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Level density of physical systems with Lanczos-type Hamiltonians

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The classification of physical systems according to their level density is studied. Here a large class of (bounded and unbounded) Lanczos-type Hamiltonians which have a very general level-density function are identified. This function is given in integral form and only depends on a few parameters which govern the asymptotic behavior of the matrix elements. These may behave differently according to whether the index is even or odd. Several previous findings of various authors are found as particular cases. Enlarged subclasses of Hamiltonians having for their level density functions of regular, uniform, Wigner, Weyl, Karamata, and hypergeometric types are explicitly given. There exist a rich variety of physical systems characterized by these kinds of Hamiltonians.

Lanczos-type Hamiltonians characterize numerous physical systems[1,2] ranging from atoms and molecules[3] to disordered materials[4] and nuclei;[5] see also Ref. 6 for a brief summary. Their matrix representation is of Jacobi type (i.e., a tridiagonal symmetric matrix) which is usually truncated so that the associated eigenvalue problem can be computed.[1-5]

At times the N-dimensional Lanczos Hamiltonian matrix H is bounded, that is, its only nonvanishing entries $H_{n,n}=a_n$, $H_{n,n+1}=H_{n+1,n}=b_n$ have finite limits as the index goes to infinity. The authors have shown[7] that the quantum systems with a bounded Lanczos Hamiltonian satisfying

$$\lim_{n\to\infty} a_n = a \in R \quad \text{and} \quad \lim_{n\to\infty} b_n = b \geq 0 \tag{1}$$

(R is the set of real numbers) have a regular level-energy behavior, i.e., the level energies are distributed according to an inverted semicircle law.

However, unbounded Hamiltonians H seem to be closer to reality. Recently,[6,8] the total density of levels, with the appropriate scaling, of the Lanczos Hamiltonians subject to

$$\lim_{n\to\infty} (a_n/n^\alpha) = a \in R \quad \text{and} \quad \lim_{n\to\infty} (b_n/n^\alpha) = b/2 \geq 0 \tag{2}$$

with $\alpha \geq 0$ has been found. The resulting level density is a function of (i) Karamata or generalized Weyl type[9,10] for $b=0$ and $\alpha>0$, (ii) hypergeometric type[6] for $a=0$ and $b>0$, and (iii) Appell's hypergeometric type[8] for a and b different from zero and $\alpha>0$. Subclasses of the class of the Hamiltonians subject to the conditions (2) are formed by Hamiltonians with level-density functions of regular, uniform, Karamata (also called powerlike or generalized Weyl), logarithmic, Wigner, and hypergeometric types.

Here we will extend the previous results by means of the determination of the total level density of the Lanczos Hamiltonians H having the asymptotic behavior

$$\begin{aligned} &\lim_{n\to\infty} (a_{2n}/\lambda_{2n}) = \alpha_1, \quad \lim_{n\to\infty} (b_{2n}/\lambda_{2n}) = \beta_1 , \\ &\lim_{n\to\infty} (a_{2n+1}/\lambda_{2n}) = \alpha_2, \quad \lim_{n\to\infty} (b_{2n+1}/\lambda_{2n}) = \beta_2 , \end{aligned} \tag{3}$$

where $\lambda_m \equiv g(m)$ is a regularly varying function with exponent $\alpha \geq 0$. A regular varying function with exponent α can be written[11] as $g(x)=x^\alpha L(x)$ where $L: R^+ \to R^+$ is a function which satisfies

$$\lim_{x\to\infty} \frac{L(xt)}{L(x)} = 1 . \tag{4}$$

We note that for $\lambda_m = m^\alpha$, $\alpha_1=\alpha_2$, and $\beta_1=\beta_2$ the conditions (3) reduce to (2). Bounded [$\lambda_m=1$ or $\alpha=0$ and $L(x)=1$] and unbounded ($\alpha>0$) Hamiltonians H satisfying the conditions given by Eqs. (3) have been found to describe numerous physical systems.[2,12-14]

To do that we shall convert the eigenvalue problem of the Lanczos matrix subject to the restrictions (3) into a problem of zeros of orthogonal polynomials and then we shall use some results recently found by van Assche.[15,16] Indeed, for a general $N\times N$ Jacobi matrix H_N the characteristic polynomials of the principal submatrices for the matrix $EI_N - H_N$, I_N being the N-dimensional unit matrix, form a set of orthogonal polynomials $\{P_n(E); n=0,1,\ldots,N\}$ which satisfy the recurrence relation $P_n(E) = (E-a_n)P_{n-1}(E) - b_n^2 P_{n-2}(E), P_{-1}(E)=0$, $P_0(E)=1$. Then the eigenvalues of the matrix H_N are the zeros $\{E_i, i=1,2,\ldots,N\}$ of the polynomial of the Nth degree $P_N(E)$. On the other hand, van Assche[16] has shown the following result:

$$\lim_{N\to\infty} \frac{1}{N} \sum_{i=1}^{N} f\left[E_i/\lambda_N\right] = \int_0^1 \int_{-\infty}^{\infty} f(E)\,dF(E-\gamma t^\alpha; \delta t^\alpha, \beta t^\alpha)\,dt , \tag{5}$$

where $f(x)$ is any continuous function and δ,β,γ are given by

$$\begin{aligned} &\delta^2 = \tfrac{1}{4}(\alpha_1-\alpha_2)^2 + (\beta_1-\beta_2)^2 , \\ &\beta^2 = \tfrac{1}{4}(\alpha_1-\alpha_2)^2 + (\beta_1+\beta_2)^2, \quad \gamma = \tfrac{1}{2}(\alpha_1+\alpha_2) , \end{aligned} \tag{6}$$

and the function $F(x;\alpha,\beta)$ is

$$F(x;\alpha,\beta) = \frac{1}{\pi} \int_{-\infty}^{x} \frac{|t| I_B(t)\,dt}{(\beta^2-t^2)^{1/2}(t^2-\alpha^2)^{1/2}} . \tag{7}$$

$I_B(t)$ is the so-called indicator function of the set $B=[-\beta,-\alpha]\cup[\alpha,\beta]$, i.e., it is equal to unity if t belongs to B and vanishes otherwise. For $\lambda_N=1$, the expression (5) was previously obtained by the same author in Ref. 15.

Making $f(x)=x^M$ in Eq. (5) and taking into account the definition (7) one has for any non-negative integral number M,

$$\mu_M^* = \frac{1}{\pi}\int_0^1 dt \int_{-\infty}^{\infty} \frac{E^M\,|E-\gamma t^\alpha|\,I_B(E-\gamma t^\alpha)dE}{[\beta^2 t^{2\alpha}-(E-\gamma t^\alpha)^2]^{1/2}[(E-\gamma t^\alpha)^2-\delta^2 t^{2\alpha}]^{1/2}}\,, \tag{8}$$

where the notation

$$\mu_M^* = \lim_{N\to\infty}(1/N)\sum_{i=1}^{M}(E_i/\lambda_N)^M,\quad M=1,2,3,\ldots \tag{9}$$

has been used. These quantities are the moments around the origin of the scaled level density $\rho^*(E) = \lim_{N\to\infty}\rho_N(E\lambda_N)$, where $\rho_N(E)\equiv N^{-1}\sum_{i=1}^{N}\delta(E-E_i)$. They completely characterize the ρ^* density. Let us calculate it. From Eq. (8) one finds

$$\mu_M^* = \frac{1}{\pi(\alpha M+1)}\left[\int_{\gamma-\beta}^{\gamma-\delta}+\int_{\gamma+\delta}^{\gamma+\beta}\right]\frac{y^M\,|y-\gamma|\,dy}{[\beta^2-(y-\gamma)^2]^{1/2}[(y-\gamma)^2-\delta^2]^{1/2}}\,, \tag{10}$$

where the change of variable $E=yt^\alpha$ has been made and the notation

$$\left[\int_a^b+\int_c^d\right]G(y)dy=\int_a^b G(y)dy+\int_c^d G(y)dy$$

has been adopted. Then the characteristic function of the E variable defined[17] by $\Psi(s)=\sum_{M=0}^{\infty}(is)^M/M!\,\mu_M^*$ will have the expression

$$\Psi(s)=\frac{1}{\pi}\left[\int_{\gamma-\beta}^{\gamma-\delta}+\int_{\gamma+\beta}^{\gamma+\delta}\right]\frac{|y-\gamma|\,e^{iys}\Phi(1,1+1/\alpha;-iys)dy}{[\beta^2-(y-\gamma)^2]^{1/2}[(y-\gamma)^2-\delta^2]^{1/2}}$$

once the μ values given by Eq. (10) have been used. The Φ symbol denotes the known confluent hypergeometric function (Ref. 18, p. 940).

The Fourier transform of $\Psi(s)$ gives the wanted density of levels $\rho^*(E)$ as[17] $\rho^*(E)=1/2\pi\int_{-\infty}^{\infty}e^{-iEs}\Psi(s)ds$.

Taking into account the last two equations and performing the integration over the infinite interval, one finds the following general expression for the level density:

$$\rho^*(E)=\frac{1}{\pi\alpha}\left[\int_{\gamma-\beta}^{\gamma-\delta}+\int_{\gamma+\delta}^{\gamma+\beta}\right]\frac{|y-\gamma|\,(E/y)^{1/\alpha-1}}{[\beta^2-(y-\gamma)^2]^{1/2}[(y-\gamma)^2-\delta^2]^{1/2}}\frac{dy}{|y|} \tag{11}$$

if $|1-(2E/y)|<1$. Notice that sign (E)=sign (y) and that the density vanishes if E does not belong to the set $[\gamma-\beta,\gamma-\delta]\cup[\gamma+\delta,\gamma+\beta]$. This expression gives the density of levels of the physical systems with Lanczos Hamiltonians subject to the general conditions (3).

From the general expression (11) one can immediately find many particular results of great interest. Let us point out some of them.

(1) If $\gamma+\delta\geq 0$ and $\gamma-\beta\geq 0$, then the level density is

$$\rho^*(E)=\frac{1}{\pi\alpha}E^{(1/\alpha)-1}\left[\int_E^{\gamma+\beta}\frac{(y-\gamma)y^{-1/\alpha}dy}{[\beta^2-(y-\gamma)^2]^{1/2}[(y-\gamma)^2-\delta^2]^{1/2}}I_{[\gamma+\delta,\gamma+\beta]}(E)\right.$$
$$\left.+\int_E^{\gamma-\delta}\frac{|y-\gamma|\,y^{-1/\alpha}dy}{[\beta^2-(y-\alpha)^2]^{1/2}[(y-\gamma)^2-\delta^2]^{1/2}}I_{[\gamma-\beta,\gamma-\delta]}(E)\right].$$

Similar expressions can be easily obtained from Eq. (11) for the remaining possibilities of $\gamma+\delta$, $\gamma-\beta$, and/or $\gamma-\delta$ not considered here.

(2) If $\gamma=0$, i.e., if $\alpha_1+\alpha_2=0$, then

$$\rho^*(E)=\frac{1}{\pi\alpha}E^{(1/\alpha)-1}\int_E^{\beta}\frac{y^{1-(1/\alpha)}dy}{(\beta^2-y^2)^{1/2}(y^2-\delta^2)^{1/2}}I_{[\delta,\beta]}(E)+\frac{|E|^{(1/\alpha)-1}}{\pi\alpha}\int_{|E|}^{\beta}\frac{y^{1-(1/\alpha)}dy}{(\beta^2-y^2)^{1/2}(y^2-\delta^2)^{1/2}}I_{[-\beta,-\delta]}(E)\,. \tag{12}$$

Here one has an even density of levels since $\rho^*(E)=\rho^*(-E)$. This density function can be expressed in terms of elliptic integrals (Ref. 18, p. 904). So, for $\alpha=1$ it only depends on the elliptic integral of the first kind; for $\alpha=\frac{1}{3}$ the only elliptic integral of the second kind. For $\alpha=\frac{1}{5}$, a combination of the two mentioned elliptic integrals is needed.

An important subcase is when $\delta=0$, that is $\alpha_1=\alpha_2=0$ and $\beta_1=\beta_2=b/2$. Then $\beta^2=b^2$ according to Eq. (6), and the density of levels becomes

$$\rho^*(E)=\frac{|E|^{(1/\alpha)-1}}{\pi\alpha}\int_{|E|}^{b}\frac{dy}{y^{(1/\alpha)}(b^2-y^2)^{1/2}}\quad \text{for } -b<E<b\ , \tag{13}$$

which can be expressed by means of a hypergeometric function and gives rise to Eq. (5) of Ref. 6, so considerably enlarging the class of Lanczos Hamiltonians having such a level behavior firstly identified in the above-mentioned reference. It is interesting to remark that for $\alpha=\frac{1}{2}$ this density function reduces to

$$\rho^*(E)=(2/\pi b)(1-E^2/b^2)^{1/2}I_{[-b,b]}\ ,$$

that is, Wigner's famous semicircle law[19] which plays a relevant role in the statistical theories of complex nuclear spectra.[20] It is worth while make this result more explicit: The quantum systems characterized by a Lanczos Hamiltonian satisfying the conditions

$$\lim_{n\to\infty}(a_n/\lambda_n)=0,\quad \lim_{n\to\infty}(b_n/\lambda_n)=b/2>0,$$

with $\lambda_n=n^{1/2}L(n)$, where $L(x)$ is defined by Eq. (4), have the Wigner level-energy behavior. This result extends the previous findings of several authors.[21,22]

(3) If $\alpha_1=\alpha_2\equiv a$ and $\beta_1=\beta_2\equiv b/2$, then $\delta=0$, $\beta=b$, and $\gamma=a$. According to Eq. (11) the density of levels is

$$\rho^*(E)=\frac{1}{\pi\alpha}\int_{a-b}^{a+b}\frac{(E/y)^{(1/\alpha)-1}dy}{|y|[b^2-(y-a)^2]^{1/2}}\quad \text{for } |1-2E/y|<1\ ,$$

which can be expressed by means of Appell's hypergeometric function of $F_1(\alpha,\beta,\beta';\gamma;x,y)$ type[18] as already obtained in Ref. 8. So this class of physical systems which have this function for the density of levels is much larger than pointed out in Ref. 8. Indeed, all the Lanczos Hamiltonians satisfying

$$\lim_{n\to\infty}(a_n/\lambda_n)=0,\quad \lim_{n\to\infty}(b_n/\lambda_n)=b/2>0\ , \tag{14}$$

where $\lambda_n=g(n)$ is a regularly varying sequence of exponent $\alpha\geq 0$, have the level behavior defined by the density function given by Eq. (7) in Ref. 8. In this reference, only the case $\lambda_n=n^{\alpha}$ was considered.

Finally, two special cases of the general expression (11) will be discussed.

(a) For $\alpha=0$, it is convenient to start not from Eq. (11) but previously from Eq. (8) and to remember that the moments μ_M^* can also be written as $\mu_M^*=\int_{-\infty}^{\infty}E^M\rho^*(E)dE$. Then it is straightforward to show that the level density is

$$\rho^*(E)=\frac{1}{\pi}\frac{|E-\gamma|}{[\beta^2-(E-\gamma)^2]^{1/2}[(E-\gamma)^2-\delta^2]^{1/2}}$$

if E belongs to the set $[\gamma-\beta,\gamma-\delta]\cup[\gamma+\delta,\gamma+\beta]$, and is equal to zero otherwise. An important subcase occurs for $\alpha_1=\alpha_2=a$ and $\beta_1=\beta_2=b/2$; then $\delta=0$, $\beta=b$, and $\gamma=a$, and the Hamiltonian has a regular density of levels, i.e.,

$$\rho^*(E)=(1/\pi)[b^2-(E-a)^2]^{-1/2}\ \text{ if } a-b\leq E\leq a+b\ .$$

This subcase considerably enlarges the class of Lanczos Hamiltonians with a regular level-energy behavior found in Ref. 7. We see that this class is formed by those Hamiltonians subject to conditions (14) where $\lambda_n=L(n)$, $L(x)$ being a non-negative measurable function which satisfies the limiting restriction (4). We note that for those systems in which $L(n)$ is a bounded function, the ρ^* function coincides with the real (i.e., not scaled) density of levels. Systems with a regular level density may be found in, e.g., condensed matter.[23]

(b) Another special case occurs when β_1 or β_2 (or both) is equal to zero. Then $\delta=\beta$ according to Eq. (6). In this case it is more convenient to start from Eq. (5). One obtains that Eq. (5) reduces to (Ref. 16, Sec. IV)

$$\lim_{N\to\infty}(1/N)\sum_{i=1}^{N}f(E_i/\lambda_N)=\tfrac{1}{2}\int_0^1\{f[(\gamma+\beta')t^{\alpha}]+f[(\gamma-\beta')t^{\alpha}]\}dt\ ,$$

where f is a continuous function and

$$\beta'^2=\tfrac{1}{4}(\alpha_1-\alpha_2)^2+\beta''^2,\quad \beta''=\max(\beta_1,\beta_2)\ .$$

Making $f(x)=x^M$ for $M=0,1,2,\ldots$, one has that the moments of the scaled level density $\rho^*(E)$ are given by

$$\mu_M^*=\frac{1}{2(\alpha M+1)}[(\gamma+\beta')^M+(\gamma-\beta')^M]\ .$$

Operating as indicated above, one finds that these moments correspond to the density function

$$\rho^*(E)=\frac{1}{2\alpha}\left[\frac{1}{|\gamma+\beta'|}\left[\frac{E}{\gamma+\beta'}\right]^{(1/\alpha)-1}I_{[0,\gamma+\beta']}(E)+\frac{1}{|\gamma-\beta'|}\left[\frac{E}{\gamma-\beta'}\right]^{(1/\alpha)-1}I_{[0,\gamma-\beta']}(E)\right]\ ,$$

where the indicator function $I_{[a,b]}(E)$, which is equal to unity if $E\in[a,b]$ and zero otherwise, has been used again.

An interesting subcase occurs for $\alpha_1=\alpha_2\equiv a$ and $\beta_1=\beta_2=0$. Then $\beta'=0$ and $\gamma=a$, and the level density reduces to

$$\rho^*(E)=(1/\alpha|a|)(E/a)^{(1/\alpha)-1}I_{[0,a]}\ , \tag{15}$$

a result already found in Ref. 6 although only when $\lambda_n=n^{\alpha}$. Here we have just shown that it is valid in a more general sense, precisely when λ_n is a regularly varying sequence with exponent $\alpha\geq 0$. One should remark that if $\alpha=1$, this level density is a uniform or rectangular function. This result allows one to enlarge, in the above-mentioned sense, the class of Lanczos Hamiltonians having a uniform level-energy behavior as already identified in Ref. 6. It is also important to point out that for $\alpha=\frac{2}{3}$ the resulting level density is the Weyl's function[24] of great interest among physicists and mathematicians.[10,25] To the best of our knowledge, the characterization of Weyl's quadratic law as the asymptotic eigenvalue density of Lanczos Hamiltonians has not been investigated except in a recent previous work of the authors[6] where no explicit mention of it was made.

Density functions given by Eq. (15) are of Karamata type[9,10] and are usually used for generalized Weyl or powerlike functions. They also appear as densities of states of some disordered tight-binding materials,[26] and for $\alpha=2,3,4,\ldots$ characterize the spectra of one-dimensional random chains of Dyson type.[27]

Another subcase of this special case is for $\alpha_1 \neq \alpha_2$ and $\beta_1=\beta_2=0$. Then $\gamma+\beta'=\alpha_1$ and $\gamma-\beta'=\alpha_2$. The corresponding level density is

$$\rho^*(E)=\frac{1}{2\alpha}\left[\frac{1}{|\alpha_1|}\left[\frac{E}{\alpha_1}\right]^{(1/\alpha)-1} I_{[0,\alpha_1]}(E) + \frac{1}{|\alpha_2|}\left[\frac{E}{\alpha_2}\right]^{(1/\alpha)-1} I_{[0,\alpha_2]}(E)\right] . \quad (16)$$

In addition, if $\alpha_1=-\alpha_2$, one immediately has

$$\rho^*(E)=\frac{1}{2|\alpha_1|\alpha}\left[\left|\frac{E}{\alpha_1}\right|\right]^{(1/\alpha)-1} I_{[-|\alpha_1|,|\alpha_1|]} .$$

And for $\alpha=1$, one gets that the ρ^* density is a uniform function centered at the origin, a result not encountered so far. In Ref. 6 we also found uniform level densities but they were never centered at the origin. Physical systems with a level density of type (16) for $\alpha=1$ can be found in, e.g., atomic physics[28] and condensed matter.[23]

In conclusion, we have analytically determined the asymptotic eigenvalue density of a large class of Lanczos Hamiltonians which have a different limiting behavior according to whether the index of their nonvanishing matrix elements is even or odd, as shown by Eq. (3). This class contains Hamiltonians of bounded type and those of unbounded type with the regular variation property. Since these Hamiltonians characterize a great number of physical systems, one can classify these systems according to their density of levels. Several previous results about this problem naturally arise as a consequence of the general level-density function given by Eq. (11). In doing so, we have identified enlarged subclasses of Hamiltonians having for their level density a function of regular, uniform, Wigner, Weyl, Karamata, or powerlike and hypergeometric types. Finally, it is worthwhile to point out that this classification is made from the Lanczos Hamiltonian of the system. We are aware that it would be desirable to do it directly from the two-body interaction dominant in the system, but this is an extremely difficult problem not yet solved.

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