_{as} with the opposite sign for the argument of the last exponential and the power law, explicitly $2^{9/8}e^B|2\pi s + 1|^{-1/8}e^{-(\pi^2/4)s^2-(\pi/2)s}$. This term was not included in DH because it made a negligible contribution [26]. Likewise, we find here that such a term affects the moments of $P^{[4]}(s)$ by at most 0.00001, negligible at the precision we consider.
[26] Barbara Dietz, private communication.