Quantum systems with uniform- and regular-level-energy behaviors

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We consider the problem of identification and characterization of (Hamiltonian operators of) quantum systems which have a uniform-level-energy behavior (i.e., the level distribution follows a rectangular law) and a regular-level-energy behavior (i.e., the level energies are distributed according to an inverted semicircle law). Here we find a large class of Hamiltonians with these level-energy behaviors in terms of the matrix elements of their associated Lanczos matrix forms.

A global statistical property which plays an important role in the study of spectra of quantum systems is the density of levels (i.e., the number of levels per unit of energy interval) as a function of the excitation energy. In this Brief Report we will consider the problem of identification and characterization of (Hamiltonian operators of) systems with a common density of levels.

A pioneering work is that of Wigner[1] who proved that the distributions of levels of a random matrix follows a semicircle law. Then one says that the matrix has a semicircular eigenvalue behavior. This behavior was observed in random models of Hamiltonians to describe a large variety of quantum systems.[2–5] Recently it has been shown that the Wigner semicircle behavior has a deterministic origin.[6–8] In particular there exists a large class of nonrandom Hamiltonians with the semicircle law as the asymptotic eigenvalue density[8] (AED).

We will discuss the identification of the quantum Hamiltonians that have (1) a uniform eigenvalue behavior (i.e., the AED is a uniform density function) and (2) a regular eigenvalue behavior (i.e., the AED is an inverted semicircle). We will not find all the Hamiltonians which exhibit these eigenvalue behaviors but we will identify a large class of them having these properties in terms of the matrix elements of the associated Lanczos matrix forms.

For a large number of quantum systems,[9–11] the Lanczos method[12] allows us to transform the Hamiltonian operator into a N-dimensional tridiagonal matrix which is usually called the Lanczos Hamiltonian. The only nonvanishing matrix elements of this Hamiltonian are denoted by

$$H_{n,n}=a_n \ , \qquad H_{n,n+1}=H_{n+1,n}=b_n \ . \tag{1}$$

The (discrete) normalized-to-unity eigenvalue density $\rho_N(E)$ of this Hamiltonian is defined by

$$\rho_N(E)=\frac{1}{N}\sum_{i=1}^{N}\delta(E-E_i)=\frac{1}{N}\mathrm{Tr}\,\delta(E-H) \ .$$

The moments around the origin of this function are

$$\mu_r'^{(N)}=\frac{1}{N}\mathrm{Tr}\,H^r=\frac{1}{N}\sum_{i=1}^{N}E_i^r; \quad r=0,1,2,\ldots \ . \tag{2}$$

Also, the asymptotic eigenvalue density $\rho(E)$ and its moments around the origin are given by

$$\rho(E)=\lim_{N\to\infty}\rho_N(E) \ , \qquad \mu_r'=\lim_{N\to\infty}\mu_r'^{(N)}; \quad r=0,1,2,\ldots \ . \tag{3}$$

Here we will solve the above mentioned problem in terms of the matrix elements a_n and b_n. Our first result is the following: If

$$\lim_{n\to\infty}\frac{a_n}{n}=q\in R, \quad \lim_{n\to\infty}\frac{b_n}{n}=0 \tag{4}$$

(R denotes the set of real numbers), then the moments around the origin of the scaled eigenvalue density $\rho^*(E)=\lim_{N\to\infty}\rho_N(E/N)$ are

$$\mu_r''=\frac{q^r}{r+1}, \quad r=0,1,2,\ldots \ , \tag{5}$$

which correspond to a uniform or rectangular density function over the interval $[0,q]$.

Secondly, we will show that if the matrix elements of the Lanczos Hamiltonian satisfy the conditions

$$\text{(i) } a_n=a\in R \ , \qquad \text{(ii) } 0<b_{n-1}^2\leqslant b^2, \quad n\geqslant 2 \ , \qquad \text{(iii) } \lim_{n\to\infty}b_n^2=b^2 \ , \tag{6}$$

then the energy eigenvalues have a regular behavior in the interval $[a-2b,a+2b]$, that is,

$$\rho(E)=\begin{cases}\dfrac{1}{\pi}[4b^2-(E-a)^2]^{-1/2} & \text{if } a-2b\leqslant E\leqslant a+2b\\ 0, & \text{otherwise} \ .\end{cases}$$

Thirdly, if the following limiting restrictions

$$\lim_{n\to\infty}a_n=a\in R, \quad \lim_{n\to\infty}b_n=b\geqslant 0 \ , \tag{7}$$

then the eigenvalue moments μ_r' of the density $\rho(E)$ are given by

$$\mu_r'=\sum_{j=0}^{[r/2]}a^{r-2j}b^{2j}\binom{r}{2j}\binom{2j}{j} \ , \tag{8}$$

which correspond to the moments around the origin of an inverted semicircular density function centered at $E=a$ and with a support interval $[a-2b,a+2b]$.

Before proving these results let us give some direct consequences of them for those systems with a Lanczos Hamiltonian matrix of a rational Jacobi type, that is, when

$$a_n=\frac{Q_\theta(n)}{Q_\beta(n)},\quad b_n=+\left[\frac{Q_\alpha(n)}{Q_\gamma(n)}\right]^{1/2}, \tag{9a}$$

where

$$Q_\theta(n)=\sum_{i=0}^{\theta} c_i n^{\theta-i},\quad Q_\beta(n)=\sum_{i=0}^{\beta} d_i n^{\beta-i}, \tag{9b}$$

$$Q_\alpha(n)=\sum_{i=0}^{\alpha} e_i n^{\alpha-i},\quad Q_\gamma(n)=\sum_{i=0}^{\gamma} f_i n^{\gamma-i}. \tag{9c}$$

There are several consequences.

(i) If $\theta-\beta=1$ and $\alpha-\gamma<2$, then the density $\rho^*(E)$ has the level eigenvalue moments $\mu_r''=(r+1)^{-1}(c_0/d_0)^r$, which correspond to a uniform density function in the interval $[0,c_0/d_0]$.

(ii) If $\theta=\beta$ and $\alpha=\gamma$, then the moments of the eigenvalue density $\rho(E)$ are

$$\mu_r'=\sum_{j=0}^{[r/2]}\left[\frac{e_0}{f_0}\right]^j\left[\frac{c_0}{d_0}\right]^{r-2j}\binom{2j}{j}\binom{r}{2j},\quad r=0,1,\ldots,$$

which correspond to an inverted semicircle density function over the interval

$$[c_0/d_0-2\sqrt{e_0/f_0},\ c_0/d_0+2\sqrt{e_0/f_0}],$$

and centered around $E=c_0/d_0$.

(iii) If $\theta<\beta$ and $\alpha=\gamma$, then

$$\mu_{2k}'=\left[\frac{e_0}{f_0}\right]^k\binom{2k}{k},\quad \mu_{2k+1}'=0,\quad k=0,1,\ldots,$$

which are the moments of an inverted semicircle density $\rho(E)$ centered around the origin and with a support interval $[-2\sqrt{e_0/f_0},\ 2\sqrt{e_0/f_0}]$.

The starting point to prove all these results is the following well-known property of the Lanczos Hamiltonian (1): the characteristic polynomials $\{P_n(E),\ n=0,1,\ldots,N\}$ of the principal submatrices of the matrix EI_N-H, I_N being the $N\times N$ unity matrix, satisfy the recursion relation

$$P_n(E)=(E-a_n)P_{n-1}(E)-b_{n-1}^2P_{n-2}(E),$$
$$P_{-1}(E)=0,\quad P_0(E)=1,\quad n=1,2,\ldots,N. \tag{10}$$

The first and third results can be proved from the following theorem[13] of the theory of orthogonal polynomials: Let R^+ be the set of positive real numbers. Let $\phi: R^+\to R^+$ be a nondecreasing 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, $a\in R$ and $b\geq 0$ such that the coefficients in the recurrence relation (10) satisfy

$$\lim_{n\to\infty}\frac{a_n}{\phi(n)}=a,\quad \lim_{n\to\infty}\frac{b_n}{\phi(n)}=\frac{b}{2}. \tag{11}$$

Then for every non-negative integer r,

$$\lim_{n\to\infty}\frac{\sum_{k=1}^{N}E_k^r}{\int_0^N[\phi(t)]^r}=\sum_{j=0}^{[r/2]}b^{2j}a^{r-2j}2^{-2j}\binom{2j}{j}\binom{r}{2j}, \tag{12}$$

where E_k, $k=1,2,\ldots,N$ are the zeros of $P_N(E)$.

One easily notices that with the choice $\phi(x)=x^A$, $A=1$, $b=0$, and taking into account the definitions (2) and (3), the Eqs. (11) and (12) reduce to the wanted Eqs. (4) and (5), respectively. Similarly, with the choice $\phi(x)=1$, Eqs. (11) and (12) transform into Eqs. (7) and (8), respectively. Then, our first and third results have been proved.

The second result can be obtained in a straightforward manner from Maki's theorem of orthogonal polynomials and Remark 2 of Ref. 14, together with Eqs. (3)–(5) of Ref. 15. The corollaries (i), (ii), and (iii) are immediate consequences of the first and third results.

In conclusion, we have identified a large class of quantum Hamiltonians which have a uniform eigenvalue behavior. This behavior has been observed in many physical systems which go from the well-known harmonic oscillator to some atomic configurations.[16] Also, a characterization of some quantum systems with a regular-level behavior has been given.

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