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# **Eigenvalues of a statistical mechanics matrix**

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**Abstract** We consider the problem of finding the spectrum of an  $n \times n$  matrix which arises in the study of a certain model of long-range interactions in a one-dimensional statistical mechanics system. Our analysis exhibits a curious resemblance of the suitably normalized distribution of eigenvalues to the Marčenko–Pastur law in the limit  $n \rightarrow \infty$ .

Keywords Anti-triagonal matrix · Marčenko-Pastur law · Contractile ring

## **1** Introduction

The purpose of this note is the spectral analysis of certain matrices which arise in the context of a particular toy model of contractile structures from cell biology [1]. Our emphasis here is on the mathematical analysis; still, our article would be incomplete if we did not try to convey to the reader an idea of how these matrices make their appearance in a statistical mechanics system. We begin with that. By 'contractile structure' we mean any subcellular arrangement of macromolecules which exerts a measurable force when attached to an experimental apparatus (which might as well be the cell membrane itself). The example we mostly had in mind is the contractile ring which during the final stages of cytokinesis in many eukaryotes appears to help cleave

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Departamento de Matemáticas Aplicadas y Sistemas, Universidad Autónoma Metropolitana—Cuajimalpa, México, D.F. 01120, Mexico e-mail: zamora@correo.cua.uam.mx a dividing cell in two [2–4]. The chemical composition of this ring suggests a mechanism based on the myosin II-mediated interdigitating of actin filaments. We picture its dynamics locally as that of a one-dimensional arrangement of actin filaments which interact with their immediate neighbors along a random stretch of monomers at their tips, like so:



For obvious reasons, we will call such an arrangement a 'bundle'. The study of bundles in  $1 + \varepsilon$  dimensions, such as



would surely be more appealing, but they are out of our scope at present. Our question is, what can one say about the contractility of a one-dimensional bundle from a thermodynamical point of view? The bundle will certainly tend to contract the stronger the more the individual actin filaments tend to overlap, but shouldn't compact structures be entropically less favored? Leaving aside questions of bending energy or the like, it soon becomes clear that the issue boils down to counting the number of bundle configurations which correspond to a given length of the bundle. Under the hypothesis that each actin filament is composed of exactly n + 1 monomers, the respective formulas then involve an  $n \times n$  matrix of the kind

$$M_{n}(p) := \begin{pmatrix} p & p & \cdots & p & p \\ p^{2} & p^{2} & \cdots & p^{2} & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ p^{n-1} & p^{n-1} & \cdots & 0 & 0 \\ p^{n} & 0 & \cdots & 0 & 0 \end{pmatrix},$$
(1)

where p is a complex number  $\neq 0$ . One might call such matrices 'upper anti-triagonal'. Our aim in this paper is to study their eigenvalues. The problem certainly has some esthetic appeal; after all, the matrices (1) seem to carry a lot of structure, yet do not seem to belong to any of the more popular classes of matrices generally encountered in linear algebra [5]. One can see that they are irreducible, though: just set p = 1 and interpret the resulting matrix as the adjacency matrix of a digraph. Hence, the Perron-Frobenius Theorem applies, so that the thermodynamics of long bundles should be dominated by their largest eigenvalue. For our analysis, we shall find it convenient to write  $p =: q^{-2}$ , and then to focus on the *inverses* of the matrices  $M_n(q^{-2})$ , normalized by  $q^{n+1}$ :

$$\mathcal{M}_{n}(q) := \frac{1}{q^{n+1}} M_{n}^{-1}(q^{-2})$$

$$= \begin{pmatrix} 0 & 0 & \cdots & 0 & q^{n-1} \\ 0 & 0 & \cdots & q^{n-3} & -q^{n-1} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & q^{-(n-3)} & \cdots & 0 & 0 \\ q^{-(n-1)} & -q^{-(n-3)} & \cdots & 0 & 0 \end{pmatrix}.$$
(2)

Hence, if  $\lambda$  is an eigenvalue of  $\mathcal{M}_n(q)$ , then  $q^{-n-1}\lambda^{-1} = p^{(n+1)/2}\lambda^{-1}$  is an eigenvalue of  $\mathcal{M}_n(p)$ . It is also clear that any eigenvalue of  $\mathcal{M}_n(q)$  is an eigenvalue of  $\mathcal{M}_n(-q)$  if *n* is odd, and of  $-\mathcal{M}_n(-q)$  if *n* is even. Since we would expect both cases to behave identically as  $n \to \infty$ , the spectrum of a large matrix  $\mathcal{M}_n$  should be essentially point symmetric with respect to the origin in the complex plane. Indeed, consider the function  $x \mapsto 1 + 2qx + q^2$  from the reals into the complex numbers. Since its image is evidently a straight line somewhere in the complex plane, we can choose a branch of the square root such that the image of either of the two mappings

$$f_q^+, f_q^- : [-1, 1] \mapsto \mathbb{C},$$

$$f_q^+(x) := \sqrt{1 + 2qx + q^2}, \quad f_q^-(x) := -f_q^+(x)$$
(3)

is connected. It then turns out that the majority of eigenvalues of a large matrix  $\mathcal{M}_n$ tends to concentrate around the set  $f_q^+([-1, 1]) \cup f_q^-([-1, 1])$ . Furthermore, it will do so indiscriminately between the two components of the set, although not necessarily so within either of the two: the 'central' portions of each set will be far less crowded than the regions closer to the tips. To make this more precise, we need to recall the definition of the push-forward of a measure: given a measure  $\rho$  on a (measurable) space  $(\Omega, \mathcal{F})$ , and a measurable function f from  $\Omega$  to another measurable space  $(\Omega', \mathcal{F}')$ , we call the push-forward of the measure  $\rho$  under the function f the measure  $f \# \rho$  on  $(\Omega', \mathcal{F}')$  for which  $f \# \rho(A') = \rho(f^{-1}(A'))$  for every  $A' \in \mathcal{F}'$ . Let us choose for  $\rho$  a measure on the interval [-1, 1] with density

$$\frac{d\rho(x)}{dx} = \frac{1}{2\pi\sqrt{1-x^2}} \,. \tag{4}$$

Except for the factor  $\frac{1}{2}$ , this is just a shifted version of the familiar arcsine distribution. We now have the following

#### **Theorem** Let

$$\rho_n := \frac{1}{n} \sum_{k=1}^n \delta_{\lambda_k} \tag{5}$$

denote the empirical distribution of eigenvalues of the  $n \times n$  matrix  $\mathcal{M}_n(q)$  in Eq. (2), and let  $f_q^+$  and  $f_q^-$  be as defined in (3). Then  $\lim_{n\to\infty} \rho_n =: \rho_q$  exists in the sense of

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weak convergence, and decomposes into the push-forwards  $f_q^+ \# \rho$  and  $f_q^- \# \rho$  of the distribution (4) under each of the two mappings  $f_q^+$  and  $f_q^-$ .

In particular,  $\rho_q$  cannot have a density with respect to complex Lebesgue measure. However, we have as a direct consequence of the theorem and the definition of a push-forward that, say,

$$\int_{f_q^+([-1,x])} d(f_q^+ \# \rho)(z) = \int_{-1}^x d\rho(x) ,$$

which after differentiation with respect to x gives

$$\frac{q}{\sqrt{1+2qx+q^2}} \left. \frac{d(f_q^+ \# \rho)(z)}{dz} \right|_{z=f_q^+(x)} = \frac{1}{2\pi\sqrt{1-x^2}} \,,$$

or

$$\frac{d(f_q^+ \# \rho)(z)}{dz} = \frac{z}{\pi \sqrt{\left((q+1)^2 - z^2\right)\left(z^2 - (q-1)^2\right)}} \,. \tag{6}$$

One can call the expression (6) the density of  $\rho_q$  in this sense. There is no reason why this quantity should be non-negative, or even real; it only relates to the measure  $\rho_q$  through a certain way of integration. Its similarity with the Marčenko–Pastur law [6] cannot be overlooked, yet we do not have an intuitive explanation for this. Rather, we prove our result by direct calculation.

## 2 Proof of the theorem

Our strategy of proof will be to show that the moment-generating functions of the empirical measures defined in (5) converge to the moment-generating function of the limiting distribution  $\rho_q$ . We calculate the latter first: by point symmetry of  $\rho_q$  with respect to 0, its odd moments are zero, whereas we have for its even moments

$$\begin{split} \mu_{2r} &= \int\limits_{f_q^+ ([-1,1])} z^{2r} \, d(f_q^+ \# \rho)(z) + \int\limits_{f_q^- ([-1,1])} z^{2r} \, d(f_q^- \# \rho)(z) \\ &= \int\limits_{-1}^1 \frac{(1+2qx+q^2)^r}{\pi\sqrt{1-x^2}} \, dx = \frac{1}{\pi} \int\limits_{0}^{\pi} (1+2q\cos\varphi+q^2)^r \, d\varphi \leq (1+|q|)^{2r} \, , \end{split}$$

again by definition of the push-forward. Hence, we have for the moment-generating function,

$$m_q(\lambda) := \sum_{r=0}^{\infty} \mu_{2r} \lambda^{2r} = \frac{1}{\pi} \int_0^{\pi} \frac{1}{1 - \lambda^2 (1 + 2q \cos \varphi + q^2)} d\varphi$$
$$= \frac{1}{\pi \left(1 - (1 + q^2)\lambda^2\right)} \int_0^{\pi} \frac{1}{1 - \frac{2q\lambda^2 \cos \varphi}{1 - (1 + q^2)\lambda^2}} d\varphi$$

for any complex  $\lambda$  for which  $|\lambda| < 1 + |q|$ . But

$$\frac{1}{\pi} \int_{0}^{\pi} \cos^{2r} \varphi \, d\varphi = \frac{1}{4^{r}} \binom{2r}{r} = (-1)^{r} \binom{-1/2}{r},$$

which after a little bit of algebra gives

$$m_q(\lambda) = \frac{1}{\sqrt{1 - 2(q^2 + 1)\lambda^2 + (q^2 - 1)^2\lambda^4}} \,. \tag{7}$$

We now calculate the moment-generating functions of the empirical measures (5). We start by working out the characteristic polynomial

$$\mathcal{D}_{n} :=: \mathcal{D}_{n}(\lambda, q) := \begin{vmatrix} -\lambda & 0 & \cdots & 0 & q^{n-1} \\ 0 & -\lambda & \cdots & q^{n-3} & -q^{n-1} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & q^{-(n-3)} & \cdots & -\lambda & 0 \\ q^{-(n-1)} & -q^{-(n-3)} & \cdots & 0 & -\lambda \end{vmatrix}$$

Laplace expansion with respect to the first row yields

$$\mathcal{D}_{n} = -\lambda \begin{vmatrix} -\lambda & 0 & \cdots & q^{n-3} & -q^{n-1} \\ 0 & -\lambda & \cdots & -q^{n-3} & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ q^{-(n-3)} & -q^{-(n-5)} & \cdots & -\lambda & 0 \\ -q^{-(n-3)} & 0 & \cdots & 0 & -\lambda \end{vmatrix} \\ + (-q)^{n-1} \begin{vmatrix} 0 & -\lambda & \cdots & 0 & q^{n-3} \\ 0 & 0 & \cdots & q^{n-5} - q^{n-3} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & q^{-(n-3)} & \cdots & 0 & -\lambda \\ q^{-(n-1)} - q^{-(n-3)} & \cdots & 0 & 0 \end{vmatrix}$$

We 'rotate' the first determinant by  $180^{\circ}$ —that is to say, we interchange the *k*th and (n - k)th rows and columns for  $k = 1, 2, ..., \lceil n/2 \rceil$ , and then divide the result by  $(-q)^{n-1}$ . This amounts to dividing each entry in the determinant by -q, hence

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$$\begin{vmatrix} \lambda/q & 0 & \cdots & 0 & q^{-(n-2)} \\ 0 & \lambda/q & \cdots & q^{-(n-4)} & -q^{-(n-2)} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & q^{n-4} & \cdots & \lambda/q & 0 \\ q^{n-2} & -q^{n-4} & \cdots & 0 & \lambda/q \end{vmatrix} = \mathcal{D}_{n-1}(-\lambda/q, 1/q) \, .$$

Then we Laplace expand the second determinant with respect to the final row. Overall,

$$-\mathcal{D}_n(\lambda,q) = (-q)^{n-1}\lambda \mathcal{D}_{n-1}(-\lambda/q,1/q) + \mathcal{D}_{n-2}(\lambda,q), \qquad (8)$$

which can be iterated if one treats the odd and even cases separately; for brevity, we focus on n = 2m + 1 odd, and obtain

$$\frac{\mathcal{D}_{2m+1}}{q^{2m}} = \frac{\lambda^2 - 1}{q^2} \frac{\mathcal{D}_{2m-1}}{q^{2m-2}} - (-1)^m \left(\lambda + \frac{\lambda^2}{q^2} \sum_{k=0}^{m-2} (-1)^k \frac{\mathcal{D}_{2k+1}}{q^{2k}}\right).$$
(9)

This is a linear recurrence (in the unknowns  $q^{-2m}\mathcal{D}_{2m+1}$ ) with uniformly bounded coefficients, and therefore cannot grow too fast. In particular, we can assume that the generating function

$$g(z) := \sum_{m=1}^{\infty} \mathcal{D}_{2m+1} z^{2m+1}$$

has a non-zero radius of convergence. It is now an easy matter to deduce from (9) that

$$g(z) = \frac{q^2 z^3 - (\lambda - 1)z}{q^2 (z^4 + z^2) - (\lambda^2 - 1)z^2 + 1}$$

and then, making use of (8), that

$$\eta(z) := \sum_{m=0}^{\infty} \mathcal{D}_{2m} z^{2m} = \frac{1 + (q^2 + q\lambda)z^2}{q^2(z^4 + z^2) - (\lambda^2 - 1)z^2 + 1}$$

(we agree on  $\mathcal{D}_0 = 1$  for convenience). To proceed, we write  $\lambda$  in the form

$$\lambda^2 = q^2 + q\left(\nu + \frac{1}{\nu}\right) + 1 \tag{10}$$

for some complex  $\nu \neq 0$ , where for definiteness we can require  $|\nu| \ge 1$ . The denominator of both generating functions now factors into  $(qz^2 - \nu)(qz^2 - 1/\nu)$ , and we obtain

$$g(z) = \nu \frac{q^2 z^3 - (\lambda - 1)z}{\nu^2 - 1} \sum_{m=0}^{\infty} q^m (\nu^{m+1} - \nu^{-m-1}) z^{2m} , \qquad (11)$$

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and a similar formula for  $\eta(z)$ . It follows that  $\lambda$  is an eigenvalue<sup>1</sup> of  $\mathcal{M}_{2m+1}$  if and only if

$$\frac{\nu}{\nu^2 - 1} \left( q^{m+1} (\nu^m - \nu^{-m}) - (\lambda - 1) q^m (\nu^{m+1} - \nu^{-m-1}) \right) = 0.$$
 (12)

We quickly check whether  $\nu = \pm 1$  is a solution. If so, we find from l'Hôpital that

$$\lambda = 1 \pm q \; \frac{m}{m+1} \; ,$$

whereas (10) implies  $\lambda^2 = (1 \pm q)^2$ . This is a contradiction for  $m < \infty$ . We also deduce from (12) that if  $\nu^{m+1} - \nu^{-m-1} = 0$ , then certainly  $\nu^m - \nu^{-m} = 0$  as well, so that  $\nu^{m+1} - \nu^{-m-1} = \nu^{m-1}(\nu^2 - 1) = 0$  or  $\nu = \pm 1$  again, which we have just ruled out. Thus we can safely write

$$\lambda = 1 + q \, \frac{\nu^m - \nu^{-m}}{\nu^{m+1} - \nu^{-m-1}} = 1 + \frac{q}{\nu} - q(\nu - \nu^{-1}) \sum_{k=1}^{\infty} \nu^{-2k(m+1)} \,, \tag{13}$$

provided, of course, that  $|\nu| > 1$ . We now solve our problem for q = 1: in this case, we immediately find from (10) that  $\pm \lambda = \sqrt{\nu} + 1/\sqrt{\nu}$ , and therefore

$$(1 - \sqrt{\nu} - 1/\sqrt{\nu})(\nu^{2m+2} - 1) + \nu^{2m+1} - \nu$$
  
=  $\frac{(\nu^{2m+1}\sqrt{\nu} + 1)(1 - \sqrt{\nu} + \nu - \nu\sqrt{\nu})}{\sqrt{\nu}} = 0.$ 

The second factor here is zero for  $\sqrt{\nu} = 1$ , *i*, and -i, all of which would result in  $\nu = \pm 1$ , and we have already seen that this is impossible. Hence  $\sqrt{\nu}$  is a 4m + 3rd root of -1, and we finally arrive at

$$\lambda_k = (-1)^{n+1} 2\cos\frac{(2k-1)\pi}{2n+1}, \quad k = 1, 2, \dots, n$$
(14)

for a matrix of size n = 2m + 1. (Incidentally, this formula holds for even values of n as well.) There seems to be little hope of solving Eqs. (10) and (13) in terms of  $\nu$  for arbitrary values of q, but we still can use them to obtain valuable information on the magnitude of the eigenvalues: if  $|\nu| = 1$ , then  $\lambda^2 = 1 + 2q \cos \varphi + q^2$  for some  $\varphi \in [0, 2\pi)$ , by Eq. (10). Or, if  $|\nu| > 1$ , then  $\lambda = 1 + q/\nu + O(\nu^{-n})$ , by Eq. (13). Either way, it now follows that  $|\lambda|$  is at most O(1 + |q|) in order of magnitude, so that  $\lambda^n \mathcal{D}_n(\lambda^{-1}, q)$  is non-zero for  $\lambda$  in a sufficiently small neighbourhood of 0. But this implies that  $\log (\lambda^n \mathcal{D}_n(\lambda^{-1}, q))$  is analytic there, and we can write

<sup>&</sup>lt;sup>1</sup> We denote by  $\lambda$  a generic eigenvalue as well as the indeterminate in the characteristic polynomial of a matrix.

$$-\frac{\partial}{\partial\lambda}\log\left(\lambda^{n}\mathcal{D}_{n}(\lambda^{-1},q)\right) = \sum_{k=1}^{n}\frac{\lambda_{k}}{1-\lambda_{k}\lambda} = \sum_{r=1}^{\infty}\left(\sum_{k=1}^{n}\lambda_{k}^{r}\right)\lambda^{r-1}.$$

The term in brackets is *n* times the *r*th moment of the empirical measure  $\rho_n$  in (5), which gives

$$m_n(\lambda) := \frac{1}{n} \sum_{r=0}^{\infty} \mu_r \lambda^r = -\lambda \frac{\partial}{\partial \lambda} \log \sqrt[n]{\mathcal{D}_n(\lambda^{-1}, q)}$$

for the corresponding moment generating function. We are 'weakly' done if we can show that  $\lim_{n\to\infty} m_n(\lambda)$  agrees with (7). This is straightforward: because everything is analytic, we can interchange differentiation and passage to the limit and only need to calculate  $\lim_{n\to\infty} \sqrt[n]{\mathcal{D}_n(\lambda^{-1}, q)}$ . Now (10) implies that  $|\nu| \neq 1$  for  $\lambda$  large enough, so that  $\lim_{n\to\infty} \sqrt[n]{\mathcal{D}_n(\lambda^{-1}, q)}$  is just the square root of the larger<sup>2</sup> of  $\nu$  and  $\nu^{-1}$  in Eq. (11), hence

$$\lim_{n \to \infty} m_n(\lambda) = -\frac{\lambda}{2} \frac{\partial}{\partial \lambda} \left( \frac{\lambda^{-2} - q^2 - 1 + \sqrt{\lambda^{-4} - 2(q^2 + 1)\lambda^{-2} + (q^2 - 1)^2}}{2q} \right)$$
$$= \frac{1}{\sqrt{1 - 2(q^2 + 1)\lambda^2 + (q^2 - 1)^2\lambda^4}}.$$

This was to be proved.

#### 3 An exceptional eigenvalue

It is clear that our analysis of the matrices  $M_n$  might have missed a finite number of eigenvalues of absolute value less than 1. This is somewhat unfortunate, as numerical analysis and a closer look at the matrices  $M_n(p)$  for |p| < 1 suggest the presence of an eigenvalue of size approximately  $p(1 - p)^{-1}$ —indeed, the vector  $(1, p, p^2, \dots, p^{n-1})^{\top}$  is almost a corresponding eigenvector. Since this is a reasonable candidate for the largest eigenvalue of  $M_n(p)$  when p is a Boltzmann weight, its study is of considerable interest for the statistical mechanics model [7]. To begin, we first observe that if the matrix  $M_n(p)$  has an eigenvalue of size close to  $p(1-p)^{-1}$  (or to any value which does not depend on the size of the matrix), then the matrix  $\mathcal{M}_n(q)$  will have an eigenvalue of size comparable to  $q^{-n}$ . Moreover, the system of Eqs. (10) and (13) can readily be solved in terms of q (or  $q^{-1}$ , which under |q| > 1 is of greater interest to us) for any given value of  $\nu$ . In fact,

<sup>&</sup>lt;sup>2</sup> More precisely, the one of larger absolute value.

$$q^{-1} = \frac{\left(\frac{\nu^m - \nu^{-m}}{\nu^{m+1} - \nu^{-m-1}}\right)^2 - 1}{\nu + \nu^{-1} - 2\frac{\nu^m - \nu^{-m}}{\nu^{m+1} - \nu^{-m-1}}} = -\nu^{-1} + O(\nu^{-3}),$$

so that  $q^{-1}$  is given by a power series in  $v^{-1}$  with zero constant term and a non-zero coefficient of  $v^{-1}$ . The implicit function theorem then implies (the catchphrase here might be Lagrange inversion) that  $v^{-1}$ , and therefore  $\lambda$ , can be represented as a Laurent series in  $q^{-1}$ . We calculate its first few terms by means of successive approximation: setting  $\lambda = 0$  in (10) yields v = -q, which by (13) gives

$$\lambda = (1 - q^{-2}) \left( q^{-2m} + O(q^{-4m-2}) \right)$$

If now we insert this into (10), we obtain  $\nu = -q + (1 - q^{-2})q^{-4m-3} + O(q^{-8m-5})$ , and then again, from (13),

$$\lambda = (1 - q^{-2}) \left( q^{-2m} + \left( 2m + 1 - (2m + 2)q^{-2} \right) q^{-6m-2} \right) + O(q^{-10m-4}) \,.$$

Hence, the approximation  $p(1-p)^{-1}$  for the largest eigenvalue of  $M_n(p)$  is correct up to terms of order  $p^{n+1}$ . In particular, the eigenvalue remains finite as  $n \to \infty$ , whereas (14) gives an essentially linear growth

$$\frac{1}{2\cos\left(\frac{n\pi}{2n+1}\right)} \sim \frac{2n+1}{\pi}$$

of the largest eigenvalue of  $M_n(1)$ .

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