^{163}Lu - Energy Ellipsoid

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1 Calculations

The initial energy function $\mathscr{H}$ is given in terms of the polar coordinates (θ,φ).

1.1 Cartesian coordinate system - calculations

The maximal MOI is around 1-axis. As a result, quantization axis is the 1-axis. Thus, the coordinate system becomes:

$$\begin{cases} x_1 = I\cos\theta, \\ x_2 = I\sin\theta\cos\varphi, \\ x_3 = I\sin\theta\sin\varphi. \end{cases} \tag{1}$$

The energy function, in Cartesian form, will have the following expression:

$$H = c_0 + c_1(x_1) + c_2(x_1,x_2,x_3)\ . \tag{2}$$

The constant (free-term) can be ignored, so we focus on the analytical expression for the last two terms, namely c_1 and c_2.

$$c_1(x_1) = -2jA_1\sqrt{I^2 - x_1^2} \tag{3}$$

and

$$c_2(x_1,x_2,x_3) = (A_3 - a_3)x_1^2 + (A_1 - a_1)x_2^2 + (A_2 - a_2)x_3^2 \tag{4}$$

with $a_k = \frac{A_k}{2I}$. *Full calculations can be seen in the attached hand-written notes at the end of this document.*

2 Features of the Energy Function - Cartesian form

Based on the expressions given in 3 and 4, one can see that:

- The energy function has an **ellipsoidal** shape, given by the *main* term c_2.
- The contribution of the x_1-dependent term has a negative sign and $c_1 \approx x_1$. This will create a shift in the ellipsoid, along the x_1-direction.
- Since c_0 doesn't have any dependence on the Cartesian coordinates, it can be neglected during the graphical representation procedure.

3 Appendix: Hand-written notes

$$
\mathcal{H} = \frac{I}{2}(A_1 + A_2) + A_3 I^2 + I(I - \frac{1}{2}) \sin^2\theta \left(A_1 \cos^2\varphi + A_2 \sin^2\varphi - A_3\right)
$$
$$
+ \frac{j}{2}(A_2 + A_3) + A_1 j^2 - 2A_1 I j \sin\theta - V\frac{2j-1}{j+1} \sin\left(\gamma + \frac{\pi}{6}\right).
$$

$$
H(\theta, \varphi) = \underbrace{h_0}_{\text{const.}} + \underbrace{h_\theta}_{f(\theta)} + \underbrace{h_1}_{g(\theta,\varphi)}
$$

$$
\begin{cases} x_1 = I\cos\theta \\ x_2 = I \sin\theta\cos\varphi \\ x_3 = I \sin\theta\sin\varphi \end{cases}
$$

x_1 – rotation MOI

$$
h_0 = \frac{I}{2}(A_1 + A_2) + A_3 I^2 + \frac{j}{2}(A_2 + A_3) + A_1 j^2 - V\frac{2j-1}{j+1}\sin\left[\gamma + \frac{\pi}{6}\right]
$$

↳ constant (can be ignored)

$$
h_\theta = -2Ij A_1 \sin\theta = -2jA_1\sqrt{I^2 - I^2\cos^2\theta}
$$
$$
= -2jA_1\sqrt{I^2 - x_1^2}
$$

↳ $x_1^2 \leq I^2$

$|x_1| \leq I$

$$
h_1 = I\left(I - \frac{1}{2}\right)\sin^2\theta\left(A_1\cos^2\varphi + A_2\sin^2\varphi - A_3\right)
$$

$$
a_k = \frac{A_k}{2I}
$$

$$
= A_1 I^2 \sin^2\theta\cos^2\varphi + A_2 I^2 \sin^2\theta\sin^2\varphi - I^2\sin^2\theta A_3 -
$$
$$
- \frac{A_1}{2} I \sin^2\theta\cos^2\varphi - \frac{A_2}{2} I \sin^2\theta\sin^2\varphi + \frac{A_3 I}{2}\sin^2\theta
$$
$$
= A_1 x_2^2 + A_2 x_3^2 - A_3 I^2(1 - \cos^2\theta) - a_1 x_2^2 - a_2 x_3^2 + a_3 I^2(1 - \cos^2\theta)
$$
$$
= (A_1 - a_1)x_2^2 + (A_2 - a_2)x_3^2 + A_3 x_1^2 - A_3 I^2 + a_3 I^2 - a_3 x_1^2
$$
$$
= (A_3 - a_3)x_1^2 + (A_1 - a_1)x_2^2 + (A_2 - a_2)x_3^2 - (A_3 - a_3)I^2
$$

cartesian form of H

$$H = h_0 - \overset{C_1(x_1)}{\left(2 j A_1 \sqrt{I^2 - x_1^2}\right)} + \overbrace{(A_3 - a_3)x_1^2 + (A_1 - a_1)x_2^2 + (A_2 - a_2)x_3^2}^{C_2(x_1, x_2, x_3)} - (A_3 - a_3) I^2$$

cartesian expression of H

$$H = C_0 + C_1(x_1) + C_2(x_1, x_2, x_3)$$