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Spectral inequalities for the quantum asymmetric top

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Abstract
We consider the spectrum of the quantum asymmetric top. Unlike in the case when two or three moments of inertia are equal, when the moments of inertia are distinct all degeneracy in the spectrum of the operator is removed. We derive inequalities for the spectra based on recent results on the interlacing of Van Vleck zeros.

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1. Introduction

Given any three positive numbers $\alpha_1, \alpha_2, \alpha_3$, the quantum top is defined as the operator

$$L_\alpha := \alpha_1 L_x^2 + \alpha_2 L_y^2 + \alpha_3 L_z^2, \tag{1.1}$$

where L_x, L_y and L_z are the components of the angular momentum, i.e.

$$L_x = -\mathrm{i}(y\partial_z - z\partial_y), \qquad L_y = -\mathrm{i}(z\partial_x - x\partial_z), \qquad L_z = -\mathrm{i}(x\partial_y - y\partial_x).$$

The quantum spherical top corresponds to the case $\alpha_1 = \alpha_2 = \alpha_3$ and the quantum symmetrical top to the case $\alpha_1 = \alpha_2 \neq \alpha_3$. When all three α's are distinct, L_α is known as the quantum asymmetric top or the quantum Euler top.

Since L_α and Δ_{S^2}, the constant curvature Laplacian on S^2, are commuting, self-adjoint elliptic operators on $L^2(S^2)$, they possess a Hilbert basis of joint eigenfunctions. In the case of the spherical and symmetrical tops, the joint eigenfunctions are given by the standard spherical harmonics

$$Y_k^m(\theta, \phi) = P_k^m(\cos\theta)\,\mathrm{e}^{\mathrm{i}m\phi}, \qquad |m| \leqslant k, \quad k \in \mathbb{N},$$

where P_k^m is the associated Legendre function of the first kind. The corresponding eigenvalues are given by $\alpha_1 k(k+1)$ in the case of the spherical top, and by $\alpha_1 k(k+1) + (\alpha_3 - \alpha_1)m^2$, $|m| \leqslant k$ for the symmetrical top. For each k there are $2k + 1$ harmonics, so the spherical top has a

$2k+1$ degeneracy for each eigenvalue and the symmetrical top has a double degeneracy for each nonzero eigenvalue.

However, the situation for the asymmetric top is not as simple. In this case the degeneracy of the eigenvalues is removed completely, and as noted by Landau and Lifshitz [10], the calculation of the energy levels in a general form is impossible. To obtain a basis of joint eigenfunctions, it is customary to introduce a new set of coordinates on S^2, the sphero-conal or elliptic coordinates [14]. In terms of these coordinates, one can separate variables to express the joint eigenfunctions as the product

$$\psi_k^\gamma(u_1, u_2) = \phi_k^\gamma(u_1)\phi_k^\gamma(u_2),$$

where the function ϕ_k^γ is given by

$$\phi_k^\gamma(x) = \prod_{j=1}^{3} |x - \alpha_j|^{\gamma_i/2} P_m(x). \tag{1.2}$$

Here, $\gamma = (\gamma_1, \gamma_2, \gamma_3)$ is a multi-index with $\gamma_j \in \{0, 1\}$ and $P_m(x)$ is a polynomial of degree $m := (k - |\gamma|)/2$. In addition, $\phi_k^\gamma(x)$ is a solution of the *Lamé equation*:

$$\frac{\mathrm{d}^2}{\mathrm{d}x^2}\phi_k^\gamma(x) + \frac{1}{2}\sum_{j=1}^{3}\frac{1}{x-\alpha_j}\frac{\mathrm{d}}{\mathrm{d}x}\phi_k^\gamma(x) = \frac{1}{4}\frac{k(k+1)x - E}{\prod_{j=1}^{3}(x-\alpha_j)}\phi_k^\gamma(x). \tag{1.3}$$

Originally, these observations were made by Kramers and Ittman [8, 9]; we refer the reader to [1] for more detailed derivations of these facts. Accordingly, the spherical harmonics ψ_k^γ are known as *Lamé harmonics*. It is well known that for each $k \in \mathbb{N}$, there exist $2k+1$ linearly independent Lamé harmonics of degree k, so the ψ_k^γ form a basis of spherical harmonics.

The separation constant E appearing on the right-hand side of (1.3) is the eigenvalue of L_α associated with the eigenfunction ψ_k^γ. It is well known that the eigenvalues are real and simple. For each k, it is customary to divide the spectrum σ_k of L_α into four disjoint subsets

$$\sigma_k = \begin{cases} \sigma_k^{0,0,0} \cup \sigma_k^{1,1,0} \cup \sigma_k^{1,0,1} \cup \sigma_k^{0,1,1} & \text{if} \quad k \text{ is even} \\ \sigma_k^{1,0,0} \cup \sigma_k^{1,0,0} \cup \sigma_k^{0,0,1} \cup \sigma_k^{1,1,1} & \text{if} \quad k \text{ is odd} \end{cases}$$

where σ_k^γ is the set of all eigenvalues of L_α corresponding to eigenfunctions of the form ψ_k^γ. The cardinality of each subset is equal to $m+1$, where m is the degree of the polynomial P_m defined above. More precisely, we have

$$\left|\sigma_k^{0,0,0}\right| = k/2 + 1, \left|\sigma_k^{1,0,0}\right| = \left|\sigma_k^{0,1,0}\right| = \left|\sigma_k^{0,0,1}\right| = (k+1)/2,$$
$$\left|\sigma_k^{1,1,0}\right| = \left|\sigma_k^{1,0,1}\right| = \left|\sigma_k^{0,1,1}\right| = k/2, \left|\sigma_k^{1,1,1}\right| = (k-1)/2.$$

Note that for k even,

$$|\sigma_k| = \left|\sigma_k^{0,0,0}\right| + \left|\sigma_k^{1,1,0}\right| + \left|\sigma_k^{1,0,1}\right| + \left|\sigma_k^{0,1,1}\right| = 2k+1$$

and similarly for k odd. In the following, we denote by $E_{k,j}^\gamma$, $j = 1, \ldots, \left|\sigma_k^\gamma\right|$ the ordered eigenvalues of L_α that belong to σ_k^γ. The main result of this paper is a separation theorem for the spectrum of L_α.

Theorem 1.1. *For every multi-index $\gamma \in \{0, 1\}^3$, the following inequalities hold:*

$$(i) \quad \frac{E_{k+2,j}^\gamma}{\mu_{k+2}^\gamma} < \frac{E_{k,j}^\gamma}{\mu_k^\gamma} \qquad \text{where} \quad \mu_k^\gamma = (k - |\gamma|)(k + |\gamma| + 1) \tag{1.4}$$

$$(ii) \quad E_{k,j}^\gamma < E_{k+2,j+1}^\gamma \qquad \text{for} \quad j = 1, \ldots, \left|\sigma_k^\gamma\right|. \tag{1.5}$$

Although there exists an extensive literature on the quantum asymmetric top, as far as we are aware, these inequalities do not appear anywhere in the literature.

2. The generalized Lamé equation

The Lamé equation (1.3) is a special case (with $\rho_1 = \rho_2 = \rho_3 = 1/2$) of the following Heun equation [4]:

$$y''(x) + \sum_{j=1}^{3} \frac{\rho_j}{x - \alpha_j} y'(x) = \frac{\mu(x - \nu)}{\prod_{j=1}^{3}(x - \alpha_j)} y(x). \tag{2.1}$$

Here, we assume that $\alpha_1 < \alpha_2 < \alpha_3$ and $\rho_j > 0$. We will refer to the above equation (2.1) as the generalized Lamé equation (GLE), although we note that it appears under several different names in the literature. The GLE plays an important role in the integrability of quantum systems [7], as well as in electrostatic systems with logarithmic potential [3, 5, 6, 12].

It is well known that for each $k \in \mathbb{N}$, there exist exactly $k+1$ distinct values of ν for which (2.1) has a polynomial solution y of degree k. These polynomial solutions are usually referred to as the Stieltjes polynomials. The corresponding linear polynomials $V(x) := \mu(x - \nu)$ are known as Van Vleck polynomials.

In 1898, Van Vleck [13] showed that the zeros ν of $V(x)$ lie inside the interval (α_1, α_3), and for each $k \in \mathbb{N}$, the $k + 1$ possible values of ν are distinct. Very few results on the zeros of $V(x)$ have been obtained since then. One of the most striking results since those of Van Vleck is the following interlacing property [2]; if we denote by

$$\nu_{1,k} < \nu_{2,k} < \cdots < \nu_{k+1,k}$$

the $k+1$ ordered Van Vleck zeros corresponding to Stieltjes polynomials of degree k, then the following inequalities hold:

$$\nu_{1,k+1} < \nu_{1,k} < \nu_{2,k+1} < \cdots < \nu_{k+1,k} < \nu_{k+2,k+1}. \tag{2.2}$$

2.1. *Proof of theorem 1.1*

Using the interlacing property, it is now easy to prove theorem 1.1. Indeed, substituting the corresponding Lamé function $\phi_k^{\gamma}(x)$ from (1.2) into (1.3), then one can verify after some straightforward computations that the polynomial P_m satisfies the GLE:

$$\frac{\mathrm{d}^2 P_m}{\mathrm{d}x^2} + \sum_{j=1}^{3} \frac{\gamma_j + 1/2}{x - \alpha_j} \frac{\mathrm{d}P_m}{\mathrm{d}x} = \frac{\mu_k^{\gamma} x - E + D(\alpha, \gamma)}{4(x - \alpha_1)(x - \alpha_2)(x - \alpha_3)} P_m, \tag{2.3}$$

where $D(\alpha, \gamma)$ is the constant given by

$$D(\alpha, \gamma) = (\gamma_2 + \gamma_3)^2 \alpha_1 + (\gamma_1 + \gamma_3)^2 \alpha_2 + (\gamma_1 + \gamma_2)^2 \alpha_3.$$

As a consequence of (2.2) applied to the Van Vleck zeros

$$\nu_{j,m} = \frac{E_{k,j}^{\gamma} - D(\alpha, \gamma)}{\mu_k^{\gamma}} \qquad (j = 1, \ldots, m),$$

we obtain

$$\frac{E_{k+2,j}^{\gamma} - D(\alpha, \gamma)}{\mu_{k+2}^{\gamma}} < \frac{E_{k,j}^{\gamma} - D(\alpha, \gamma)}{\mu_k^{\gamma}} < \frac{E_{k+2,j+1}^{\gamma} - D(\alpha, \gamma)}{\mu_{k+2}^{\gamma}} \tag{2.4}$$

for $j = 1, \ldots, m$. Theorem 1.1 is then an immediate consequence of these inequalities and the fact $\mu_k^{\gamma} < \mu_{k+2}^{\gamma}$.

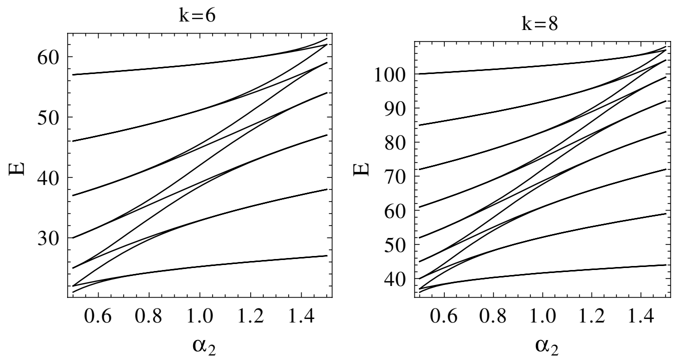

Figure 1. Spectra of the quantum top for $k = 6$ and $k = 8$ with $\alpha_1 = 1/2$ and $\alpha_3 = 3/2$. The energy levels of the prolate symmetrical top are at $\alpha_2 = 1/2$ and of the oblate symmetrical top are at $\alpha_2 = 3/2$. Values of $1/2 < \alpha_2 < 3/2$ represent the energy levels of the asymmetrical top.

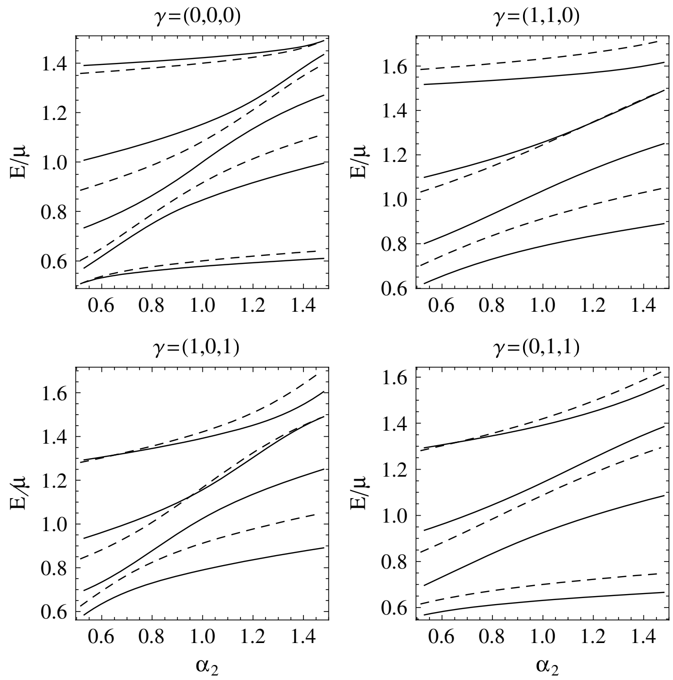

Figure 2. Scaled spectra of the quantum top. The $E^{\gamma}_{6,j}/\mu^{\gamma}_{6}$ are plotted as dashed curves and the $E^{\gamma}_{8,j}/\mu^{\gamma}_{8}$ are plotted as solid curves.

2.2. *Distribution of the eigenvalues*

As mentioned above, Van Vleck [13] showed that the Van Vleck zeros lie in the interval (α_1, α_3). Thus each $E = E^{\gamma}_{k,j}$ satisfies

$$\alpha_1(k - |\gamma|)\,(k + |\gamma| + 1) + D(\alpha, \gamma) < E < \alpha_3(k - |\gamma|)\,(k + |\gamma| + 1) + D(\alpha, \gamma).$$

A straightforward calculation shows that this is equivalent to

$$\alpha_1 k(k+1) + (\alpha_2 - \alpha_1)\,(\gamma_1 + \gamma_3)^2 + (\alpha_3 - \alpha_1)\,(\gamma_1 + \gamma_2)^2 < E$$
$$< \alpha_3 k(k+1) - (\alpha_3 - \alpha_2)\,(\gamma_1 + \gamma_3)^2 - (\alpha_3 - \alpha_1)\,(\gamma_2 + \gamma_3)^2 .$$

Thus, in the limiting case $\alpha_1 = \alpha_2 = \alpha_3$, we recover the fact that the eigenvalues of the spherical top are $\alpha_1 k(k+1)$. As $\alpha_1, \alpha_2, \alpha_3$ separate the eigenvalues split. We have the following slight improvement of theorem 2.2 of [1]:

Theorem 2.1. *Suppose that* $0 < \alpha_1 < \alpha_2 < \alpha_3$. *The part of the spectrum* σ_k *of* $-L_\alpha$ *corresponding to the Lamé harmonics of degree* k *lie inside the interval* $(\alpha_1 k(k+1), \alpha_3 k(k+1))$.

The situation is illustrated in figures 1 and 2. Here we fix $\alpha_1 = 1/2$ and $\alpha_3 = 3/2$, and allow α_2 to vary between $1/2$ and $3/2$. The cases when $\alpha_2 = 1/2$ or $3/2$ correspond to symmetrical tops with prolate or oblate symmetry, respectively [11]. The two kinds of symmetry depend on whether the moment of inertia of the two equal moments is greater than or less than the unequal moment. As α_2 becomes greater than $1/2$ the eigenvalues split and as α_2 approaches $3/2$ they coalesce, but at different levels. Figure 1 shows the plots of $E = E^{\gamma}_{k,j}$ for two fixed values of k, namely $k = 6$ and $k = 8$.

In figure 2 we illustrate the interlacing property. Here we plot the scaled values of the energy $E^{\gamma}_{k,j}$ for $k = 6$ and $k = 8$ for the four possible values of γ. When $\gamma = (0, 0, 0)$, $D(\alpha, \gamma) = 0$, so the $E^{\gamma}_{6,j}/\mu^{\gamma}_6$ and $E^{\gamma}_{8,j}/\mu^{\gamma}_8$ interlace for all values of α such that $\alpha_1 < \alpha_2 < \alpha_3$ (upper left panel). In the other three cases, the scaled energy levels do not interlace for all α due to the presence of the nonzero $D(\alpha, \gamma)$ term in (2.4).

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