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LETTER TO THE EDITOR

The eigenvalue density of rational Jacobi matrices

Jesús S Dehesa

Departamento de Física Nuclear, Facultad de Ciencias, Universidad de Granada, Granada, Spain

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Abstract. The calculation of the density of states of certain physical systems (e.g. the electronic state density of some disordered materials, the nuclear level density, etc) often reduces to the determination of the density of eigenvalues of a rational Jacobi matrix (i.e. a Jacobi matrix whose elements are rational functions of the suffix) when its dimension $N \to \infty$. Here the asymptotical ($N \to \infty$) density of eigenvalues of such a matrix is investigated.

The Hamiltonian of a physical system can often be expressed as a Jacobi matrix, i.e. a real, N-dimensional and symmetric matrix such that the only non-vanishing elements are $H_{ii} = a_i$ and $H_{i,i+1} = H_{i+1,i} = b_i$. This is the case of certain disordered materials in the tight-binding approximation (see e.g. Haydock 1976, Jones 1975 and references therein). Likewise, the nuclear Hamiltonian in the shell model can be written in such a form by means of the Lanczos method of tridiagonalisation (see e.g. Whitehead *et al* 1977 and references therein).

In many cases (see e.g. Gaspard and Cyrot-Lackmann 1973) the Jacobi Hamiltonian H is a rational Jacobi matrix (i.e. it has entries which are rational functions of the suffix) whose elements a_m and b_m have expressions which are instances of the following general one:

$$\begin{aligned} a_m &= Q_\theta(m)/Q_\beta(m) \\ b_m^2 &= Q_\alpha(m)/Q_\gamma(m) \end{aligned} \tag{1}$$

where $Q_\theta(m)$, $Q_\beta(m)$, $Q_\alpha(m)$ and $Q_\gamma(m)$ are polynomials of degree θ, β, α and γ respectively, that is

$$\begin{aligned} Q_\theta(m) &= \sum_{i=0}^{\theta} c_i m^{\theta-i}; \qquad & Q_\beta(m) &= \sum_{i=0}^{\beta} d_i m^{\beta-i} \\ Q_\alpha(m) &= \sum_{i=0}^{\alpha} e_i m^{\alpha-i}; \qquad & Q_\gamma(m) &= \sum_{i=0}^{\gamma} f_i m^{\gamma-i}. \end{aligned} \tag{2}$$

All the c_i's, d_i's, e_i's and f_i's are supposed to be real numbers. Then the calculation of level average properties of certain physical systems often reduces to the determination of spectral average properties of the rational Jacobi matrices. Of special importance among these properties is the asymptotical ($N \to \infty$) level density of the system. The asymptotical eigenvalue density $\rho(x)$ of the Jacobi matrix H is $\rho(x) = \lim_{N\to\infty} \rho^{(N)}(x)$, where $\rho^{(N)}(x)$ is the discrete eigenvalue density of the N-dimensional matrix H. The

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function $\rho^{(N)}(x)$ can be completely characterised by the knowledge of its moments $\mu_r'^{(N)}$, whose expression is as follows (see e.g. Jones 1975 and Whitehead *et al* 1977)

$$\mu_r'^{(N)} = \frac{1}{N} \operatorname{Tr} H^r = \frac{1}{N} \sum_{k=1}^{N} E_r^k; \qquad r = 0, 1, 2, \ldots \tag{3}$$

where $\{E_i, i = 1, \ldots, N\}$ are the eigenvalues of the matrix H. Therefore the moments μ_r' of the asymptotical density $\rho(x)$ are given by

$$\mu_r' = \lim_{N\to\infty} \mu_r'^{(N)}; \qquad r = 0, 1, 2, \ldots. \tag{4}$$

In this letter, compact expressions of the moments of the asymptotical eigenvalue density of the rational Jacobi matrices given by (1) and (2) are explicitly found in terms of the parameters θ, β, α, γ, c_0, d_0, e_0 and f_0. To calculate these quantities we shall proceed as follows. It is known that the characteristic polynomials of the principal submatrices of a Jacobi matrix H form a system of orthogonal polynomials $\{P_n(x)\}_{n=1}^{N}$ which verifies the following recurrence relation

$$\begin{aligned} &P_n(x) = (x - a_n)P_{n-1}(x) - b_{n-1}^2 P_{n-2}(x) \\ &P_{-1} \equiv 0, \qquad P_0 = 1, \qquad n = 1, 2, \ldots, N. \end{aligned} \tag{5}$$

Furthermore the eigenvalues $\{E_k, k = 1, \ldots, N\}$ of the Jacobi matrix H are equal to the zeros $\{x_{kN}, k = 1, \ldots, N\}$ of the polynomial $P_N(x)$. Recently the following result has been shown (Nevai and Dehesa 1978).

Theorem 1

Let R and R^+ be the set of real numbers and the set of positive real numbers respectively. Let $\phi: R^+ \to R^+$ be a non-decreasing function such that for every fixed $t \in R$

$$\lim_{x\to+\infty} \frac{\phi(x+t)}{\phi(x)} = 1.$$

Assume that there exist two numbers a and $b \geq 0$ such that the coefficients in the recurrence relation (5) satisfy

$$\lim_{n\to\infty} \frac{a_n}{\phi(n)} = a \qquad \text{and} \qquad \lim_{n\to\infty} \frac{b_n}{\phi(n)} = \frac{b}{2}.$$

Then for every non-negative integer r

$$\lim_{n\to\infty} \frac{\sum_{k=1}^{n} x_{kn}^r}{\int_0^n [\phi(t)]^r \, dt} = \sum_{j=0}^{[r/2]} b^{2j} a^{r-2j} 2^{-2j} \binom{2j}{j} \binom{r}{2j} \tag{6}$$

where x_{kn} are the zeros of $P_n(x)$ and $[r/2]$ is equal to $r/2$ or $(r-1)/2$ when r is even or odd respectively.

Choosing $\phi(x) = x^A$, $A \geq 0$, one can easily get the following corollary.

Let us suppose that there exists $A \geq 0$ such that the coefficients in the recurrence relation (5) satisfy

$$\lim_{n\to\infty} \frac{a_n}{n^A} = a \in R \qquad \text{and} \qquad \lim_{n\to\infty} \frac{b_n}{n^A} = \frac{b}{2} \geq 0. \tag{7}$$

Then for $r = 0, 1, \ldots$

$$\lim_{n\to\infty} \frac{1}{n} \sum_{k=1}^{n} \left(\frac{x_{kn}}{n^A}\right)^r = \frac{1}{rA+1} \sum_{j=0}^{[r/2]} b^{2j} a^{r-2j} 2^{-2j} \binom{2j}{j} \binom{r}{2j}. \tag{8}$$

For $n = N$, the limit conditions (7) applied to the expressions (1) and (2) of a_n and b_n permit us to write that

$$\begin{aligned} a &= \frac{c_0}{d_0} \lim_{N\to\infty} N^{\theta-(A+\beta)} \\ b &= 2\sqrt{\frac{e_0}{f_0}} \lim_{N\to\infty} N^{\alpha-(A+\gamma)}. \end{aligned} \tag{9}$$

Note that $a \in R$ and $b \geqslant 0$ happen when the following two inequalities are fulfilled:

$$\theta \leqslant A + \beta \qquad \alpha \leqslant A + \gamma. \tag{10}$$

In particular expressions (9) show that

$$\begin{aligned} \theta < A + \beta &\Rightarrow a = 0 \\ \theta = A + \beta &\Rightarrow a = c_0/d_0 \end{aligned} \tag{11}$$

and

$$\begin{aligned} \alpha < A + \gamma &\Rightarrow b = 0 \\ \alpha = A + \gamma &\Rightarrow b = 2\sqrt{e_0/f_0}. \end{aligned} \tag{12}$$

From relations (3)–(4) and (8)–(10) one can readily get the following result.

Theorem 2

The moments of the asymptotical eigenvalue density $\rho(x)$ of a rational Jacobi matrix with elements a_n and b_n given by relations (1) and (2) are expressed as follows

$$\mu'_r = \sum_{j=0}^{[r/2]} b^{2j} a^{r-2j} 2^{-2j} \binom{2j}{j} \binom{r}{2j} \qquad r = 0, 1, 2, \ldots \tag{13}$$

where a and b are given by expressions (11) and (12).

This theorem classifies the rational Jacobi matrices (1) and (2) into four different classes according to the values of the parameters θ, β, α and γ; namely, (I) matrices with $\theta < \beta$ and $\alpha < \gamma$, (II) matrices with $\theta < \beta$ and $\alpha = \gamma$, (III) matrices with $\theta = \beta$ and $\alpha < \gamma$, and (IV) matrices with $\theta = \beta$ and $\alpha = \gamma$. It is clear that rational Jacobi matrices belonging to these four classes have different values for the quantities μ'_r. Expression (13) gives these values. They are as follows.

Class I. $\theta < \beta$ and $\alpha < \gamma$. Relations (11) and (12) show that $a = 0$ and $b = 0$. Then

$$\mu'_r = 0, \qquad r = 1, 2, \ldots.$$

Class II. $\theta < \beta$ and $\alpha = \gamma$. Here $a = 0$ and $b = 2\sqrt{e_0/f_0}$. Then

$$\mu'_{2k} = \left(\frac{e_0}{f_0}\right)^k \binom{2k}{k} \qquad \mu'_{2k+1} = 0 \qquad k = 0, 1, 2, \ldots.$$

Class III: $\theta=\beta$ and $\alpha<\gamma$. Here $a=c_0/d_0$ and $b=0$. Then

$$\mu'_r=(c_0/d_0)^r, \qquad r=0,1,2,\ldots.$$

Class IV. $\theta=\beta$ and $\alpha=\gamma$. Here $a=c_0/d_0$ and $b=2\sqrt{e_0/f_0}$. Then

$$\mu'_r=\sum_{j=0}^{[r/2]}\left(\frac{e_0}{f_0}\right)^j\left(\frac{c_0}{d_0}\right)^{r-2j}\binom{2j}{j}\binom{r}{2j}, \qquad r=0,1,2\ldots.$$

Let me finally remark that a complete study and classification of the rational Jacobi matrices (1) and (2) according to their asymptotical eigenvalue density should also consider those matrices with $\theta>\beta$ and/or $\alpha>\gamma$. Such matrices do not satisfy the conditions of theorem 1. That is why they do not appear in our study. Nevertheless they are also important in physics. In fact, the theory of electron structure of disordered systems has studied (Gaspard and Cyrot-Lackmann 1973) the effect on the matrix elements a_n and b_n, of the electron energy band singularities, of internal band singularities and of band gaps. Particularly if the band is unbounded, the coefficients b_n tend to plus infinity.

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