ANOMALOUS SPECTRAL STATISTICS OF THE ASYMMETRIC ROTOR MODEL

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We investigate the spectral statistics of the asymmetric rotor model (triaxial rigid rotator). The asymmetric top is classically integrable and, according to the Berry-Tabor theory, its spectral statistics should be Poissonian. Surprisingly, our numerical results show that the nearest neighbor spacing distribution $P(s)$ and the spectral rigidity $\Delta_{3}(L)$ do not follow Poisson statistics.

1 Introduction

As is well known, in the semiclassical limit there is a clear connection between the behavior of classical systems (regular or chaotic) and the corresponding quantal ones. In particular for quantal systems, corresponding to classical regular systems, the spectral statistics ($P(s)$ and $\Delta_{3}(L)$) follow the Poisson ensemble, while for systems corresponding to chaotic ones the Wigner ensemble is followed (see, for example, Ref. 3 and references therein).

Nevertheless, some exceptions are known. The most famous case is perhaps the harmonic oscillator one, discussed in great detail in Ref. 4 and 5.

The aim of this paper is to discuss another pathological case: the classically integrable triaxial rotator model (see, for instance, Ref. 6). Incidentally, this model has been used very often in the description of the low-lying states of the even-even atomic nuclei.

The asymmetric top described by the rotor model is a classically integrable system, but an analytical formula for its quantum energy spectrum is not known. Nevertheless, numerical results can be obtained. By following the Landau approach, the Hamiltonian operator is split into 4 submatrices, corresponding to different symmetry classes. Each truncated submatrix is numerically diagonalized. Finally, the nearest-neighbor spacing distribution
$P(s)$ and the spectral rigidity $\Delta_3(L)$ are calculated. Surprisingly, the spectral statistics of energy levels do not follow the predictions of Poisson statistics. This result may suggest the presence of a hidden symmetry in the system but, to our knowledge, such a symmetry has not yet been identified.

2 The Asymmetric Rotor Model

Let us consider a system of coordinates with axes along the three principal axes of inertia of the top, and rotating with it. The classical Hamiltonian $H$ of the top is given by

$$\hat{H} = \frac{1}{2} (a\hat{J}_1^2 + b\hat{J}_2^2 + c\hat{J}_3^2),$$

where $\hat{J} = (J_1, J_2, J_3)$ is the angular momentum of the rotation and $a = 1/I_1$, $b = 1/I_2$, $c = 1/I_3$ are three parameters such that $I_1$, $I_2$ and $I_3$ are the principal moments of inertia of the top. The Hamiltonian is classically integrable and its action variables are precisely the three components $J_s$, $s = 1, 2, 3$, of the angular momentum.

The quantum Hamiltonian $\hat{H}$ is obtained by replacing the components of the angular momentum, in the classical expression of the energy, by the corresponding quantum operators $\hat{J}_1$, $\hat{J}_2$ and $\hat{J}_3$. The commutation rules for the operators of the angular momentum components in the rotating system of coordinates are given by

$$\hat{J}_r\hat{J}_s - \hat{J}_s\hat{J}_r = -ih\, \epsilon_{rst} \hat{J}_t,$$

where $\epsilon_{rst}$ is the Ricci tensor and $r, s, t = 1, 2, 3$. Note that these commutation rules differ from those in the fixed system in the sign on the right-hand side.

As usual, the two operators $\hat{J}_2 = \hat{J}_1^2 + \hat{J}_2^2 + \hat{J}_3^2$ and $\hat{J}_3$ are simultaneously diagonalized on the basis of eigenstates $|J, k\rangle$ with integer eigenvalues $J$ and $k$ ($k = -J, -J + 1, \ldots, J - 1, J$), respectively. The non-zero matrix elements of the quantum Hamiltonian $\hat{H}$ in the basis $|J, k\rangle$ are given by

$$\langle J, k | \hat{H} | J, k \rangle = \frac{\hbar^2}{4} (a + b)(J(J + 1) - k^2) + \frac{\hbar^2}{2}ck^2,$$

$$= \frac{\hbar^2}{8} (a - b) \sqrt{(J - k)(J - k - 1)(J + k + 1)(J + k + 2)}.$$

The quantum Hamiltonian $\hat{H}$ has matrix elements only for transitions with $k \to k$ or $k \pm 2$. The absence of matrix elements for transitions between states
Table 1. Number of states in each submatrix of the asymmetrical top Hamiltonian for a fixed $J$.

|       | $(E, S)$ | $(E, A)$ | $(O, S)$ | $(O, A)$ |
|-------|---------|---------|---------|---------|
| $J$ even | $J$ even | $J$ even | $J$ even | $J$ even |
| $J$ odd  | $J$ odd  | $J$ odd  | $J$ odd  | $J$ odd  |

with even and odd $k$ has the result that the matrix of degree $2J + 1$ is the direct product of two matrices of degrees $J$ and $J + 1$. One of these contains matrix elements for transitions between states with even $k$, and the other contains those for transitions between states with odd $k$.

It is useful to introduce a new basis, given by

$$|J, k; S⟩ = \frac{1}{\sqrt{2}}(|J, k⟩ + |J, -k⟩), \quad |J, 0, S⟩ = |J, 0⟩,$$

$$|J, k; A⟩ = \frac{1}{\sqrt{2}}(|J, k⟩ - |J, -k⟩), \quad k \neq 0.$$  \hspace{1cm} (5)

By using this new basis, the total Hamiltonian matrix is decomposed in the direct product of 4 submatrices by considering the parity of the quantum number $k$: even (E) or odd (O), and the symmetry of the state: symmetric (S) or anti-symmetric (A). So the submatrices are labelled as follow: (E,S), (E,A), (O,S), (O,A). These are the classes of symmetry of the system. In Table 1 we show the dimension of each submatrix for a fixed $J$.

The matrix elements of the Hamiltonian $\hat{H}$ in the new basis, with respect to the old basis, are given by

$$⟨J, k, S|\hat{H}|J, k, S⟩ = ⟨J, k, A|\hat{H}|J, k, A⟩ = ⟨J, k|\hat{H}|J, k⟩, \quad k \neq 0$$  \hspace{1cm} (6)

$$⟨J, 1, S|\hat{H}|J, 1, S⟩ = ⟨J, 1|\hat{H}|J, 1⟩ + ⟨J, 1|\hat{H}|J, -1⟩$$  \hspace{1cm} (7)

$$⟨J, 1, A|\hat{H}|J, 1, A⟩ = ⟨J, 1|\hat{H}|J, 1⟩ - ⟨J, 1|\hat{H}|J, -1⟩$$  \hspace{1cm} (8)

$$⟨J, k, S|\hat{H}|J, k + 2, S⟩ = ⟨J, k, A|\hat{H}|J, k + 2, A⟩ = ⟨J, k|\hat{H}|J, k + 2⟩, \quad k \neq 0$$  \hspace{1cm} (9)

$$⟨J, 0, S|\hat{H}|J, 2, S⟩ = \sqrt{2}⟨J, 0|\hat{H}|J, 2⟩, \quad k \neq 0$$  \hspace{1cm} (10)

We calculate the eigenvalues of each submatrix for different values of $J$ using a fast implementation, in double precision, of the Lanczos algorithm with a LAPAC code.\[8]

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In Figure 1 we plot the density of levels $\rho(E)$ of each submatrix of $\hat{H}$ and $J = 1000$. The results show that the density of levels is practically the same for the four classes. $\rho(E)$ displays a high peak at the left-center of the energy interval and a long tail for large energy values.

3 Spectral Statistics

As previously discussed, according to the Berry-Tabor theory, given a classical integrable Hamiltonian that, written in action variables $J_r$, satisfies the condition $\left| \frac{\partial^2 H}{\partial J_r \partial J_s} \right| \neq 0$, then, in the semiclassical limit, its spectral statistics should follow the Poisson statistics. Note that a system of linear harmonic oscillators, whose Hamiltonian is given by $H = \vec{\omega} \cdot \vec{I}$, does not satisfy the previous condition. In fact, a system of linear harmonic oscillators is integrable.
but it does not follow Poissonian statistics.

The triaxial rigid rotator is integrable and satisfies the previous Berry-Tabor condition. Thus, one expects that the spectral statistics of the quantized rigid rotator should be Poissonian. We shall show that is not the case.

In general, various statistics may be used to show the local correlations of the energy levels but the most used spectral statistics are $P(s)$ and $\Delta_3(L)$. $P(s)$ is the distribution of nearest-neighbor spacings $s_i = (\tilde{E}_{i+1} - \tilde{E}_i)$ of the unfolded levels $\tilde{E}_i$. It is obtained by accumulating the number of spacings that lie within the bin $(s, s + \Delta s)$ and then normalizing $P(s)$ to unit. As shown by Berry and Tabor, for quantum systems whose classical analogs...
Figure 3. Spectral rigidity $\Delta_3(L)$ of the four classes of symmetry with $J = 1000$. The dashed line is the Poisson prediction $\Delta_3(L) = L/15$. Parameters: $a = 1$, $b = \sqrt{2}$, $c = \sqrt{5}$ and $\hbar = 1$.

are integrable, $P(s)$ is expected to follow the Poisson distribution

$$P(s) = \exp(-s) . \quad (11)$$

The statistic $\Delta_3(L)$ is defined, for a fixed interval $(-L/2, L/2)$, as the least-square deviation of the staircase function $N(E)$ from the best straight line fitting it:

$$\Delta_3(L) = \frac{1}{L} \min_{A,B} \int_{-L/2}^{L/2} [N(E) - AE - B]^2 dE ,$$

where $N(E)$ is the number of levels between $E$ and zero for positive energy, between $-E$ and zero for negative energy. The $\Delta_3(L)$ statistic provides a measure of the degree of rigidity of the spectrum: for a given interval $L$, the smaller $\Delta_3(L)$ is, the stronger is the rigidity, signifying the long-range
correlations between levels. For this statistic the Poissonian prediction is

$$\Delta_3(L) = \frac{L}{15}. \quad (12)$$

It is useful to remember that Berry, on the basis of the Gutwiller semiclassical formula for the density of states, has shown that $\Delta_3(L)$ deviates from the universal Poissonian predictions for large $L$: $\Delta_3(L)$ should saturate to an asymptotic value performing damped oscillations.

In Figure 2 the spectral statistic $P(s)$ is plotted for the four submatrices of $\hat{H}$ and $J = 1000$. Note that the level spectrum is mapped into unfolded levels with quasi-uniform level density by using a standard procedure described in Ref. 13. As expected from the previous analysis of density of levels, $P(s)$ is practically the same for the four classes of symmetry. Moreover, $P(s)$ has a pathological behavior: a peak near $s = 1$ and nothing elsewhere.

Compared to $P(s)$, the spectral rigidity $\Delta_3(L)$ is less pathological. As shown in Figure 3, $\Delta_3(L)$ follows quite well the Poisson prediction $\Delta_3(L) = L/15$ for small $L$ but for larger values of $L$ it gets a constant mean value with fluctuations around this mean value. These fluctuations becomes very large by increasing $L$, in contrast with the Berry prediction.

The behavior of the density of levels $\rho(E)$ and of the spectral statistics $P(s)$ and $\Delta_3(L)$ does not change by changing the matrix dimension, namely the quantum number $J$. In Figure 4 we plot the density of levels and the spectral statistics for $J = 2000$ and $J = 4000$.

Conclusions

The main conclusion of this paper is that the asymmetric rotor is, like the harmonic oscillator, another pathological case with respect to the classical-quantum correspondence between integrability and Poisson statistics. In our opinion, the pathology of the asymmetric rotor model is more interesting because, unlike the harmonic oscillator, the asymmetric rotor satisfies the conditions of the Berry-Tabor theory. The presence of hidden symmetries could explain the pathological behavior of spectral statistics but such symmetries have not yet been identified.

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Figure 4. Density of levels $\rho(E)$, Nearest neighbor spacing distribution $P(s)$ and spectral rigidity $\Delta(L)$ of the $(E,S)$ class of symmetry, with $J = 2000$ (top) and $J = 4000$ (bottom). Dashed lines are Poisson predictions. Parameters: $a = 1$, $b = \sqrt{2}$, $c = \sqrt{5}$ and $\hbar = 1$.

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