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A Possible Form of NNS Distribution for Degenerate Spectra

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To expose the statistical properties of the degenerated spectrum, with the aid of the random matrix theory, a possible form of the NNS distribution function of the degenerate spectrum was proposed by providing a solution in terms of the same-degeneracy case. The results indicate that the target spectrum is transformed into two sub-spectra: a random one and a regular one, and that the repulsion level of the regular spectrum is also decreased.

Key words: NNS distribution, Degenerate spectum, Random matrix theory

I. INTRODUCTION

Since the foundation of the random matrix theory (RMT) in the 1960s, the basic research work about level fluctuation spectra has made rapid progress [1-14]. As a result of this work, a series of statistical theories and the corresponding models of level fluctuation have been established. In addition, the focus of research has expanded from nuclear to atomic and molecular systems, and from observed spectra to eigenvalue spectra. Furthermore, the close relationship between quantum chaos and the statistical regularities of the fluctuation spectra has further greatly promoted the research on level statistics for various quantum systems such as a nucleus, an atom, a molecule, and even quantum dots. To date, these theories have been limited to non-degenerate spectra, with little focus on degenerate ones. In the case of a degenerate spectrum, the original nearest neighbor spacing (NNS) distribution theory for non-degenerate spectra had a breakdown because of both the degeneracy and the NNS distribution. Meanwhile, the statistical analysis complicated by the complex interlacing of degeneracy and the strength in the spectral lines, and it is particularly difficult to study. These are the challenges we seek to solve, i.e. how to extract an intrinsic concept of the distribution which not only reflects the dual characteristics of the degenerate spectra, but also directly relates to the non-integrality of the corresponding dynamic systems. Based on this intrinsic approach we can establish a NNS distribution for degenerate spectra as an extension to the theoretical formalism of the original NNS distribution and an enrichment of the quantum chaos theory. It appears that the development of the statistical theory of fluctuations in degenerate spectra will enable further research on level statistics and will help to penetrate the complex structure of various quantum systems. Therefore, whether theoretical or empirical, discoveries and research of this kind of extension and development is of great necessity.

Fortunately, with the aid of the weighted statistical method, a few interesting results about the degenerate spectra were obtained [14]. However, the analytical expression for degenerate spectra is still unknown. Using the framework of RMT, a possible form of the NNS distribution function for degenerate spectra is proposed in this work.

II. THEORY

Usually a spectrum can be separated, in a general sense, into a smoothly varying average part and a fluctuating part describing the deviations from the average. The statistical analysis then concentrates on the fluctuating part. It is known that complex systems exhibit universal fluctuation properties. Two types are particularly important: Poisson law which describes the uncorrelated random level spectra (Poisson spectrum), and Wigner law describing the Gaussian orthogonal ensemble of the random matrix spectra. The NNS distribution functions for these are given as

$$P(s) = \begin{cases} e^{-s} & \text{(Poisson)} \\ \frac{\pi}{2} s \exp\left(-\frac{\pi s^2}{4}\right) & \text{(Wigner)} \end{cases} \quad (1)$$

Through level repulsion, both the Poisson distribution and the Wigner one can be derived from a simple probability argument, which results in an integral equation for the distribution $P(s)$,

$$P(s) = r(s) \int_s^\infty P(x)\mathrm{d}x \quad (2)$$

The Poisson law follows if the level repulsion function $r(s)$ is unity (no level repulsion), whereas the Wigner's follows from the assumption of linear repulsion as $r(s) \propto s$. Therefore the level repulsion function

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is a very important factor in describing the statistical properties of a level spectrum.

All these are valid for the non-degenerate spectra. In fact, theoretical studying on the degenerate spectra have already to be reported. However, the statistical properties of a degenerate spectrum can be easily obtained through the weighted statistical method, and we have made some progress in the study of degenerate spectra recently [14]. For a numerical studying, as opposed to the relationship between the degeneracies and symmetries of the system, we pay attention to the analysis of the data of the energy levels obtained from experimental measurements or numerical calculations. Considering a given degenerate spectrum

$$\{e_i, g_i\} \qquad (i = 1, 2, \cdots, n) \tag{3}$$

where e_i is ith energy level of Eq.(3), and g_i the corresponding level's degeneracy ($\sum g_i = N$, N is the total number of levels). We know that levels in Eq.(3) are correlated, and the correlations among them come from three factors: (a) relations among the degenerate levels, (b) relations among the non-degenerate levels, and (c) relations between degenerate and non-degenerate levels. It is easy to find that the neighbor spacings between degenerate levels are 0, and that the level repulsions among them are also 0, so these degenerate levels make up of a sub-spectrum of Eq.(3). Obviously, this is a random spectrum. The other two correlations (b) and (c) constitute another sub-spectrum of Eq.(3)

$$\{e_i\}, \quad \{g_i\} \qquad (i = 1, 2, \cdots, n) \tag{4}$$

which is called the regular spectrum of Eq.(3). As the random spectrum follows Poisson's law, it cannot reveal the special characteristics of the system considered. Therefore, to get more information about the system, further investigations on Eq.(4) are needed. For simplicity, if only the correlation (b) is considered, Eq.(4) reduces to a non degenerate spectrum

$$\{e_i\} \qquad (i = 1, 2, \cdots, n) \tag{5}$$

Obviously, Eq.(5) is the reduced non-degenerate spectrum of Eq.(4). We believe that there must be some relationship between Eq.(4) and Eq.(5). As a non degenerate spectrum, the statistical characteristics of Eq.(5) are easy to get. Considering the degeneracy as the level's weight, the statistical character of Eq.(4) can also be analyzed through the weighted statistical method [14]. The relations between Eq.(4) and Eq.(5) can then be exposed in this way. However, in this work, we try to study these relations through RMT, and compare the results obtained through RMT with the results determined through the weighted statistical method. So, we briefly review the weighted statistical method. Then, in the framework of RMT, a possible form of the NNS distribution function for the degenerate spectrum is proposed. The correctness of this NNS distribution function will be tested against the weighted statistical method.

A. Weighted statistical method for degenerate spectrum

Considering the regular spectrum of Eq.(4), the cumulative function is

$$N_d(e_i) = \sum_{i=1}^{n} g_i \Theta(e - e_i) \tag{6}$$

here $\Theta(x) = \begin{cases} 0 & (x \le 0) \\ 1 & (x > 0) \end{cases}$ is the unit step function. If we suppose that the fitting polynomial function

$$N_d{}'(e_i) = b + \sum_{j=1}^{m} a_j {e_i}^j \tag{7}$$

can be taken as the average part of $N_d(e_i)$, then the fluctuation part is

$$\epsilon_i = N_d(e_i) - N_d{}'(e_i) \tag{8}$$

and the degenerate fluctuation spectrum of Eq.(4) is

$$\{\epsilon_i\}, \quad \{g_i\} \qquad (i = 1, 2, \cdots, n) \tag{9}$$

The covariance between Eq.(6) and Eq.(7) is

$$\begin{aligned} Q &= \sum_{i=1}^{n} g_i [N_d(e_i) - N_d{}'(e_i)] \\ &= \sum_{i=1}^{n} g_i \Big[N_d(e_i) - b - \sum_{j=1}^{m} a_j {e_i}^j \Big] \end{aligned} \tag{10}$$

and the coefficients b and a_j (where $j = 1, 2, \cdots, m$) are determined through

$$\frac{\partial Q}{\partial b} = 0, \quad \frac{\partial Q}{\partial a_j} = 0 \qquad (j = 1, 2, \cdots, m) \tag{11}$$

and m is determined by the fitting precision.

Usually NNS distribution, spectral rigidity, fractal dimension (FD) function, etc., are used to describe the statistical properties of a spectrum. The NNS distribution is simply the probability $P(s)$ of finding a separation s between neighbor levels in the fluctuation spectrum. Obviously, the number of $s = 0$ among the ith levels e_i is $g_i - 1$ due to the degeneracy, therefore the total number of zero spacing is $\sum_{i=1}^{n} (g_i - 1) = N - n$ and the probability of finding a zero spacing is $(N - n)/N$. On the other hand, the probability of finding a non zero space $s \neq 0$ is

$$P(s) = \lim_{\Delta s \to 0} \frac{\sum_{i=1}^{n-1} \theta(|\varepsilon_{i+1} - \varepsilon_i| - s_i| - \Delta s) g_i}{N \Delta s} \tag{12}$$

If the accumulative function

$$N(\varepsilon) = \sum_{i=1}^{n} g_i \Theta(\varepsilon - \varepsilon_i) \tag{13}$$

of the fluctuation spectrum of Eq.(9) is divided into M sub-stretches by the unit of length L, the spectral rigidity is the average of the least-square deviation of the accumulative function in each sub-stretch, i.e.,

$$\Delta_3(L) = \frac{1}{M}\sum_{i=1}^{M}\frac{1}{L}\Big\{\min_{A_j,B_j}\sum_{n_j}[N(\varepsilon_j) - A_j\varepsilon_j - B_j]\Big\} \tag{14}$$

where the coefficients A_j and B_j are determined through the linear fitting. The FD function for energy levels was introduced by Cederbaum *et al.* [9]. They firstly mapped the spectrum into a set of n points in the interval [0;1]. Each point is covered by a bar of length δ with $\delta/2$ on each side of the point. Once δ exceeds the smallest distance between two points, the bars overlap and the coarse graining is done by the union of the overlapping bars being now of lengths l_i, $i = 1, 2, \cdots, m$. Then the fractal dimensional function for energy levels is

$$D = \frac{\sum_{i=1}^{m} P_i \ln P_i}{\sum_{i=1}^{m} P_i \ln l_i} \tag{15}$$

where P_i is the probability that a point falls into the line of coarse l_i and can be calculated as

$$P_i = \frac{\sum_{j=1}^{k(l_i)} g_{k(j,l_i)}}{N} \tag{16}$$

where $k(l_i)$ is the number of points consisting of the coarse graining l_i, $k(j, l_i)$ the serial number of level corresponding to the jth point in l_i.

Through Eqs.(12)-(15), we can determined the statistical characteristics of the regular spectrum of Eq.(4), a sub-spectrum of Eq.(3). However, the analytical expression for the NNS distribution function, spectral rigidity and the FD function are still unknown. In the following pages, we try to give a possible form of the NNS distribution function for the regular spectrum of a degenerate spectrum.

B. A possible form of NNS distribution function for degenerate spectrum in the framework of RMT

We note that RMT is no longer valid for the degenerate spectra. According to RMT, the invariant volume element of a $N\times N$ random Hamiltonian matrix H is defined by [1]

$$\mathrm{d}V_H = 2^{N(N-1)/4}\mathrm{d}h_{11}\cdots\mathrm{d}h_{N-1,N} \tag{17}$$

where $\mathrm{d}h_{11}, \cdots, \mathrm{d}h_{N-1,N}$ are the elements of $\mathrm{d}H$, while $\mathrm{d}H$ corresponds to the differential increment of H, i.e.

$$\mathrm{d}H = \begin{bmatrix} \mathrm{d}h_{11} & \mathrm{d}h_{12} & \cdots & \mathrm{d}h_{1N} \\ \mathrm{d}h_{21} & \mathrm{d}h_{22} & \cdots & \mathrm{d}h_{2N} \\ \vdots & \vdots & \ddots & \vdots \\ \mathrm{d}h_{N1} & \mathrm{d}h_{N2} & \cdots & \mathrm{d}h_{NN} \end{bmatrix} \tag{18}$$

For real symmetric Hamiltonian matrixes, i.e. Gaussian orthogonal ensembles (GOE), $\mathrm{d}V_H$ will take the form [1]

$$\mathrm{d}V_H^{\mathrm{GOE}} = 2^{N(N-1)/4} f\left(\alpha_1, \cdots, \alpha_{N(N-1)/2}\right) \cdot\Big\{\prod_{i<j=1}^{N}|e_j - e_i|\Big\}\mathrm{d}e_1\cdots\mathrm{d}e_N\mathrm{d}\alpha_1\cdots\mathrm{d}\alpha_{N(N-1)} \tag{19}$$

whereas for Gaussian unitary ensemble (GUE), $\mathrm{d}V_H$ shifts to

$$\mathrm{d}V_H^{\mathrm{GUE}} = 2^{N(N-1)/4} f\left(\alpha_1, \cdots, \alpha_{N(N-1)/2}\right) \cdot\Big\{\prod_{i<j=1}^{N}|e_j - e_i|^2\Big\}\mathrm{d}e_1\cdots\mathrm{d}e_N\mathrm{d}\alpha_1\cdots\mathrm{d}\alpha_{N(N-1)} \tag{20}$$

where e_i represents the eigenvalues of H, $f(\alpha_1, \cdots, \alpha_{N(N-1)/2})$ appears as a function of the parameters α_i involved in the corresponding orthogonal matrix O, while $\prod_{i<j=1}^{N}|e_j - e_i|$ and $\prod_{i<j=1}^{N}|e_j - e_i|^2$ are the weight factors of GOE and GUE respectively. Evidently, when e_i=e_j, both $\mathrm{d}V_H^{\mathrm{GOE}}$ and $\mathrm{d}V_H^{\mathrm{GUE}}$ will tend to be trivial, which leads to the inevitable singularity of the statistical distribution for degenerate spectra. However, we can't exclude the possibility of degeneracy because dynamic symmetry very likely exists in any quantum system, so we have to extend the original statistical theory to include the case of degeneracy. The only way to do this is to revise the above formulas, the foundation of the theory as well as the deductions made from it.

For a symmetric matrix, whether its eigenvalues are degenerate or not, there must exist an orthogonal transformation to make it diagonal. If degeneracy appears, the number of independent matrix elements will decrease and both the Jacobi determinant of the orthogonal transformation and the invariant volume element of the matrix will change. Take the GOE type as an example. We can write out a 2×2 symmetric matrix H and its corresponding orthogonal matrix O as well as the final diagonal matrix H_D as follows [1]

$$\begin{aligned} H &= \begin{bmatrix} h_{11} & h_{12} \\ h_{12} & h_{22} \end{bmatrix} \\ H_D &= \begin{bmatrix} e_1 & 0 \\ 0 & e_2 \end{bmatrix} \\ O &= \begin{bmatrix} \cos\alpha & \sin\alpha \\ -\sin\alpha & \cos\alpha \end{bmatrix} \end{aligned} \tag{21}$$

After taking the orthogonal transformation [1], we have the matrix elements as

$$\begin{aligned} h_{11} &= e_1\cos^2\alpha + e_2\sin^2\alpha \\ h_{12} &= (e_2-e_1)\cos\alpha\sin\alpha \\ h_{22} &= e_1\sin^2\alpha + e_2\cos^2\alpha \end{aligned} \tag{22}$$

and the invariant volume element as

$$\mathrm{d}h_{11}\mathrm{d}h_{12}\mathrm{d}h_{22} = J\begin{pmatrix} h_{11} & h_{12} & h_{22} \\ e_1 & e_2 & \alpha \end{pmatrix}\mathrm{d}e_1\mathrm{d}e_2\mathrm{d}\alpha \tag{23}$$

in which

$$J\begin{pmatrix} h_{11} & h_{12} & h_{22} \\ e_1 & e_2 & \alpha \end{pmatrix} = \begin{vmatrix} \dfrac{\partial h_{11}}{\partial e_1} & \dfrac{\partial h_{11}}{\partial e_2} & \dfrac{\partial h_{11}}{\partial \alpha} \\ \dfrac{\partial h_{12}}{\partial e_1} & \dfrac{\partial h_{12}}{\partial e_2} & \dfrac{\partial h_{12}}{\partial \alpha} \\ \dfrac{\partial h_{22}}{\partial e_1} & \dfrac{\partial h_{22}}{\partial e_2} & \dfrac{\partial h_{22}}{\partial \alpha} \end{vmatrix} \tag{24}$$

From Eq.(22), it's evident that when e_1=e_2, i.e. e_1 and e_2 are degenerate, h_{12} vanishes. As a result, in addition to the decrease of the number of the independent matrix elements, the Jacobi determinant J of this transformation is no longer trivial because of the disappearance of the $|e_1-e_2|$ item.

To obtain a possible expression for the NNS distribution of degenerate spectra, we assume that a diagonalized matrix with degenerate eigenvalues can be written as

$$\begin{vmatrix} e_1I_1 & 0 & \cdots & 0 \\ 0 & e_2I_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & e_nI_n \end{vmatrix} \tag{25}$$

where I_i is the g_i-dimensional unit matrix, g_i is the degeneracy of eigenvalue e_i. Obviously, the diagonalized matrix of its reduced nondegenerate spectrum is

$$\begin{vmatrix} e_1 & 0 & \cdots & 0 \\ 0 & e_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & e_n \end{vmatrix} \tag{26}$$

We also assume that if $P(H)$ is the probability distribution function of the eigenvalue spectrum corresponding to the Hamiltonian matrix H, then the information of this matrix will be in the form of

$$I = \int \mathrm{d}V_H P(H)\ln P(H) \tag{27}$$

It is subject to the following two constraining conditions [1]

$$\int \mathrm{d}V_H (TrHH^+)P(H) = C \tag{28}$$

$$\int \mathrm{d}V_H P(H) = 1 \tag{29}$$

where C is a constant. According to the maximum information principle, the distribution function $P(H)$ can be finally deduced to be

$$P(H) = \exp\{-(1+\lambda_0+\lambda_1 Tr[(HH^+)]\} \tag{30}$$

where λ_0 and λ_1 are the Lagrange multipliers. Introducing the scaling transformation $x_i = \sqrt{2\lambda_1}e_i$, for the regular part, the above formula shifts to

$$\begin{aligned} P_1(x_1,\cdots,x_n) = C_{ng}\prod_{i<j=1}^{N}|e_j-e_i|^q \\ \cdot\exp\left[-\frac{1}{2}\sum {g_i}^2{x_i}^2\right] \end{aligned} \tag{31}$$

for its reduced non-degenerate part, it's

$$P_2(x_1,\cdots,x_n) = C_n\prod_{i<j=1}^{N}|e_j-e_i|^q\exp\left[-\frac{1}{2}\sum {x_i}^2\right] \tag{32}$$

When q=1, it is the GOE type; while when q=2, it is the GUE type. For simplification, we consider a matrix only having two different eigenvalues e_1 and e_2 with degeneracies g_1 and g_2 respectively. Examining Eqs.(31) and (32), we conclude that the probability of the eigenvalue pair being in the intervals $e_2 \to e_2+\mathrm{d}e_2$ and $e_1 \to e_1+\mathrm{d}e_1$:

$$\begin{aligned} P_1(e_1,e_2)\,\mathrm{d}{e_1}^{g_1}\mathrm{d}{e_2}^{g_2} &= C_{2g}|e_j-e_i|^q \\ \cdot\exp\left[-\frac{1}{2}\left({g_1}^2{e_1}^2+{g_2}^2{e_2}^2\right)\right](\mathrm{d}e_1)^{g_1}(\mathrm{d}e_2)^{g_2} \end{aligned} \tag{33}$$

$$\begin{aligned} P_2(e_1,e_2)\,\mathrm{d}e_1\mathrm{d}e_2 &= C_2|e_j-e_i|^q \\ \cdot\exp\left[-\frac{1}{2}\left({e_1}^2+{e_2}^2\right)\right]\mathrm{d}e_1\mathrm{d}e_2 \end{aligned} \tag{34}$$

They satisfy the normalization condition

$$\int\int (\mathrm{d}e_1)^{g_1}(\mathrm{d}e_2)^{g_2}P_1(e_1,e_2) = 1 \tag{35}$$

$$\int\int \mathrm{d}e_1\mathrm{d}e_2 P_2(e_1,e_2) = 1 \tag{36}$$

respectively. Obviously, in this theoretical formalism, it is very difficult to determine the general solution for $P(s)$. However, we deal with the following special case in an attempt to propose a possible form of NNS distribution for degenerate spectra. As a special case, we assume $g_1 = g_2 = g$, i.e. the different eigenvalues of the matrix have the same degeneracy. After taking advantage of the following transformation

$$\overline{e} = \frac{1}{2}(e_1+e_2), \qquad s = |e_1-e_2| \tag{37}$$

Eqs.(33) and (34) turn into

$$P_1(s,\bar{e})\mathrm{d}s^g\mathrm{d}\bar{e}^g \propto C_{2g}s^q\exp\left(-\frac{4\bar{e}^2+g^2s^2}{8\alpha^2}\right)(\mathrm{d}s)^g(\mathrm{d}\bar{e})^g \quad (38)$$

$$P_2(s,\bar{e})\mathrm{d}s\mathrm{d}\bar{e} \propto C_2 s^q\exp\left(-\frac{4\bar{e}^2+s^2}{8\alpha^2}\right)\mathrm{d}s\mathrm{d}\bar{e} \quad (39)$$

Integrating over the variable $\bar{e}$ (i.e. the average energy), we have the realization probability of the spacing s in the interval $s \to s+\mathrm{d}s$

$$P_1(s)\mathrm{d}s = C'_{2g}s^{q/g}\exp\left(-\frac{gs^2}{8\alpha^2}\right)\mathrm{d}s \quad (40)$$

$$P_2(s)\mathrm{d}s = C'_2 s^q\exp\left(-\frac{s^2}{8\alpha^2}\right)\mathrm{d}s \quad (41)$$

It's easy to extend the above conclusion to the GOE type having n different eigenvalues but the same degeneracy g, and the corresponding probability function yields

$$P_1(s) = C'_{ng}s^{q/g}\exp\left(-\frac{gs^2}{8\alpha^2}\right) \quad (42)$$

$$P_2(s) = C'_n s^q\exp\left(-\frac{s^2}{8\alpha^2}\right) \quad (43)$$

For the degenerate spectra with different degeneracies, we try to briefly demonstrate its character through its average degeneracy, since in general according to the idea of RMT, except for the symmetry of the matrix. The matrix elements are allowed to change randomly, for any degenerate spectrum, and every eigenvalue is likely to experience degeneracy. If the probability of eigenvalues encountering degeneracy is presumed to be the same for each energy level, the degeneracy of every eigenvalue can be evaluated over the degeneracy ensemble $\{g_i\}$ and then the average degeneracy of eigenvalue e_i is

$$\overline{g}_{e_i} = \frac{\sum g_i}{n} = \frac{N}{n} \quad (44)$$

Evidently, all of the eigenvalues of the random matrix have the same average degeneracy $g \equiv \overline{g} = \overline{g}_{e_i}$. Therefore, we can use the conclusion of Eq.(42) of the equal-degeneracy case to describe the general degenerate spectra briefly, and thus

$$P(s) = Cs^{q/g}\exp\left(-\frac{gs^2}{8\alpha^2}\right) = Cs^{nq/N}\exp\left(-\frac{ns^2}{8N\alpha^2}\right) \quad (45)$$

Additionally, taking into account the random spectra of the degeneracy case characterized by $s=0$ with relative ratio $(N-n)/N$, we finally obtain the complete form of the NNS distribution for degenerate spectra as follows:

$$P(s) = \begin{cases} \frac{N-n}{N} & (s=0) \\ \frac{n}{N}Cs^{\frac{n}{N}q}\exp\left(-\frac{ns^2}{8N\alpha^2}\right) & (s\neq 0) \end{cases} \quad (46)$$

All the coefficients C, C_2, C_{2g}, C_n, C_{ng}, C'_2, C'_{2g}, C'_n and C'_{ng} are used to normalize the distribution function. Even though this expression is derived in terms of the special case, it is enormously useful that it exposes physical insights required for the degenerate spectra. The expression shows the whole set of degenerate spectra can be decomposed into two parts: when $s=0$, $P(s)$ describes the random spectrum; when $s\neq 0$, the regular spectrum. When compared with Eqs.(42) and (43), it's easy to see that, for the reduced non degenerate spectrum, the level repulsion is s^q, for the regular part of the degenerate spectrum, it is $s^{(n/N)q}$, i.e., the level repulsion of the regular part is smaller than its reduced part. Clearly, this result is interesting.

III. RESULTS

The statistical characteristcs is calculated by the quantum self-trapped theory [15-17]. In the spectrum, the two levels are taken to be degenerate when their interval is smaller than 1 cm^{-1}. When doing so, it was found that the average degeneracy of H_2O was 1.4. The statistical characteristics of the regular spectrum and its reduced non-degenerate spectrum of the vibrational energy levels of H_2O, are obtained through weighted statistical method, and demonstrated in Fig.1-Fig.4, respectively. From Fig.1 and Fig.2, few obvious differences are found in the NNS distributions between the regular spectrum and its reduced non degenerate spectrum; however, Fig.3 and Fig.4 show clearly that both the spectral rigidity and FD function of the regular part fall closer to the Poisson law than the reduced non degenerate spectrum does. This means that the level repulsion of the regular spectrum is smaller than

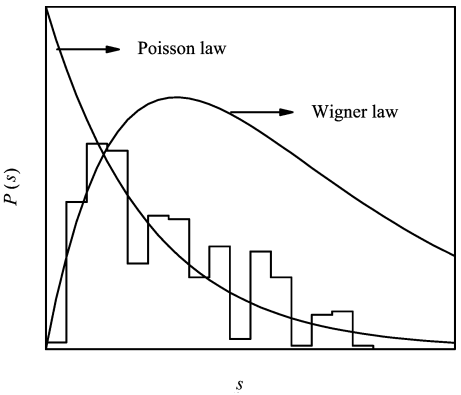

FIG. 1 The NNS distribution of the regular spectrum of the vibrational energy levels of H_2O.

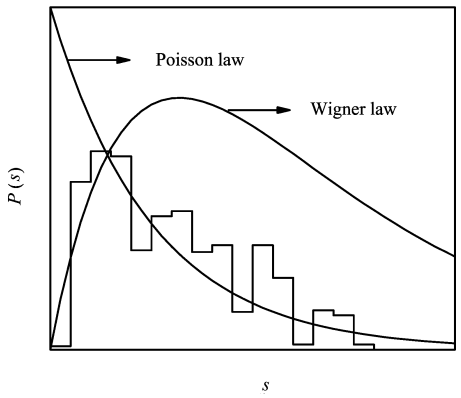

FIG. 2 The NNS distribution of the reduced non-degenerate spectrum of the vibrational energy levels of H_2O.

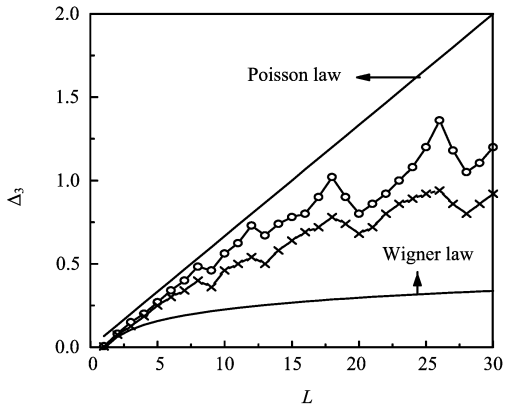

FIG. 3 The spectral rigidity, where Δ_3 is the spectral rigidity, L the length of the measured unit. The curves consists of "×" or " ○" are for the regular spectrum or the reduced non-degenerate spectrum of the vibrational energy levels of H_2O respectively.

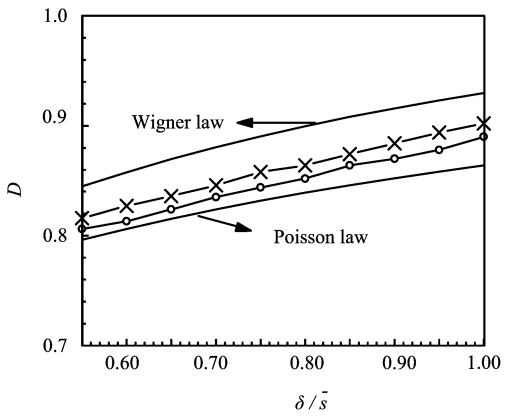

FIG. 4 The FD function, where D is the FD function, $\delta/\bar{s}$ the ratio of the measured length δ to the average value $\bar{s}$ of levels. The curves consists of "×" or "○" are for the regular spectrum or the reduced non-degenerate spectrum of the vibrational energy levels of H_2O respectively.

that of the reduced reduced non degenerate spectrum, since the level repulsion of a random spectrum which follows the Poisson law is 0, and the closer to Poisson law, the smaller the level repulsion will be. This is just in accordance with above conclusion derived from RMT. There is no doubt that the difference between $s^{(n/N)q}$ and s^q is very small if n/N will near to 1. Therefore, we see that the results derived from the RMT theory through a very special case expose the physical insights of the degenerate spectra in a way.

IV. CONCLUSION

By considering the same-degeneracy special case, we explicitly obtain a possible form of the NNS distribution for degenerate spectra. Our result shows that the degenerate spectrum is actually composed of two subspectrum, the random spectrum and regular spectrum, according to the ratios $(N-n)/N$ and n/N. In addition, it turns out that the level repulsion of the regular spectrum is smaller than that of the reduced non-degenerate spectrum because of degeneracy.

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[1] L. Reichl, *Translation to chaos*, New York: Spinger-Verlag, 248-285 (1922).
[2] T. A. Brody, J. Flores, P. A. Mell, *et al.* Rev. Mod. Phys. **53**, 385 (1981).
[3] A. Honiig and D. Wintgen, Phys. Rev. A **39**, 5642 (1989).
[4] P. Pechukas, Phys. Rev. Lett. **51**, 943 (1983).
[5] M. Robonik, J. Phys. A **20**, L495(1987).
[6] T. Yukawa, Phys. Rev. Lett. **54**, 1993 (1985).
[7] T. Yukawa, Phys. Lett. A **116**, 227 (1986).
[8] H. Hasegawa, Phys. Rev. A **38**, 395 (1988).
[9] L. S. Cederbaum, E. Haller and P. Pfeifer. Phys. Rev. A **31**, 1869 (1985).
[10] Thomas Guhr, Axel Muller-Groeling and Hans A. Weidenmuller, Phys. Rep. **299**, 189 (1998).
[11] C. M. Xiao and J. L. Luo, Sci. China Ser. B **41**, 207 (1998).
[12] C. Y. Tao, J. L. Luo and G. S. Yan, Chem. J. Chin. Univ. **14**, 75 (1993).
[13] C. Y. Tao, J. L. Luo and G. S. Yan, Chin. J. Chem. Phys. **6**, 148 (1993).
[14] C. M. Xiao and J. L. Luo, Chin. J. Chem. Phys. **13**, 181 (2000).
[15] A. C. Scott and J. C. Eilbeck, Chem. Phys. Lett. **132**, 23 (1986).
[16] J. C. Eilbeck, P. S. Lomdahl and A. C. Scott, Physica D **16**, 318 (1985).
[17] A. C. Scott, P. S. Lomdahl and J. C. Eilbeck, Chem. Phys. Lett. **113**, 29 (1985).