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On the Nature of the Lee–Yang Measure for Ising Ferromagnets

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For the two- and three-dimensional nearest neighbors Ising model in the presence of a magnetic field, we study numerically asymptotic properties of the set of orthogonal polynomials associated with the Lee–Yang measure. This provides an insight into the nature of this measure near its end points, on the Lee–Yang circle. We introduce a smoothness index which analyzes the structure of the measure. Its value is found to be equal to 2 within 10^{-3} for all the models tested in two and three dimensions, at any temperatures. The results strongly suggest the absence of any singular part (continuous or pure point) in the measure, even in dimension 3. We also confirm, using a different method, known results on the behavior of the measure near its end points.

KEY WORDS: Lee–Yang measure; end-point singularities; orthogonal polynomials.

INTRODUCTION

Many thermodynamical properties of the ferromagnetic Ising model are related to a positive measure $d\phi_T(\theta)$ defined on the unit circle $z = e^{i\theta}$ of the activity z plane, as proved by Lee and Yang.[1,2] The analytic form of $d\phi_T(\theta)$ is not known and even its support $|\theta| \geqslant \theta_0(T)$, which above the critical temperature T_c is no longer the full circle,[3] remains to be determined.

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Table I. Complete List of Relavant Parameters for the Diamond and the Square Lattice, at the Critical Temperature[a]

n	$\alpha(n)$	$\beta(n)$	n	$\alpha(n)$	$\beta(n)$
0	2.4556630		0	2.3431458	
1	2.6183532	3.2227693	1	2.4365942	2.8629150
2	2.6019630	1.7004798	2	2.4186407	1.4691123
3	2.5953538	1.6873476	3	2.4162785	1.4609487
4	2.5931886	1.6822806	4	2.4153710	1.4590917
5	2.5920938	1.6803256	5	2.4149786	1.4582799
6	2.5915162	1.6793190	6	2.4147502	1.4578737
			7	2.4146053	1.4576594

n	$x_{n,n}$	extrapolated	n	$\sigma_n^{(1)}$	extrapolated	n	$x_{n,n}$	extrapolated	n	$\sigma_n^{(1)}$	extrapolated
1	2.4556630	2.4556630	1	−.3096874	−.3096874	1	2.3431458	2.3431458	1	−.3285207	−.3285207
2	4.3340575	6.2124519	2	−.3529589	−.3962304	2	4.0825301	5.82119144	2	−.3824543	−.4363878
3	4.7828793	5.5135212	3	−.3707555	−.4134171	3	4.4846003	5.1284396	3	−.4060066	−.4660757
4	4.9511531	5.0976430	4	−.3801919	−.4060873	4	4.6323313	4.7557874	4	−.4192738	−.4670162
5	5.0315480	5.1827451	5	−.3859313	−.4060873	5	4.7020571	4.8306452	5	−.4277866	−.4667896
6	5.0760265	5.1803692	6	−.3897269	−.3970940	6	4.7403166	4.8283300	6	−.4337116	−.4667312
7	5.1031697	5.1802921				7	4.7635248	4.8284274	7	−.4380746	−.4667877
						8	4.7786472	4.8284615			

	$s_n^{(1)}$			$\sigma_n^{(2)}$			$s_n^{(1)}$			$\sigma_n^{(2)}$	
1	1.1693524	1.1693524	1	−.0828159	−.0828158	1	1.2035535	1.2035535	1	−.1155343	−.1155343
2	1.5118440	1.8543355	2	−.3881904	−.6935649	2	1.5488992	1.8942448	2	−.4546212	−.7937082
3	1.6523589	1.9883858	3	−.3952645	−.4026742	3	1.6846040	1.9959982	3	−.4600308	−.4656158
4	1.7291167	1.9915067	4	−.3982300	−.4059557	4	1.7575563	2.0017012	4	−.4620340	−.4666040
5	1.7775126	1.9912950	5	−.3995328	−.4035049	5	1.8031112	2.0001684	5	−.4630976	−.4666861
6	1.8108161	1.9930780	6	−.4001310	−.3981880	6	1.8342546	1.9996412	6	−.4637776	−.4665757
						7	1.8568959	2.0000889	7	−.4642364	−.4667822
	$s_n^{(2)}$			$\sigma_n^{(3)}$			$s_n^{(2)}$			$\sigma_n^{(3)}$	
1	1.4315466	1.4315466	1	.5452969	.5452969	1	1.4646596	1.4646596	1	.5276110	.5276110
2	1.9620675	2.4925884	2	−.1000689	−.7454347	2	2.0024678	2.5402760	2	−.1506231	−.8288571
3	2.2159274	2.9356630	3	−.2083727	−.3603575	3	2.2524683	2.9367883	3	−.2649704	−.4256933
4	2.3677748	2.9865649	4	−.2619087	−.4212564	4	2.4007142	3.0007305	4	−.3195380	−.4775273
5	2.4693977	2.9914061	5	−.2928470	−.4067395	5	2.4994221	2.9992338	5	−.3514051	−.4724344
			6	−.3128320	−.4028627	6	2.5700001	3.0198965	6	−.3721837	−.4590598
									7	−.3866999	−.4910598

[a] The largest zero $x_{n,n}$ is extrapolated using the interpolation points $1/n^2$, the endpoint singularity index σ is extrapolated with $1/n$.

Our question of interest was to know more about the nature of the measure $d\phi_T(\theta)$. From the decomposition theorem we know that a positive measure is the sum of three parts: absolutely continuous, pure point, and singular continuous. In particular one can ask if there would be a dramatic change in the nature of the measure when one goes from two to three dimensions. To try to answer such questions one must enter into the delicate analysis of the way in which the zeroes of the orthogonal polynomials associated to the measure approach asymptotically their limits, and also of the way the coefficients of the three terms recursive relation, that such polynomials fulfill, behave for large indices. It is the purpose of this paper to give some insight into these questions.

Numerical approximations to the gap $\theta_0(T)$, to the density of $d\phi_T(\theta)$, and to the index σ of its behavior at θ_0 given by $\phi'_T(\theta) \sim (\theta - \theta_0)^\sigma$ have been obtained from high temperature series and/or high field series for various models.[4] The high temperature limits have been subsequently improved[5] and the result for dimension two $\sigma = -0.163 \pm 0.003$ is in excellent agreement with the exact result $\sigma = -\frac{1}{6}$ recently determined.[6,7] Other investigations based on renormalization group techniques[8–10] suggest a very complex structure of the Yang–Lee edge, confirmed by Ref. 11.

In this note we carry out a new analysis of the Lee–Yang measure $d\phi_T(\theta)$ for various models starting from its trigonometric moments, given by the coefficients of the Mayer–Yvon expansion. After transforming the trigonometric moment problem into a moment problem on the real line[12] we compute the related orthogonal polynomials. The available coefficients α_{n-1}, β_n $(n \leqslant N)$ on the associated Jacobi matrix rapidly approach constant values α, β so that we can approximate the measure with an explicitly computable measure whose Jacobi matrix has $\alpha_{n-1} = \alpha$ and $\beta_n = \beta$ for $n > N$. The convergence of α_n and β_n to α and β shows that the measure consists of a continuous part, whose points of increase are dense in $[\alpha - 2\sqrt{\beta}, \alpha + 2\sqrt{\beta}]$ and a (at most denumerable) set of mass points outside $(\alpha - 2\sqrt{\beta}, \alpha + 2\sqrt{\beta})$ with possible accumulation points at $\alpha \pm 2\sqrt{\beta}$. All the others parameters $\theta_0(T)$ and $\sigma(T)$ of the measure can also be estimated by using some asymptotic properties of the orthogonal polynomials and their zeroes. For $T \leqslant T_c$ the functions $\theta_0(T)$ and $\sigma(T)$ are known: indeed $\theta_0(T) = 0$ for $T \leqslant T_c$ and if we assume $\phi'_T(\theta) = \theta^{\sigma(T)}\, \Phi_T(\theta)$ where $\Phi_T(\theta)$ is analytic in a neighborhood of $\theta = 0$, then the existence of a spontaneous magnetization $M = M_0$ for $T < T_c$ and the critical behavior $M \sim H^{1/\delta}$ at $T = T_c$ imply $\sigma(T) = -\frac{1}{2}$ for $T < T_c$ and $\sigma(T_c) = \frac{1}{2}(1/\delta - 1)$.

Below the critical temperature the known values of θ_0 and σ are reproduced with a very high accuracy using extrapolation techniques. At the critical temperature the accuracy is still high (see Table I) even though the results are affected by the uncertainty on T_c itself for the three-dimensional models. Above the critical temperature the extrapolated values for $\theta_0(T)$ are still accurate, while for $\sigma(T)$, which itself depends on $\theta_0(T)$, the results are rather poor since some extrapolations are no longer reliable (see Figs. 2 and 3).

The present analysis provides an approximation to the measure *which is not a simple fit* but satisfies all the constraints of a Stieltjes moment problem and suggests that the measure has a smooth Jacobi-like density. The largest zero $x_{n,n}$ of the nth degree orthogonal polynomial converges to a limit as n^{-s} for $n \to \infty$, and an extrapolation procedure allows the determination of s with a good accuracy. The value $s=2$ within 10^{-3} found for all the tested models at several temperatures suggests the absence of pure point masses outside the support of the absolutely continuous part of the measure (see Appendix 2). No essential difference appears between two- and three-dimensional models as far as the smoothness of the masure is concerned.

1. THE LEE–YANG REPRESENTATION

We consider a ferromagnetic Ising model on a lattice of dimensions d with c nearest neighbors. The partition function for a subset of N spins is given by

$$Z_N = \sum_{\{\sigma\}} \exp\left[-\beta\left(-J\sum_{i,j}{}^{*}\sigma_i\sigma_j - H\sum_i \sigma_i\right)\right] \tag{1.1}$$

where $\sigma_i \pm 1$, J is a real positive constant, H is the magnetic field, $\beta = 1/kT$ is the inverse temperature and the sum $\sum^*$ runs over the nearest neighbors. We use the following variables

$$x = e^{-2\beta J} \qquad z = e^{-2\beta H} \tag{1.2}$$

where $x \in [0, 1]$ and $z \in [0, 1]$, $H > 0$.

Lee and Yang[2] have proved that all the zeroes of Z_N are on the unit circle $|z| = 1$ and the free energy per spin $F_N = -1/(\beta N) \log Z_N$ has a limit when $N \to \infty$ given by the following representation

$$F(z, x) = \lim_{N \to \infty} F_N = -H - \frac{c}{2} J - \int_{\theta_0(x)}^{\pi} \log(1 - 2z\cos\theta + z^2)\, d\phi_x(\theta) \tag{1.3}$$

The magnetization is given by

$$M(z, x) = -\frac{\partial F}{\partial H} = 2(1 - z^2) \int_{\theta_0(x)}^{\pi} \frac{d\phi_x(\theta)}{1 - 2z\cos\theta + z^2} \tag{1.4}$$

and since this is an odd function of the magnetic field H its symmetry in the variable z reads

$$M(z, x) = -M(1/z, x) \tag{1.5}$$

so that we can restrict our analysis to $z \in [0, 1]$. The measure is normalized on the circle, namely,

$$2 \int_{\theta_0(x)}^{\pi} d\phi_x(\theta) = 1 \tag{1.6}$$

The Mayer–Yvon expansion of $M(z, x)$ around $z = 0$ reads

$$M(z, x) = 1 - 2 \sum_{l=1}^{\infty} l\mathscr{M}_l(x) z^l \tag{1.7}$$

and $-l\mathscr{M}_l$ are the trigonometric moments of the measure $2d\phi_x(\theta)$

$$-l\mathscr{M}_l(x) = 2 \int_{\theta_0(x)}^{\pi} \cos l\theta \, d\phi_z(\theta) \tag{1.8}$$

In order to approximate the measure and θ_0 we first transform the moment problem (1.8) into a moment problem on the real line.[12] Introducing the variable

$$v = \frac{4z}{(1+z)^2} = \frac{1}{\cosh^2 \beta H} \tag{1.9}$$

the magnetization can be written as

$$M = \bar{M}\sqrt{1-v} = 2\sqrt{1-v} \int_{\theta_0(x)}^{\pi} \frac{d\phi_x(\theta)}{1 - v\cos^2(\theta/2)} \tag{1.10}$$

After the change of variables defined by

$$\tau = \frac{4}{1-u} \cos^2 \frac{\theta}{2} \qquad w = \frac{v}{4}(1-u) \tag{1.11}$$

where

$$u = \begin{cases} x & c \text{ odd} \\ x^2 & c \text{ even} \end{cases} \tag{1.12}$$

the function $\bar{M}$ can be written as

$$\bar{M}(w, u) = \int_0^{4/(1-u)\cos^2(\theta_0/2)} \frac{d\hat{\phi}_u(\tau)}{1 - w\tau} \tag{1.13}$$

where $d\hat{\phi}_u(\tau)$ is related to $d\phi_x(\theta)$ by

$$d\hat{\phi}_u(\tau) = d\phi_x\left(2 \arccos \sqrt{\frac{1-u}{4}\,\tau}\right) \tag{1.14}$$

When $d\hat{\phi}_u$ has a density we can write

$$\hat{\phi}'_u(\tau) = 2\sqrt{\tau\left(\frac{4}{1-u} - \tau\right)}\,\phi'_x\left(2 \arccos \sqrt{\frac{1-u}{4}\,\tau}\right)$$

Observe that the range of integration in (1.13) is always finite because of the inequality

$$\pi - \theta_0 \leqslant \frac{c}{2}(\pi - \psi)$$

where $x = \sin \psi/2$ and $\psi > \pi/2$[12,13] (c is the coordination number of the lattice). The expansion of $\bar{M}$ around $w = 0$ reads

$$\bar{M}(w, u) = 1 + \sum_{l=1}^{\infty} w^l \mathscr{P}_l(u) \tag{1.15}$$

where $\mathscr{P}_l(u)$ defined by

$$\mathscr{P}_l(u) = \int_0^{4/(1-u)\cos^2(\theta_0/2)} \tau^l \, d\hat{\phi}_u(\tau) \tag{1.16}$$

are polynomials in u.[13] The relation with the Mayer–Yvon coefficients is given by

$$(1-u)^l \mathscr{P}_l(u) = \frac{1}{2}\binom{2l}{l} - \sum_{j=1}^{l} j \binom{2l}{l-j} \mathscr{M}_j(x) \tag{1.17}$$

So we are faced with a moment problem for a measure $d\hat{\phi}_u(\tau)$ defined in the interval

$$\left[0,\ A(u) = \frac{4}{1-u}\cos^2\frac{\theta_0}{2}\right]$$

where $A(u)$ is exactly known only for $T \leqslant T_c$ when $\theta_0 = 0$. We shall first assume that $d\hat{\phi}_u(\theta)$ is absolutely continuous in the neighborhood of $A(u)$ and that $\hat{\phi}'_u(\tau)$ has a singularity at $A(u)$ of the form

$$\hat{\phi}'_u(\tau) \sim [A(u) - \tau]^{\sigma(u)} \qquad \tau \to A(u) \tag{1.18}$$

One can easily show that a singularity occurs in $\bar{M}$ for $w = A^{-1}(u)$, that is $i\beta H = \theta_0/2$, when $\sigma < 0$

$$\bar{M}(w, u) \sim [1 - wA(u)]^{\sigma(u)} \qquad w \to A^{-1}(u) \tag{1.19}$$

Below the critical temperature the end point singularity of $\bar{M}$ corresponds to $H = 0$ and implies

$$M(v, x) \sim (1 - v)^{1/2}(1 - v)^{\sigma(u)} \sim H^{1 + 2\sigma(u)} \qquad v \to 1;\ H \to 0 \tag{1.20}$$

Comparing with the expected behavior of the magnetization $M \sim M_0 + o(1)$ for $T < T_c$ and $M \sim H^{1/\delta}$ for $T = T_c$ we argue that

$$\sigma(u) = \begin{cases} -\dfrac{1}{2} & u < u_c \\ \dfrac{1}{2}\left(\dfrac{1}{\delta} - 1\right) & u = u_c \end{cases}$$

2. ORTHOGONAL POLYNOMIALS AND APPROXIMATIONS TO THE MEASURE

Let $d\phi(\tau)$ be a measure defined on $[0, A]$, $M(w)$ the associated Stieltjes function and $\mathscr{P}_l$ its moments

$$M(w) = \int_0^A \frac{d\phi(\tau)}{1 - w\tau} = 1 + \sum_{l=1}^{\infty} w^l \mathscr{P}_l \tag{2.1}$$

Given the moments $\mathscr{P}_0, \mathscr{P}_1, \ldots, \mathscr{P}_{2N+1}$ then, using standard algorithms, one can compute the Jacobi matrix J_N truncated at order N

$$J_N = \begin{pmatrix} \alpha_0 & \beta_1 & & 0 \\ \beta_1 & \alpha_1 & \beta_2 & \\ & \ddots & \ddots & \ddots \\ 0 & & \beta_N & \alpha_N \end{pmatrix} \tag{2.2}$$

The monic orthogonal polynomials with respect to $d\phi(\tau)$ are given by the recursion relation

$$P_{n+1}(y) = (y - \alpha_n)\, P_n(y) - \beta_n P_{n-1}(y) \tag{2.3}$$

with $P_{-1}(y) = 0$ and $P_0(y) = 1$. The associated orthogonal polynomials are defined by

$$Q_n(y) = (y - \alpha_n)\, Q_{n-1}(y) - \beta_n Q_{n-2}(y)$$

with $Q_{-1}(y)=0$ and $Q_0(y)=1$, and the $[n-1/n]$ Padé approximants to $(1/w)\,M(1/w)$ are given by

$$[n-1/n](w)=\frac{Q_{n-1}(w)}{P_n(w)} \tag{2.4}$$

We denote by $x_{j,n}$ the zeroes in increasing order of the orthogonal polynomial $P_n(x)$ and recall the following results:

Theorem 1. If for some $\varepsilon>0$ the measure $d\phi(\tau)$ is absolutely continuous in $[A-\varepsilon, A]$ and $\phi'(\tau)\approx(A-\tau)^{\sigma}$ $(\sigma>-1)$ for $\tau\in[A-\varepsilon, A]$, then

$$x_{n,n}-A\approx\frac{1}{n^2} \qquad n\to\infty \tag{2.5}$$

Theorem 2. Under the same conditions on $d\phi(\tau)$ as in Theorem 1 but with $-1<\sigma<0$

$$[n-1/n](A)\approx n^{-2\sigma} \qquad n\to\infty \tag{2.6}$$

Let $p_n(x)$ denote the normalized orthogonal polynomials whose recurrence is given by

$$\sqrt{\beta_{n+1}}\,p_{n+1}(y)=(y-\alpha_n)\,p_n(y)-\sqrt{\beta_n}\,p_{n-1}(y) \tag{2.7}$$

with initial conditions $p_{-1}(y)=0$ and $p_0(y)=1$, then one has the following.

Theorem 3. If $d\phi(\tau)$ is absolutely continuous and if $\phi'(\tau)=(A-\tau)^{\sigma}f(\tau)$ with $\sigma>-1$ and $f(\tau)=\chi(\tau)\prod_{k=1}^{m}|t_k-\tau|^{\sigma_k}$, $(0\leqslant t_k<A,\ \sigma_k>-1,\ k=1,\dots,m)$ where $\chi(\tau)$ is a positive continuous function with a "smooth" behavior, then

$$p_n(A)\approx n^{\sigma+1/2} \qquad p_n(x_{n+1,n+1})\approx n^{\sigma-1/2} \qquad n\to\infty \tag{2.8}$$

In Appendix 1 we give a proof of Theorem 2 and references to the proofs of Theorems 1 and 3. We also fix the notation $\approx$ and the precise meaning of "smooth" there. Given the sequence r_n defined by

$$r_n=a+c_0n^{\omega}\left(1+\frac{c_1}{n}+\cdots+\frac{c_k}{n^k}+\cdots\right) \tag{2.9}$$

then we can compute ω as the limit of a new sequence $\omega_n^{(1)}$

$$\omega_n^{(1)}=n\log\frac{r_{n+1}-a}{r_n-a}=\omega+O\left(\frac{1}{n}\right) \tag{2.10}$$

or if a is not known of the sequence $\omega_n^{(2)}$

$$\omega_n^{(2)} = n \log \frac{r_{n+1} - r_n}{r_n - r_{n-1}} = \omega - 1 + O\left(\frac{1}{n}\right) \tag{2.11}$$

The limit of the sequences (2.10) and (2.11) can be obtained by extrapolation algorithms such as Thiele continued fraction (see Appendix 3).

Smooth approximations to the measure can be given if the sequences α_n and β_n rapidly converge to limit values α and β. In fact the measure $d\phi(\tau)$ corresponding to the truncated Jacobi matrix J_N is a sum of N δ functions, but if we consider an infinite Jacobi matrix J_N^* where the diagonal sequences α_n^* and β_{n+1}^* have the constant values α and β for $n \geqslant N$ then the corresponding measure $d\phi_N^*(\tau)$ has a continuous density and possibly a finite number of δ functions. In Appendix 2 we explain that for a Jacobi matrix J_N^* defined by

$$\begin{cases} \alpha_n^* = \alpha_n, \\ \beta_{n+1}^* = \beta_{n+1}, \end{cases} \quad n < N \qquad \begin{cases} \alpha_n^* = \alpha, \\ \beta_{n+1}^* = \beta, \end{cases} \quad n \geqslant N$$

the corresponding measure is given by the following density (provided point masses are absent)

$$\phi_N^{*\prime}(\tau) = \frac{1}{2\pi} \frac{\sqrt{4\beta - (\tau - \alpha)^2}}{\beta p_N^2(\tau) - \beta_N p_{N-1}^2(\tau) - (\tau - \alpha)\sqrt{\beta_N}\, p_N(\tau)\, p_{N-1}(\tau)} \tag{2.12}$$

where $p_n(\tau)$ are the normalized orthogonal polynomials which can be computed by (2.7). We further observe that if α and β are the limits of the sequences α_n and β_n then the relations with the endpoints 0 and A of the interval of orthogonality are given by (still provided there are no point masses)

$$\alpha - 2\sqrt{\beta} = 0 \qquad \alpha + 2\sqrt{\beta} = A \tag{2.13}$$

These relations are useful to check the accuracy of the numerical guesses for the limits of the sequences α_n and β_n.

3. LEE–YANG MEASURE AND RELATED PARAMETERS

We have computed using formal languages the moments $\mathscr{P}_l(u)$ for the square, triangular, honeycomb two-dimensional lattices and cubic, diamond three-dimensional lattices using the available tables for the coefficients of the polynomials.[13] For the square lattice the moments are available up to order $l=15$, for the triangular up to $l=10$ and for the remaining models moments up to $l=13$. We have also computed the moments for the Bethe lattice with coordination number $c=3, 4, 6$ up to order $l=15$.

Starting from the $l=2N+1$ available moments the coefficients $\alpha_0, \alpha_1,..., \alpha_N$ and $\beta_1,..., \beta_N$ of the corresponding Jacobi matrix J_N were computed and the zeroes $x_{1,n} < x_{2,n} < \cdots < x_{n,n}$ of the orthogonal polynomials $P_n(y) = \det[yI - J_{n-1}]$ determined. The limits α, β and $\bar{x}$ of the sequences α_n, β_n and $x_{n,n}$ were computed with an extrapolation procedure based on the Thiele continued fraction (see Appendix 3) and the relations $\alpha = 2\sqrt{\beta}$ and $\bar{x} = 2\alpha = A$ were found to be satisfied with a good accuracy (at least 10^{-3} as can be checked for instance in Table I). The gap angle θ_0 was determined above the critical temperature according to

$$\theta_0 = 2 \arccos \sqrt{\frac{\bar{x}}{4}(1-u)} \tag{3.1}$$

In Fig. 1 a plot of θ_0 as a function of T/T_c is given for four different models (we did not plot the triangular lattice being almost coincident with the square lattice).

If we assume that $x_{n,n} = A + c_0 n^{-s}(1 + c_1/n + c_2/n^2 + \cdots +)$, even though we have no a priori arguments to exclude nonanalytic corrections in $1/n$ to the leading order, then s can be determined by extrapolating with

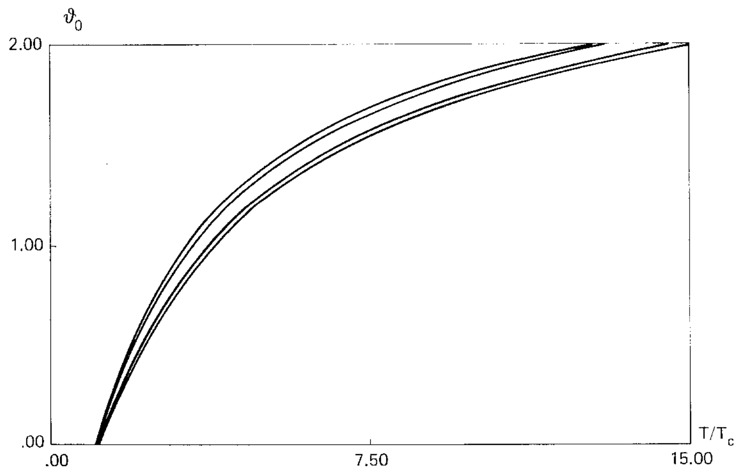


Fig. 1. The Lee–Yang edge θ_0 as a function of T/T_c. From top to bottom we have the cubic, the diamond, the square, and the honeycomb lattice.

the Thiele algorithm the sequences $s_n^{(1)}$, $s_n^{(2)}$ computed according to (2.10), (2.11). The results obtained for all the tested models in a wide range of temperatures are compatible with $s=2$ (see also Table I, where the rapid convergence of the extrapolations, to be expected if the corrections to the leading order are analytic, can be observed). This is also a good indication that the measure $d\phi'_u(\tau)$ has no point masses above $\alpha+2\sqrt{\beta}=A$.

The index $\sigma(u)$ of the singularity $\hat{\phi}'_u(\tau)\sim[A(u)-\tau]^\sigma$ of the measure at the endpoint $A(u)$ was computed following three different methods summarized by (2.6) and (2.8).

The sequences

$$\sigma_n^{(1)} = -\frac{n}{2}\log\frac{Q_n(A)\,P_n(A)}{P_{n+1}(A)\,Q_{n-1}(A)}$$

$$\sigma_n^{(2)} = -\frac{1}{2}+n\log\frac{p_{n+1}(A)}{p_n(A)} \tag{3.2}$$

$$\sigma_n^{(3)} = \frac{1}{2}+n\log\frac{p_n(x_{n+1,n+1})}{p_{n-1}(x_{n,n})}$$

all converge to σ (the first one only for $\sigma<0$) and were all computed for all the models at various temperatures. When A is exactly known, that is below the critical temperature, the extrapolations (see Appendix 3) greatly improve the convergence of the sequences $\sigma_n^{(1)}$, $\sigma_n^{(2)}$: for instance at $T=\frac{1}{2}T_c$ one obtains $\sigma=-\frac{1}{2}$ with an error less than 10^{-6}.

At the critical temperature the extrapolations are still reliable and the rate of convergence of the sequences α_n, β_n, $x_{n,n}$, $s_n^{(1)}$, $s_n^{(2)}$, $\sigma_n^{(1)}$, $\sigma_n^{(2)}$, $\sigma_n^{(3)}$ $(n=1,\dots,N)$ and their extrapolations for the square and the diamond lattices can be read in Table I. (We recall that $-s_n^{(1)}$, $-s_n^{(2)}$ are defined by (2.10), (2.11) where r_n, ω, a are replaced by $x_{n,n}$, $-s$, A and that their limits differ by one unit). The top values of the σ sequences $\sigma_N^{(1)}$, $\sigma_N^{(2)}$, $\sigma_N^{(3)}$ and their extrapolations for all the other tested models are quoted in Table II. As we mentioned in the introduction one should compare them with $\sigma(T_c)=\frac{1}{2}(1/\delta-1)$ that is $\sigma(T_c)=-\frac{7}{15}$ for the two-dimensional models and $\sigma(T_c)=-\frac{1}{3}$ for the Bethe lattice; for the three-dimensional models δ is not exactly known and if we rely on Domb[14] as we did for the critical temperatures then $\sigma(T_c)\simeq-\frac{2}{5}$ while more recent estimates of the magnetic susceptibility based on the renormalization group[15] $(\delta=4.80\pm0.03)$ give $\sigma(T_c)=-0.3958\pm0.0006$. If one excludes the cubic lattice, the extrapolations on $\sigma_n^{(2)}(T_c)$ for all the tested models agree with the expected values within 10^{-3}, the extrapolations on $\sigma_n^{(1)}(T_c)$ exhibit the same

Table II. Values of the Lee–Yang Edge Singularity σ Computed by Three Different Methods (3.2) at the Critical Temperature and at Very High Temperature[a]

	$\sigma_N^{(1)}$	$\sigma_N^{(2)}$	$\sigma_N^{(3)}$	
Square lattice	−.438 (−.467)	−.464 (−.467)	−.387 (−.491)	$T=T_c$
(15 moments)	−.207 (−.199)	−.142 (−.149)	−.078 (−.179)	$T=\infty$
Honeycomb lattice	−.436 (−.465)	−.464 (−.464)	−.361 (−.475)	$T=T_c$
(13 moments)	−.226 (−.232)	−.213 (−.241)	−.053 (−.168)	$T=\infty$
Triangular lattice	−.418 (−.467)	−.463 (−.466)	−.319 (−.480)	$T=T_c$
(10 moments)	−.206 (−.207)	−.152 (−.039)	.004 (−.212)	$T=\infty$
Diamond lattice	−.390 (−.397)	−.400 (−.398)	−.313 (−.403)	$T=T_c$
(13 moments)		.087 (.046)	.154 (.066)	$T=\infty$
Cubic lattice	−.371 (−.321)	−.370 (−.315)	−.294 (−.357)	$T=T_c$
(13 moments)		.099 (.048)	.175 (.078)	$T=\infty$
Bethe ($c=3$)	−.372 (−.341)	−.350 (−.333)	−.293 (−.321)	$T=T_c$
(15 moments)		.345 (.821)	.361 (.536)	$T=\infty$
Bethe ($c=4$)	−.356 (−.339)	−.338 (−.333)	−.273 (−.326)	$T=T_c$
(15 moments)		.406 (.726)	.442 (.512)	$T=\infty$
Bethe ($c=6$)	−.345 (−.337)	−.331 (−.333)	−.262 (−.329)	$T=T_c$
(15 moments)		.432 (.686)	.475 (.506)	$T=\infty$

[a] The values between brackets are the extrapolations obtained with the interpolation points $1/n$.

accuracy except for the Bethe lattice where the agreement is only within a few percent just as for the extrapolations of $\sigma_n^{(3)}$ for all the models.[4]

Above the critical temperature the extrapolations become less reliable and for $T \gg T_c$ σ is rather small or positive so that the sequence $\sigma_n^{(1)}$ does no longer converge. In Figs. 2 and 3 we plot $\sigma_N^{(1)}$, $\sigma_N^{(2)}$, $\sigma_N^{(3)}$ for all the models in the full temperature range (we recall that if we plotted the extrapolated values, for $T < T_c$ the three curves would be indistinguishable from the straight line $\sigma = -\frac{1}{2}$). The behavior of $\sigma_N^{(2)}$, $\sigma_N^{(3)}$ above the critical tem-

[4] The lower accuracy of the sequence $\sigma_n^{(3)}$ and their extrapolations is due to the lack of one piece of information, the endpoint of the cut A, as it is evident from (3.2). The loss of accuracy of the extrapolations of $\sigma_n^{(1)}$ for the Bethe lattice is due to the range of convergence of these sequences which, according to Theorem 2 is limited to $-1<\sigma<0$ rather than $-1<\sigma$. As a consequence the convergence is optimal around $\sigma = -\frac{1}{2}$ and rapidly decreases when 0 or -1 are approached, as one can check on the Jacobi polynomials $P^{(\sigma,-1/2)}(x)$. The value $\sigma = -\frac{1}{3}$ for the Bethe lattice is sufficiently further from $-\frac{1}{2}$ than for the two- and three-dimensional model to explain the observed loss of accuracy.

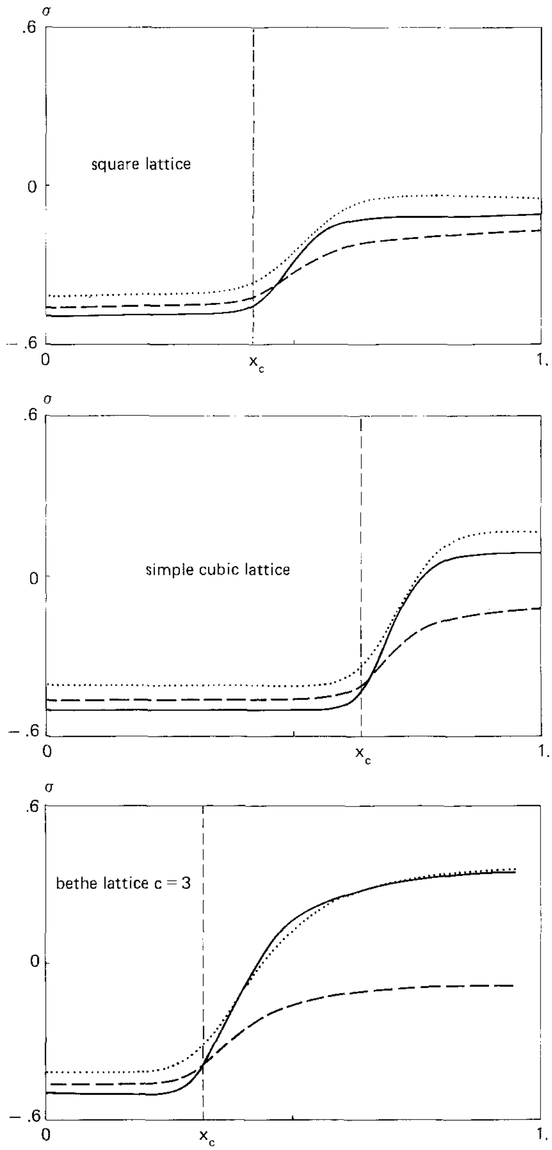


Fig. 2. The Lee–Yang edge singularity σ as a function of x. The full line is the approximation by $\sigma_N^{(2)}$, the dashed line corresponds to $\sigma_N^{(1)}$, and the pointed line is for $\sigma_N^{(3)}$. When $T > T_c$ the dashed line is only significant for the two-dimensional models.

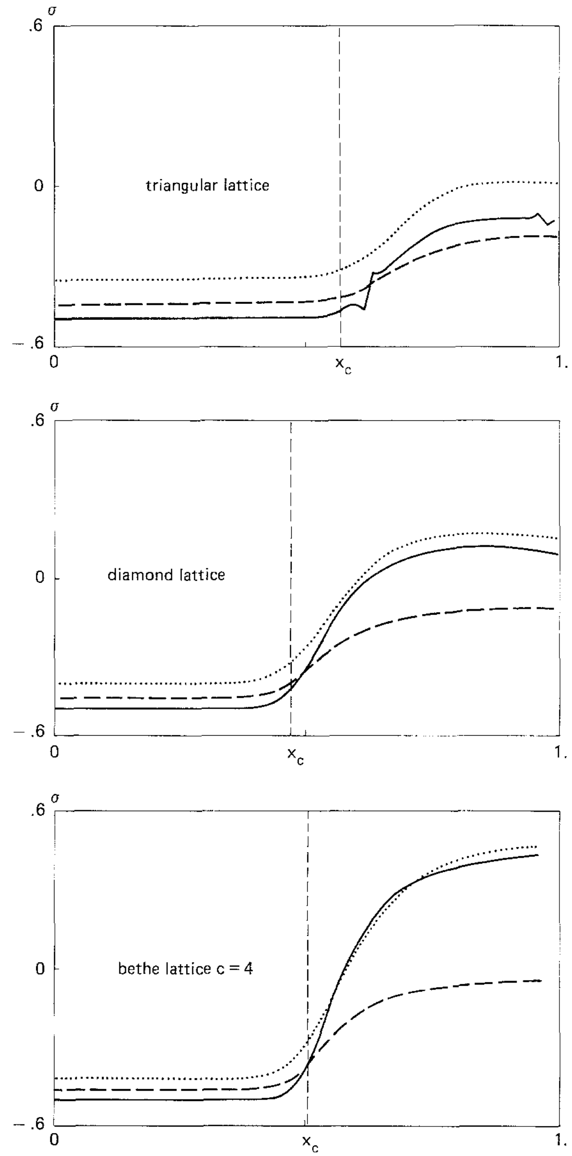


Fig. 3. The Lee–Yang edge singularity σ as a function of x. The full line is the approximation by $\sigma_N^{(2)}$, the dashed line corresponds to $\sigma_N^{(1)}$, and the pointed line is for $\sigma_N^{(3)}$. When $T > T_c$ the dashed line is only significant for the two-dimensional models.

perature is similar in all the models (if one maps the x intervals $[x_c, 1]$ into $[\frac{1}{2}, 1]$ then the curves for the models of the same dimensionality almost superimpose) but even though we know that the curve should be flat for the Bethe lattice one cannot exclude that, for the remaining models, σ is temperature dependent for $T > T_c$. The asymptotic values of $\sigma(T)$ for $T \to \infty$ are reported in Table II: the values of $\sigma_N^{(2)}$ are the closest to the exactly known value $\sigma = -1/6$ for the two-dimensional models, so that for the three-dimensional models the estimate from $\sigma_N^{(2)}$ would be $\sigma = 0.09$ in agreement with previous results.

The measure $d\hat{\phi}_u(\tau)$ was approximated by the measure $d\hat{\phi}_N^*(\tau)$ according to (2.12). The procedure is reliable since the sequences α_n and β_n converge very fast to limits α and β which were computed using the Thiele extrapolation algorithm. We have calculated the sums $\sum_{n=1}^{N} K_n$ and $\sum_{n=1}^{N} nK_n$ where

$$K_n = \left|1 - \frac{\beta_n}{\beta}\right| + \frac{|\alpha_{n-1} - \alpha|}{\sqrt{\beta}}$$

which give an idea of how fast the α_n and β_n converge to their limits α and β, as indicated in Appendix 2.

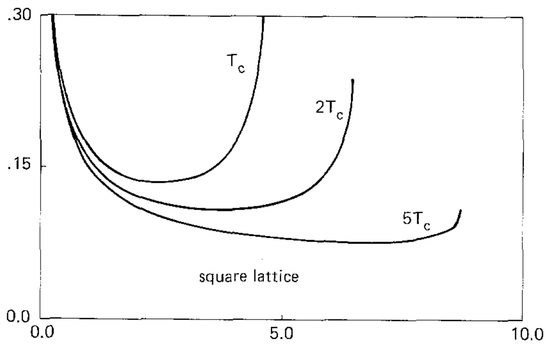
Table III. Partial Sums of the Series Specifying the Convergence of the Sequences α_n and β_n to Their Limits. Sequences

		$x = \frac{1}{2}x_c$		$x = x_c$	
	N	$\sum_{n=1}^{N} k_n$	$\sum_{n=1}^{N} nk_n$	$\sum_{n=1}^{N} k_n$	$\sum_{n=1}^{N} nk_n$
Square lattice	1	1.003069	1.003069	1.023669	1.023669
	2	1.005132	1.007196	1.050449	1.077229
	3	1.005200	1.007399	1.056753	1.096142
	4	1.005208	1.007431	1.059826	1.108433
	5	1.005209	1.007439	1.061590	1.117253
	6	1.005210	1.007440	1.062750	1.124214
	7	1.005210	1.007441	1.063574	1.129980
Diamond lattice	1	1.005073	1.005073	1.025372	1.025372
	2	1.008803	1.012533	1.061084	1.096796
	3	1.008973	1.013115	1.076309	1.142472
	4	1.009011	1.013170	1.083411	1.170877
	5	1.009012	1.013178	1.087674	1.192195
	6	1.009013	1.013180	1.090492	1.209103

We have only calculated these sums for $x=\frac{1}{2}x_c$ and $x=x_c$ because we can find the limits α and β exactly for $x<x_c$ by the equations

$$\alpha-2\sqrt{\beta}=0 \qquad \alpha+2\sqrt{\beta}=\frac{4}{1-u}$$

It is clear from Table III that below the critical temperature these sums increase very slowly as N increases. At the critical temperature we see, however, that the sum $\sum_{n=1}^{N} nK_n$ increases more rapidly, which is consistent with the fact that we find an index σ different from $\pm\frac{1}{2}$ for this temperature. Indeed, as explained in Appendix 2, when this sum converges one can only have square root singularities at the endpoints of the interval. The absence of point masses in the measure $d\hat{\phi}_N^*(\tau)$ is indicated by the convergence of



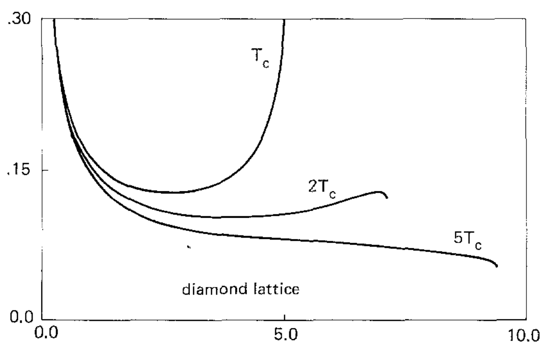


Fig. 4. The approximation to the density of the Lee–Yang measure on $[0, A(u)-\varepsilon]$ where $\varepsilon=A(u)/100$ for the square and diamond lattice at the temperatures $T=T_c$, $2T_c$, and $5T_c$.

$x_{n,n}$ to its limit: if an isolated point mass is present then this convergence would be exponential and we find instead a convergence of the order n^{-2}. The results for $d\phi_N^*(\tau)$ are shown in Figs. 4 and 5 for T_c, $2T_c$ and $5T_c$. Below the critical temperature the behavior of the measure $d\hat{\phi}_N^*(\tau)$ is always the same, characterized by end point singularities with exponent $-\frac{1}{2}$. At higher temperatures the behavior changes considerably and there is good agreement with a negative exponent at the endpoint $A(u)$ for the two-dimensional models. For the three-dimensional models the behavior of the curves at $A(u)$ is consistent with a small positive index at high temperature and an index close to $\frac{1}{2}$ comes out for the Bethe models. It can be noticed that the actual approximation $d\hat{\phi}_N^*$ has square root singularities at the endpoints 0 and A but the presence of near lying poles (the polynomials in the denominator of (2.12) have no zeros in $[0, A]$) can simulate a behavior

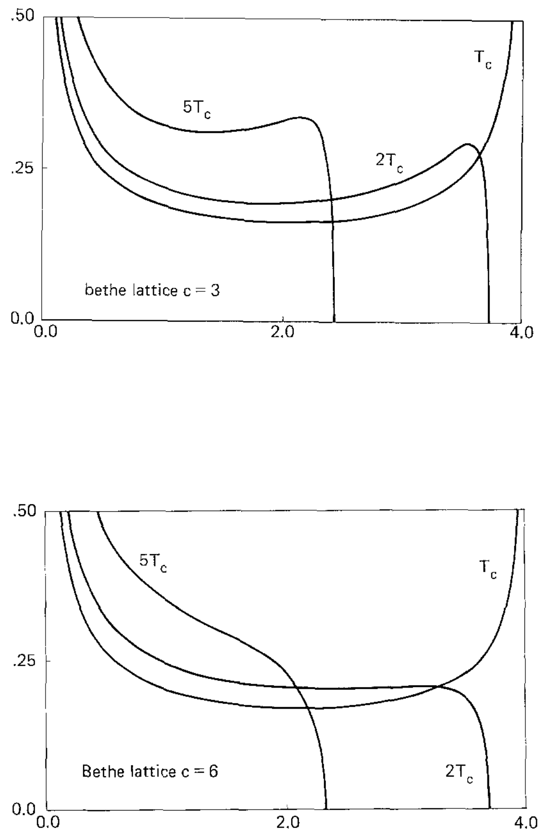


Fig. 5. The approximation of the density of the Lee–Yang measure for the Bethe lattice on $[0, 4\cos^2(\vartheta_0/2)]$ for $T=T_c$, $2T_c$ and $5T_c$.

with a different index. This is the reason why we have excluded a small neighborhood of A in plotting the density of $d\hat{\phi}_N^*$. The singularity at 0 is always consistent with $-\frac{1}{2}$ for all the models at all temperatures. The direct computation of this index using the sequences (3.2) confirms this result with high accuracy (at least 10^{-6}).

CONCLUSIONS

The method we propose to analyze the Lee–Yang measure and its relevant parameters relies upon the properties of the orthogonal polynomials associated to it rather than on best-fitting methods. Information about the regularity of the measure is obtained and smooth approximations are computed. Their behavior is consistent with the indices of the endpoint singularities computed with independent procedures.

ACKNOWLEDGMENTS

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APPENDIX 1

In this appendix we give results on the behavior of the orthonormal polynomials $p_n(x)$ belonging to a measure $d\phi(\tau)$ on the interval $[-1, 1]$. The results can easily be generalized to an arbitrary interval $[a, b]$. We will frequently use the notation $a_n \approx b_n$ which means that there exist two constants c_1 and c_2 such that, for every n, $0 < c_1 \leqslant a_n/b_n \leqslant c_2 < \infty$. As before $x_{1,n} < x_{2,n} < \cdots < x_{n,n}$ the zeroes of $p_n(x)$ in increasing order.

Theorem 1. If $d\phi(\tau)$ is absolutely continuous in $[1-\varepsilon, 1]$ for some $\varepsilon > 0$ and if $\phi'(\tau) \approx (1-\tau)^\sigma$ $(\sigma > -1)$ for $\tau \in [1-\varepsilon, 1]$, then for every $x_{n+1-j,n} \in [1-\varepsilon, 1]$

$$1 - x_{n+1-j,n} \approx \frac{j^2}{n^2} \tag{A.1}$$

Proof. Define $\vartheta_{j,n}$ by $x_{j,n} = \cos \vartheta_{j,n}$ $(j = 1,..., n)$ and set $x_{n+1,n} = 1$ $(\vartheta_{n+1,n} = 0)$, then from Theorem 21, p. 165[16] we find

$$\vartheta_{n-k,n} - \vartheta_{n+1-k,n} \approx 1/n$$

hence

$$\vartheta_{n+1-j,n} = \sum_{k=0}^{j-1} (\vartheta_{n-k,n} - \vartheta_{n+1-k,n}) \approx \frac{j}{n}$$

from which the theorem follows immediately.

The asymptotic behavior (A.1) is not always valid for absolutely continuous measures. An interesting counterexample is given by the Pollaczek polynomials for which $1 - x_{n,n} \approx 1/n$.[17] The exponent $s = 2$ is an indication that the behavior of the density near the endpoint is smooth; the Pollaczek density tends exponentially fast to zero near the endpoints ± 1.

Theorem 2. If $d\phi(\tau)$ is absolutely continuous in $[1-\varepsilon, 1]$ for some $\varepsilon > 0$ and if $\phi'(\tau) \approx (1-\tau)^\sigma$ $(\sigma > -1)$ for $\tau \in [1-\varepsilon, 1]$ then

$$[n-1/n](1) \approx \begin{cases} n^{-2\sigma} & -1 < \sigma < 0 \\ \log n & \sigma = 0 \\ 1 & \sigma > 0 \end{cases} \tag{A.2}$$

Proof. The $[n-1/n]$ Padé approximant to $\int_{-1}^{1} d\sigma(\tau)/(z-\tau)$ is given by

$$[n-1/n](z) = \sum_{j=1}^{n} \frac{\lambda_{j,n}}{z - x_{j,n}}$$

where $\{\lambda_{j,n}\ j = 1,\dots, n\}$ are the Christoffel numbers or Gauss–Jacobi weights for the measure $d\phi(\tau)$. We split up $[n-1/n](1)$ in two parts

$$[n-1/n](1) = \sum_{|1-x_{j,n}| < \varepsilon} \frac{\lambda_{j,n}}{1-x_{j,n}} + \sum_{|1-x_{j,n}| \geqslant \varepsilon} \frac{\lambda_{j,n}}{1-x_{j,n}} = S_1 + S_2$$

For the second sum one easily finds

$$S_2 \leqslant \frac{1}{\varepsilon} \sum_{j=1}^{n} \lambda_{j,n} = \frac{1}{\varepsilon}$$

$$S_2 \geqslant \frac{1}{2} \sum_{|1-x_{j,n}| \geqslant \varepsilon} \lambda_{j,n} \sim \frac{1}{2} \int_{1-\varepsilon}^{1} d\phi(\tau)$$

from which $S_2 \approx 1$ follows. According to Theorem 27 (pp. 119–120)[16] the first sum behaves as

$$S_1 \approx \frac{1}{n} \sum_{|1-x_{j,n}| < \varepsilon} \frac{\left(\sqrt{1-x_{j,n}} + \frac{1}{n}\right)^{2\sigma+1}}{1-x_{j,n}}$$

and by (A.1)

$$S_1 \approx n^{-2\sigma} \sum_{|1-x_{j,n}|<\varepsilon} j^{2\sigma-1}$$

The number of terms in this summation is approximately (Theorem 12.7.2, p. 310)[17]

$$\frac{n}{\pi}\int_{1-\varepsilon}^{1} \frac{dt}{\sqrt{1-t^2}} = n\Delta$$

so that

$$S_1 \approx n^{-2\sigma} \sum_{j=1}^{n\Delta} j^{2\sigma-1}$$

The result now follows immediately from

$$\sum_{j=1}^{n\Delta} j^{2\sigma-1} \approx \begin{cases} 1 & -1<\sigma<0 \\ \log n & \sigma=0 \\ n^{2\sigma} & \sigma>0 \end{cases}$$

Theorem 3. Suppose $d\phi(t) = w(t)\,dt$ where $w(t)$ is a generalized Jacobi weight[16,18]

$$w(t) = \chi(t)(1-t)^{\sigma}(1+t)^{\beta} \prod_{k=1}^{N} |t_k - t|^{\sigma_k} \qquad -1<t<1$$

where σ, β, $\sigma_k > -1$, $-1 < t_1 < t_2 < \cdots < t_N < 1$ and $\chi(t)$ is a positive continuous function on $[-1, 1]$ for which

$$\int_0^2 \frac{\omega(t)}{t}\,dt < \infty$$

with $\omega(\delta) = \sup\{|\chi(t) - \chi(s)|;\ |s-t| < \delta\}$. For the normalized orthogonal polynomials belonging to the weight $w(t)$ one finds

$$p_n(1) \approx n^{\sigma+1/2} \tag{A.3}$$

$$p_n(x_{n+1,n+1}) \approx n^{\sigma-1/2} \tag{A.4}$$

Proof. (i) is just Corollary 34 (p. 171)[16] while (ii) follows from Theorem 31 (p. 170)[16] combined with (A.1).

APPENDIX 2

In this appendix we review some properties of the measures $d\phi(t)$ of orthogonal polynomials for which the recurrence coefficients (the coefficients of the Jacobi matrix) converge to finite limits. Suppose a sequence $p_n(t)$ of orthogonal polynomials satisfies a three term recurrence relation

$$a_{n+1} p_{n+1}(t) + b_n p_n(t) + a_n p_{n-1}(t) = t p_n(t)$$

where $a_{n+1} > 0$, $b_n \in \mathbb{R}$ $(n = 0, 1, 2,...)$ and $p_{-1}(t) = 0$, $p_0(t) = 1$ (in this appendix we have taken $a_n = \sqrt{\beta_n}$ and $b_n = \alpha_n$). A very interesting class of such polynomials is the class for which the coefficients a_n and b_n converge to limits $a > 0$ and b. The simplest example is when all the coefficients are constant, $a_{n+1} = a$ and $b_n = b$ $(n = 0, 1, 2,...)$, which gives the Chebyshev polynomials of the second kind $U_n((x-b)/2a)$ corresponding to the measure $d\phi(t) = w(t)\,dt$ given by

$$w(t) = \frac{1}{2\pi a^2} \sqrt{4a^2 - (t-b)^2} \qquad b - 2a \leqslant t \leqslant b + 2a$$

Other cases of interest are the polynomials for which $a_{n+1} = a$ and $b_n = b$ for $n \geqslant N$. The measure $d\sigma_N(t)$ for this case consists of two parts, $d\phi_N(t) = w_N(t)\,dt + \sum_j c_j \delta(t - t_j)\,dt$ where

$$w_N(t) = \frac{1}{2\pi} \frac{\sqrt{4a^2 - (t-b)^2}}{a^2 p_N^2(t) + a_N^2 p_{N-1}^2(t) - (t-b)\, a_N p_N(t)\, p_{N-1}(t)}; \qquad t \in [b - 2a, b + 2a]$$

and the mass points t_j are the zeros of the polynomial $a^2 p_N^2(t) + a_N^2 p_{N-1}^2(t) - (t-b)\, a_N p_N(t)\, p_{N-1}(t)$ for which

$$\left| \frac{p_{N+1}(t_j)}{p_N(t_j)} \right| < 1$$

All the zeroes of that polynomial are outside $(b - 2a,\ b + 2a)$ since otherwise the density w_N would not be integrable on $(b - 2a, b + 2a)$. There may be a zero at $b \pm 2a$ so that w_N has square root singularities at $b \pm 2a$.

When the sequences a_n and b_n do not attain their asymptotic value after a finite number of steps then the measure $d\phi(t)$ for the orthogonal polynomials is the weak limit of the measure $d\phi_N(t)$. When

$$\sum_{n=1}^{\infty} n \left\{ \left| 1 - \frac{a_n^2}{a^2} \right| + \frac{|b_{n-1} - b|}{a} \right\} < \infty$$

then the truncated measure $d\phi_N(t)$ provides a good approximation to the measure $d\phi(t)$ since one can show[19-21] that $d\phi(t)$ consists again of two parts, $d\phi(t) = w(t)\,dt + \sum_j \delta(t - t_j)\,dt$, where the mass points are finite in number and outside $(b-2a, b+2a)$. The singularities of $w(t)$ at $b \pm 2a$ can only be square root singularities. The weaker condition

$$\sum_{n=1}^{\infty} \left\{ \left| 1 - \frac{a_n^2}{a^2} \right| + \frac{|b_{n-1} - b|}{a} \right\} < \infty$$

still gives a measure $d\phi(t) = w(t)\, dt + \sum c_j\, \delta(t - t_j)\, dt$ but now the number of mass points t_j may be infinite having accumulation points at $b \pm 2a$ while the singularities of $w(t)$ at $b \pm 2a$ may have an index different from $\pm \frac{1}{2}$.

In the general case were $a_n \to a$ and $b_n \to b$ the measure consists of a continuous part (whose points of increase are dense in $[b-2a, b+2a]$) and a pure point spectrum with possible accumulation points in $[b-2a, b+2a]$.[20] If the measure has a largest mass point A greater than $b+2a$ then the convergence of the largest zero $x_{n,n}$ to A is exponentially fast since $(x_{n,n} - A)^{1/n}$ converges to a positive constant less then one.[22]

APPENDIX 3

Given a sequence y_n which can be interpolated according to $y_n = f(1/n^2)$ where $f(x)$ is analytic in a neighborhood of the origin, the limit $\bar{y} = \lim_{n \to \infty} y_n$ is given by the value of $f(x)$ at the origin and approximations to $\bar{y}$ are provided by polynomial or rational interpolations.

Letting $x_n = 1/n^2$ the rational interpolations are obtained by truncating the Thiele continued fraction

$$f(x) = a_1 + \cfrac{x - x_1}{a_2 + \cfrac{x - x_2}{a_3 + \cfrac{\cdots}{a_n + \cfrac{x - x_n}{f_{n+1}(x)}}}}$$

where $f_{n+1}(x)$ is a remainder which fulfills the recurrence

$$f_n(x) = a_n + \frac{x - x_n}{f_{n+1}(x)} \qquad n \geqslant 1, \;\; f_1(x) \equiv f(x)$$

If we are given the sequence x_n, y_n, $1 \leqslant n \leqslant N$ then the a_n, $1 \leqslant n \leqslant N$ are recursively determined by

$$\left\{ a_n = f_n(x_n), f_{n+1}(x_j) = \frac{x_j - x_n}{f_n(x_j) - a_n}, n + 1 \leqslant j \leqslant N \right\} n = 1, \ldots, N-1$$

with the initialization $f_1(x_j) = f(x_j)$, $1 \leqslant j \leqslant N$.

The rational approximations of increasing order $r_n = P_n(x)/Q_n(x)$, $1 \leqslant n \leqslant N$ are given by the recurrence

$$Q_{n+1}(x) = a_{n+1} Q_n(x) + (x - x_n) Q_{n-1}$$
$$P_{n+1}(x) = a_{n+1} P_n(x) + (x - x_n) P_{n-1}$$

initialized by $P_0 = 1$, $P_1 = a_1$, $Q_0 = 0$, $Q_1 = 1$.

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