Energy Ellipsoid - 3D Rotational motion of a wobbler

A General Study for $^{135}\mathrm{Pr}$

Goals:

- [ ] Obtain the Contour Plot of the energy function H' for a triaxial rotor. Extensive study for the ellipsoid with different maximal moment of inertia:
  - [ ] MOI is oriented along the 1-axis. **dedicated case due to our obtained results**
  - [ ] MOI is oriented along the 2-axis.
  - [ ] MOI is oriented along the 3-axis.
- [ ] Obtain a spherical plot with the energy surface for H' for all the three cases of maximal MOI value.
- [ ] Represent the energy ellipsoid for a fixed value of I, together with the angular momentum sphere generated by the core.

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1. Theoretical framework

The Hamiltonian H' is expressed in terms of the classical components of the angular momentum I_1, I_2, I_3. The angular momentum components are written in a spherical coordinate system, via the angles θ (polar angle) and φ (azimuthal angle). The values for θ and φ are inside the intervals $[0, \pi]$, and $[0, 2\pi]$, respectively.

Depending on what axes has the largest MOI, different sets for $(I_1, I_2, I_3) \equiv (x_1, x_2, x_3)$ will be defined.

The expression for the energy is:

$$E = x_2^2 + u x_3^2 + 2 v_0 x_1$$

and the square of total angular momentum:

$$I^2 = x_1^2 + x_2^2 + x_3^2$$

, both being *constants of motion*.

Classical expression for the Hamiltonian of the system is given by the expression:

$$H' = I_2^2 + u I_3^2 + 2 v_0 I_1 \ .$$

2. Obtaining the contour plot

1-axis

When 1-axis has the largest MOI, it is convenient to pick it as the quantization axis, with $x_2 O x_3$ -plan being perpendicular to this axis. Expressions for the components of the angular momentum, expressed in spherical coordinates are as follow:

$$x_1 = I \cos \theta_1$$

$$x_2 = I \sin \theta_1 \cos \varphi_1$$

$$x_3 = I \sin \theta_1 \sin \varphi_1$$

with the Hamiltonian in the following form:

$$H' = (\cos^2 \varphi_1 + u \sin^2 \varphi_1)(I^2 - x_1^2) + 2 v_0 x_1$$

or, given as (easier for dealing with the spherical coordinates (I ,\theta_1,\varphi_1) For the first case, where $\mathcal{I}_1$ is the maximal moment of inertia, our numerical results are obtained directly from the *least squares fit* for the energies of the studied isotope. The values for the required parameters are:

I_1	I_2	I_3	θ_{coupling}	j
89	12	48	-71	$11/2$

Obs: The θ_{coupling} represents the angle which gives the orientation of the odd-proton's angular momentum in the inertia plane which is perpendicular to the quantization axis. It is fundamentally different from the value of θ_1, which represents the elevation of the angular momentum vector from the $x_2 O x_3$ principal plane.

Having the following values, it is possible to obtain the values for the functions u, v_0. For a certain value of total spin I, the function $v = \frac{v_0}{I}$ results immediately, together with the first component of the angular momentum, namely $x_1 = I \cos \theta_1$, where:

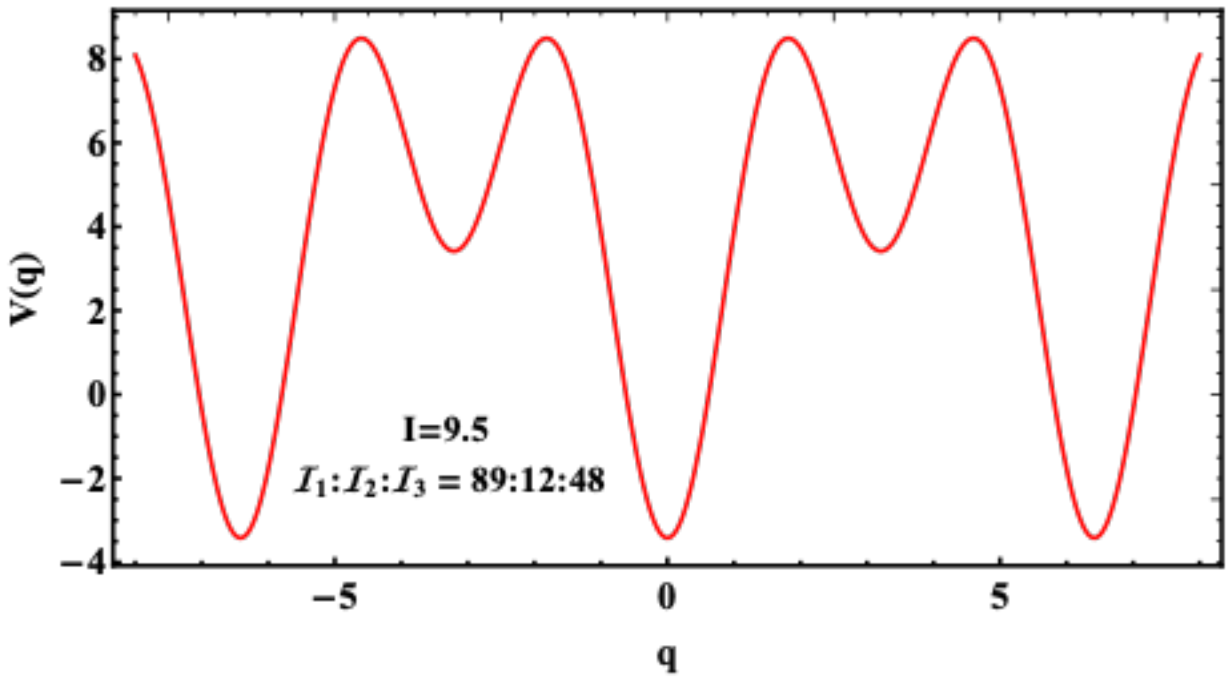
$$\theta_1 = \arccos\left(\frac{x_1}{I}\right)$$

The numerical values for the mentioned functions are calculated for a spin value fixed to $I = 19/2$. The results are as follow:

u	v_0	v	x_1
0.081531	-0.170917	-0.0179912	$\in [-19/2, 19/2]$

Rotor Potential $V(q)$

The rotor potential $V(q)$ is also calculated with the given parameters, and the figure can be seen below:



The potential for $^{135}\mathrm{Pr}$ *with the obtained fit parameters.*

Stationary points

The Hamiltonian for this case of $\mathcal{I}_1$-maximal MOI has the following stationary points:

1. $(x_1, \varphi_1) = (\frac{v_0}{u}, \frac{\pi}{2})$ - This is a **saddle point** for H' and the corresponding angular momentum components and energy is:

$$(x_1, x_2, x_3) = \left(\frac{v_0}{u}, 0, \sqrt{I^2 - \frac{v_0^2}{u^2}}\right)$$

   and:

$$E_s = \left(u + \frac{v_0^2}{u}\right) I^2 .$$

2. $(x_1, \varphi_1) = (v_0, 0)$ - This is a **maximum** for H', with the corresponding angular momentum components and energy:

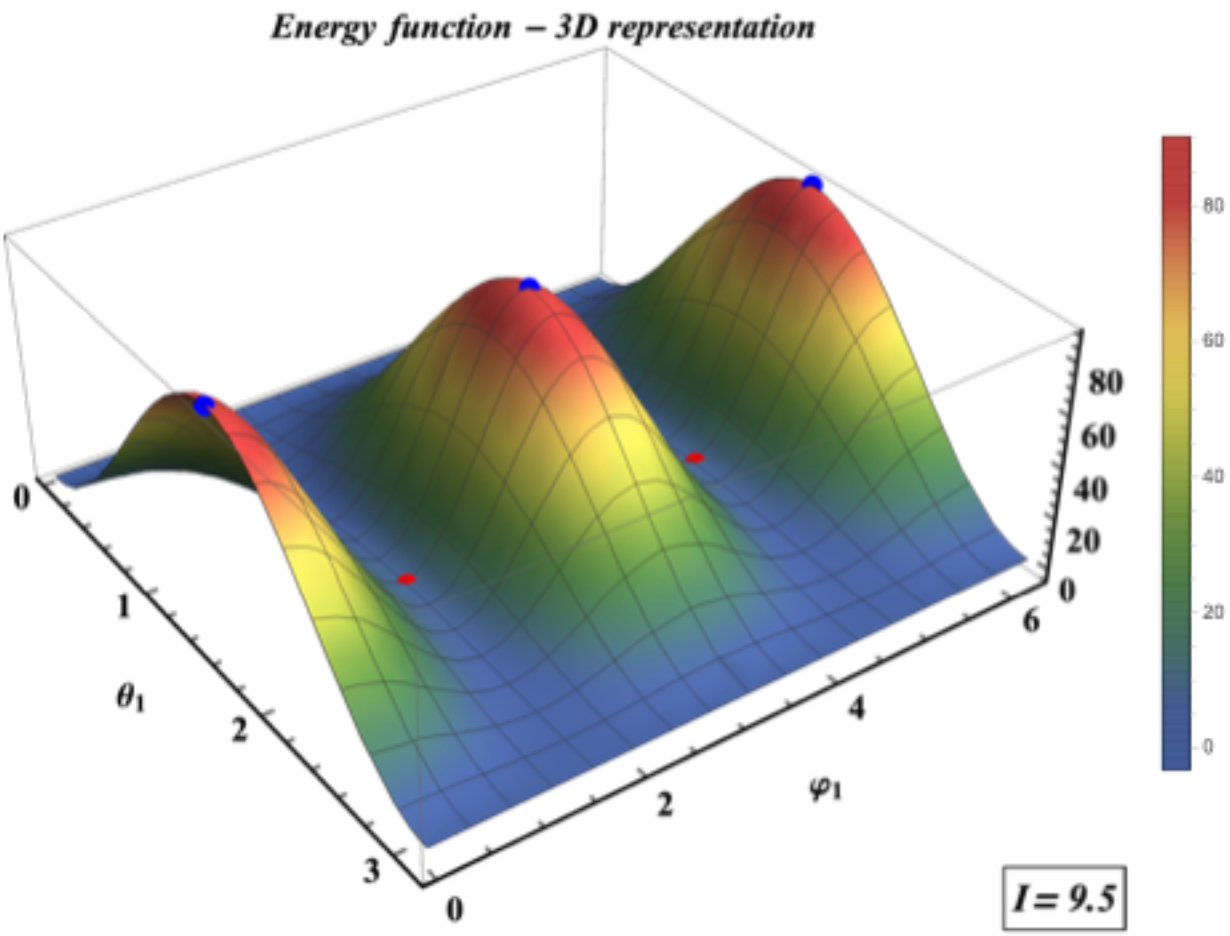
$$(x_1, x_2, x_3) = \left(v_0, \sqrt{I^2 - v_0^2}, 0\right)$$

and:

$$E_M = I^2 + v_0^2 \; .$$

3D Plot for H' as function of θ_1 and φ_1

The parameters from the above table were used in calculating H'. Value of spin is given in plot description.



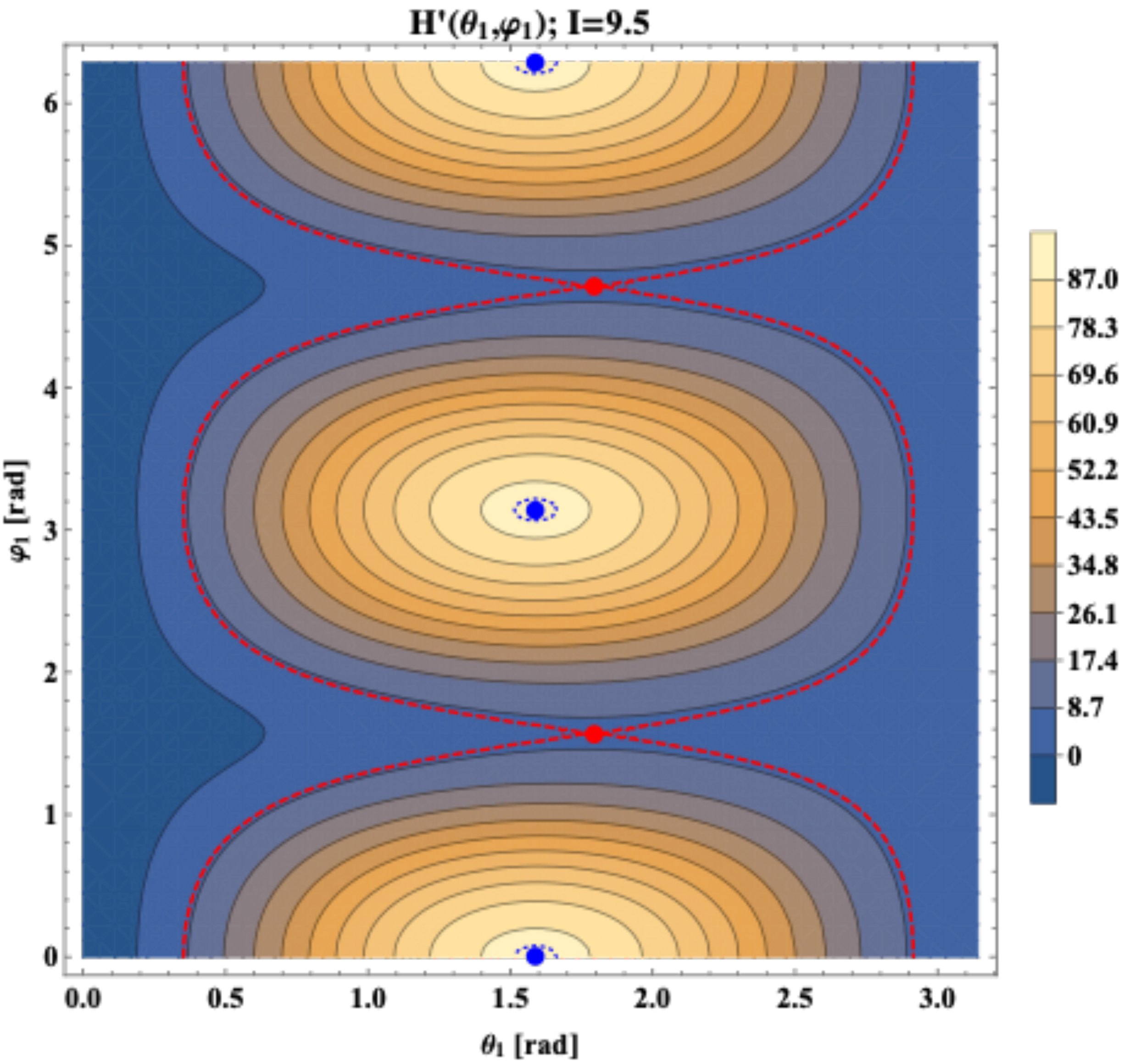
The 3D plot for the energy function H' of the triaxial rotor $^{135}\mathrm{Pr}$ using the fit parameters.

With red dots, the saddle points were represented, while the maximum points were represented by the blue dots. The three peak points where that can be seen in the figure have same height.
Obs: In this figure, there is no local minimum/maximum; only saddle point and global maximum.

Contour plot for H'

With the formula for the energy function, given in terms of the spherical coordinates, obtaining a contour plot is straightforward.

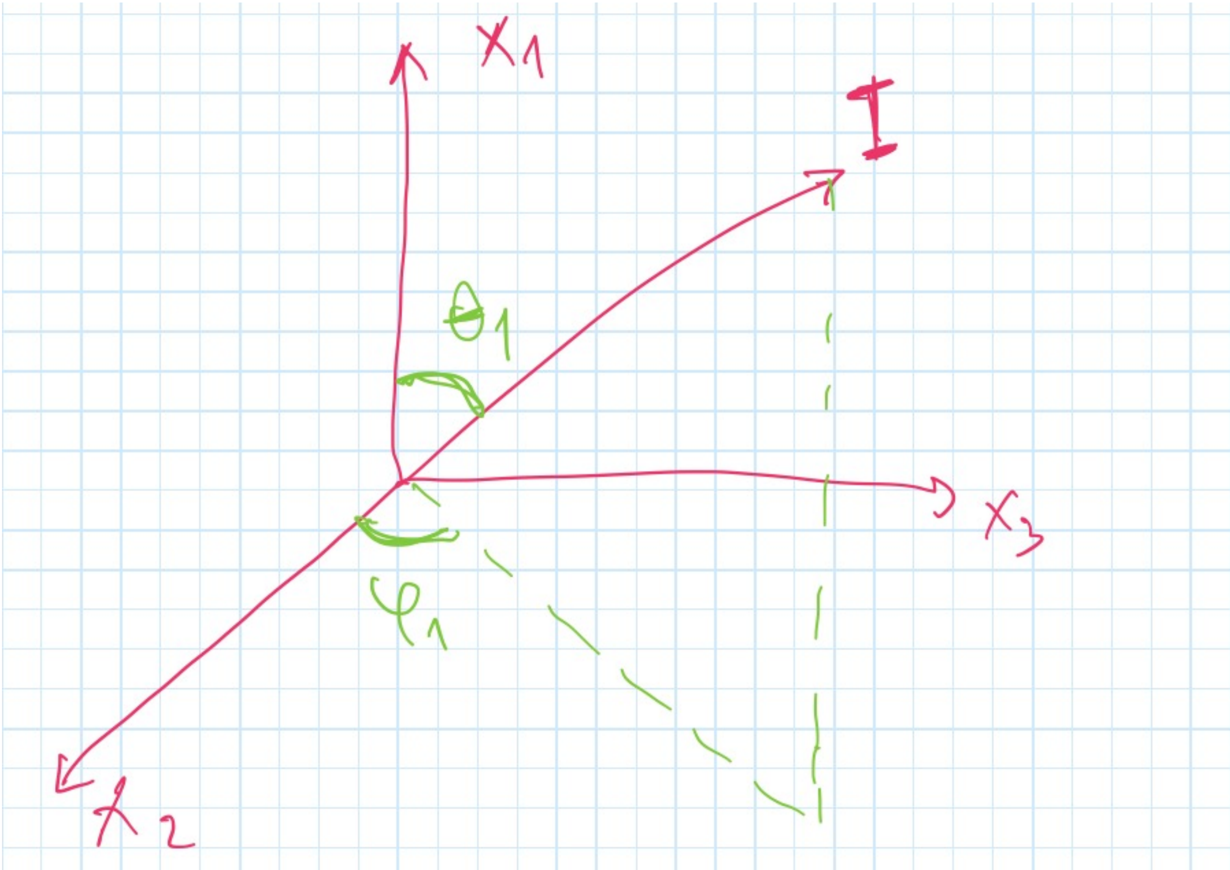
The variables are in the intervals $\theta \in [0, \pi]$ and $\varphi \in [0, 2\pi]$.



Contour plot for the energy function H'. The red lines represent the regions where the energy function equals the saddle point value $E_s^{\text{numerical}} = 7.71647$, considered for a certain spin. Meanwhile, with blue color, the maximal value of H' represented, with small circular enclosed lines marking the region very close to that maximal point $E_M^{\text{numerical}} = 90.2792$.

Obtaining the 3D-spherical plot

This is the scheme in which the approach for 3D spherical plot is considered for calculations:



Spherical coordinate plot for the 1-axes maximal MOI case.

Problems...