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Rational Jacobi matrices and certain quantum mechanical problems

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Abstract. In several branches of physics the Hamiltonian of a many-body system can be reduced to a rational Jacobi matrix (i.e. a Jacobi matrix whose elements are rational functions of the suffix) by means of a method of the Lanczos type. Here it is shown that one can calculate in a simple analytical way the asymptotic eigenvalue density of all these matrices by means of its moments without solving the corresponding eigenvalue problem. The method is applied to a large class of quantum mechanical models of Hamiltonians.

1. Introduction

The Lanczos method allows us to reduce (Mattis 1981) a large number of physical systems to a one-dimensional chain of artificial entities with nearest-neighbour coupling. This is done (Lanczos 1950, Paige 1972) by means of the transformation of the Hamiltonian of the system into a Jacobi matrix, i.e. a N-dimensional real tridiagonal and symmetric matrix. This method has been successfully used in solid state physics (Haydock 1976, Bullet *et al* 1980), nuclear physics (Whitehead *et al* 1977), statistical mechanics (Mori 1965), etc to study both individual (i.e. wavefunctions and energy levels) and collective (i.e. density of levels and states) properties of many different systems.

Often (De Brucq and Tirapegui 1968, 1970, Gaspard and Cyrot–Lackman 1973) the Jacobi Hamiltonian H is a rational matrix; that is a matrix the entries of which are rational functions of the suffix. Recently one of us (Dehesa 1978) has proposed in a paper, henceforth to be referred to as paper I, a method which allows us to calculate in a simple analytical way, the eigenvalue density of rational Jacobi matrices by means of its moments. The purpose of this paper is to complete this method and to apply it to certain matrices of this rational type encountered in certain quantum mechanical problems.

2. Main results

Let $H_{n,n} = a_n$ and $H_{n+1,n} = b_n$ be the only non-vanishing elements of the Jacobi Hamiltonian. Throughout this paper we will use the same symbols and notation as in I. In particular $\rho^{(N)}(x)$ and $\rho(x)$ denote the eigenvalue density of H and its asymptotic limit $N \to \infty$, respectively. The moments of these two density functions are $\mu_r'^{(N)}$ and μ_r', also respectively. Besides, let us consider the two following asymptotic eigenvalue densities

$$\rho^*(x) = \lim_{N\to\infty} \rho^{(N)}(x/N^{(\alpha-\gamma)/2})$$

$$\rho^{**}(x) = \lim_{N\to\infty} \rho^{(N)}(x/N^{\theta-\beta})$$

the moments of which are

$$\mu_r'' = \lim_{N\to\infty} \mu_r'^{(N)}/N^{r(\alpha-\gamma)/2}$$

$$\mu_r''' = \lim_{N\to\infty} \mu_r'^{(N)}/N^{r(\theta-\beta)}$$

$r = 0, 1, 2, \ldots$, respectively. In paper I the following result is found. Assume the existence of a real number $A \geqslant 0$ such that

$$\lim_{n\to\infty} \frac{a_n}{n^A} = a \in \mathbb{R} \qquad \text{and} \qquad \lim_{n\to\infty} \frac{b_n}{n^A} = \frac{b}{2} \geqslant 0. \tag{1}$$

Then for $r = 0, 1, 2, \ldots$

$$\lim_{N\to\infty} \frac{\mu_r'^{(N)}}{N^{rA}} = \frac{1}{rA+1} \sum_{j=0}^{[r/2]} \left(\frac{b}{2}\right)^{2j} a^{r-2j} \binom{2j}{j} \binom{r}{2j}. \tag{2}$$

Now let us apply this result to a rational Jacobi Hamiltonian, that is a Jacobi matrix with

$$a_n = Q_\theta(n)/Q_\beta(n), \qquad b_n^2 = Q_\alpha(n)/Q_\gamma(n) \tag{3}$$

where the Q's are arbitrary polynomials defined as follows

$$\begin{aligned} Q_\theta(n) &= \sum_{i=0}^{\theta} c_i n^{\theta-i}, \qquad & Q_\beta(n) &= \sum_{i=0}^{\beta} d_i n^{\beta-i}, \\ Q_\alpha(n) &= \sum_{i=0}^{\alpha} e_i n^{\alpha-i}, \qquad & Q_\gamma(n) &= \sum_{i=0}^{\gamma} f_i n^{\gamma-i}. \end{aligned} \tag{4}$$

In this case, equations (1) say that

$$a = \frac{c_0}{d_0} \lim_{N\to\infty} N^{(\theta-\beta)-A} \qquad \text{and} \qquad b = 2\left(\frac{e_0}{f_0}\right)^{1/2} \lim_{N\to\infty} N^{(\alpha-\gamma)/2-A}.$$

(Please note an error in equation (9) of paper I which however does not affect the results of it.) Then it is clear that the conditions

$$\theta - \beta \leqslant A \qquad \text{and} \qquad \tfrac{1}{2}(\alpha-\gamma) \leqslant A$$

have to be fulfilled so that $a \in \mathbb{R}$ and $b \geqslant 0$. In particular one has

$$\theta-\beta < A \Rightarrow a = 0; \qquad \tfrac{1}{2}(\alpha-\gamma) < A \Rightarrow b = 0$$

$$\theta-\beta = A \Rightarrow a = c_0/d_0; \qquad \tfrac{1}{2}(\alpha-\gamma) = A \Rightarrow b = 2(e_0/f_0)^{1/2}.$$

Thus, there are four different classes of rational Jacobi matrices (3)–(4) according to the values of the parameters θ, β, α and γ. They are as follows

Class I. $\theta<\beta$ and $\alpha<\gamma$. Here $a=0$ and $b=0$. Then

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

Class II. $\theta-\beta<\frac{1}{2}(\alpha-\gamma)$. Here $a=0$ and $b=2(e_0/f_0)^{1/2}$. Then

$$\begin{aligned}\mu''_{2k}&=\frac{1}{k(\alpha-\gamma)+1}\left(\frac{e_0}{f_0}\right)^k\binom{2k}{k}\\ \mu''_{2k-1}&=0, \qquad k=1,2,\ldots.\end{aligned} \tag{5}$$

We remark that all μ'_r will diverge unless $\alpha=\gamma$; in this case $\rho(x)=\rho^*(x)$ and $\mu'_r=\mu''_r$ for all r.

Class III. $\theta-\beta>\frac{1}{2}(\alpha-\gamma)$. Here $a=c_0/d_0$ and $b=0$. Then

$$\mu'''_r=\frac{1}{r(\theta-\beta)+1}\left(\frac{c_0}{d_0}\right)^r, \qquad r=0,1,2,\ldots$$

and all the moments μ'_r diverge unless $\theta=\beta$. In the latter case $\rho(x)=\rho^{**}(x)$ and $\mu'_r=\mu'''_r=(c_0/d_0)^r$.

Class IV. $\theta-\beta=\frac{1}{2}(\alpha-\gamma)$. Here $a=c_0/d_0$ and $b=2(e_0/f_0)^{1/2}$. Then $\rho^*(x)=\rho^{**}(x)$ with

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

for $r=0,1,2,\ldots$ and where $[r/2]$ is equal to $r/2$ or $(r-1)/2$ according to whether r is even or odd respectively. Besides, only if $\theta=\beta$ it happens that $\rho(x)=\rho^*(x)=\rho^{**}(x)$ with $\mu'_r=\mu''_r=\mu'''_r$. Otherwise all the μ'_r would diverge.

3. Application

The Hamiltonians of a class of quantum field theory models in zero dimensions can be represented in a suitable basis of Hilbert space by rational Jacobi matrices (De Brucq and Tirapegui 1968, 1970). Indeed, let us consider the class of models defined by the Lagrangian (the fields φ only depend on time t) (De Brucq and Tirapegui 1968)

$$L=\varphi^+(\mathrm{i}\,\partial/\partial t-\mu)\varphi-g(\varphi^{+v}\varphi^u+\varphi^{+u}\varphi^v) \tag{6}$$

where u and v are integers such that $v>u\geqslant1$, the symbol T^+ stands for the adjoint of the operator T, and g is a coupling constant. For these models the corresponding Hamiltonians are as follows:

$$H\doteq\mu b^+b+g(b^{+v}b^u+b^{+u}b^v)$$

where $\varphi(t)=b\exp(-\mathrm{i}\mu t)$ has been used, and the operators b and b^+ satisfy the commutation relation $[b,b^+]=1$. In the invariant space $E^{(k)}$ (i.e. the subspace of the Hilbert space of any of these models which is spanned by the orthonormal basis $(|(n-1)q+k\rangle,\ n\geqslant1,\ k=1,2,\ldots,\ q\equiv v-u)$ the Hamiltonian H can be represented by the Jacobi matrix of elements

$$a_n = [(n-1)q + k]\mu, \qquad n \geq 1$$
$$b_n^2 = g^2 \frac{(nq+k)![(n-1)q+k]!}{\{[(n-1)v - nu + k]!\}^2}. \tag{7}$$

These expressions are of the rational form (3)–(4) with

$$\theta = 1, \qquad c_0 = q\mu, \qquad \beta = 0, \qquad d_0 = 1$$

and

$$\tfrac{1}{2}(\alpha - \gamma) = \tfrac{1}{2}(v+u) > 1, \qquad e_0/f_0 = g^2 q^{v+u}.$$

Then $\theta - \beta = 1$ is smaller than $\frac{1}{2}(\alpha - \gamma)$. Therefore the Jacobi Hamiltonian (7) belongs to class II. As a consequence of this, all the moments μ'_r of the asymptotic eigenvalue density $\rho(x)$ are diverging. In this case, however, one can divide all the eigenvalues of the spectrum by $N^{(\alpha-\gamma)/2} = N^{(v+u)/2}$ and then study the eigenvalue distribution in the limit $N \to \infty$ by means of the density function $\rho^*(x) = \lim_{N\to\infty} \rho^{(N)}(x/N^{(v+u)/2})$, the moments of which are according to (5) as follows

$$\mu''_{2k} = \frac{g^{2k} q^{(v+u)k}}{k(v+u)+1} \binom{2k}{k}$$
$$\mu''_{2k-1} = 0, \qquad k = 1, 2, \ldots.$$

These quantities completely specify how the eigenenergies, if appropriately scaled, of the Hamiltonian H are concentrated or better distributed all over the spectrum in the asymptotic case. In particular since all the moments of odd order vanish, the distribution is symmetric around the origin. Besides, the second and fourth moments allow us to find the variance and the excess of such a distribution.

Finally let us say that the class of models (6) has been only used with the purpose of illustrating the applicability of our method to determining the asymptotic eigenvalue distribution without the need to solve the associated eigenvalue problem. The method can be applied in the same straightforward way as described here to other classes of Lagrangians more general than (6) encountered in some quantum mechanical problems (De Brucq and Tirapegui 1970), to several types of tight-binding Hamiltonians of disordered materials (Cyrot-Lackman 1973, Dehesa 1984), etc.

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