Oscillateur harmonique anisotrope à trois dimensions

1) Séparation des variables $\Rightarrow$ trois équations $\hat{H} = \hat{H}_x + \hat{H}_y + \hat{H}_z$

$$\hat{H}_x = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{m\omega^2}{2}\left(1+\frac{2\alpha}{3}\right)x^2 \quad ; \quad \hat{H}_x\psi(x) = E_x\psi(x)$$

$$\hat{H}_y = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial y^2} + \frac{m\omega^2}{2}\left(1+\frac{2\alpha}{3}\right)y^2 \quad ; \quad \hat{H}_y\psi(y) = E_y\psi(y)$$

$$\hat{H}_z = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial z^2} + \frac{m\omega^2}{2}\left(1-\frac{4\alpha}{3}\right)z^2 \quad ; \quad \hat{H}_z\psi(z) = E_z\psi(z)$$

$$\psi(\vec{r}) = \psi(x)\psi(y)\psi(z)$$

2) • $-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2} + \frac{m\omega^2}{2}\left(1+\frac{2\alpha}{3}\right)x^2\psi(x) = E_x\psi(x)$ avec $\psi(x) = k e^{-\alpha x^2}$ $(n_x=0)$

$$\Rightarrow \frac{\partial^2\psi(x)}{\partial x^2} = (4\alpha^2x^2 - 2\alpha)\psi(x)$$

$$-\frac{\hbar^2}{2m}(4\alpha^2x^2-2\alpha)\psi(x) + \frac{m\omega^2}{2}\left(1+\frac{2\alpha}{3}\right)x^2\psi(x) = E_x\psi(x)$$

$$\frac{\hbar^2\alpha}{m} = E_x \quad \text{avec } \alpha \text{ tel que } -\frac{2\hbar^2\alpha^2}{m} + \frac{m\omega^2}{2}\left(1+\frac{2\alpha}{3}\right) = 0$$

annulation du terme en x^2 !

$$\Leftrightarrow E_x^2 = \frac{\hbar^4\alpha^2}{m^2} \qquad \Leftrightarrow \alpha^2 = \frac{m^2\omega^2}{4\hbar^2}\left(1+\frac{2\alpha}{3}\right)$$

soit $E_x^2 = \frac{\hbar^2\omega^2}{4}\left(1+\frac{2\alpha}{3}\right) \Rightarrow E_x = \frac{\hbar\omega}{2}\sqrt{1+\frac{2\alpha}{3}}$

• Calcul identique pour l'oscillateur selon Oy $\Rightarrow E_y = \frac{\hbar\omega}{2}\sqrt{1+\frac{2\alpha}{3}}$ $(n_y=0)$

• Même principe selon Oz $\Rightarrow E_z = \frac{\hbar\omega}{2}\sqrt{1-\frac{4\alpha}{3}}$ $(n_z=0)$

$\Rightarrow$ En conclusion

$$\omega_x = \omega\sqrt{1+\frac{2\alpha}{3}} = \omega_y \quad ; \quad \omega_z = \omega\sqrt{1-\frac{4\alpha}{3}}$$

$\alpha = 1/2 + 1/2$ (1/2 quantum par degré x et y)

$\gamma = 1/2$

$+\ \beta = 1/2$ (racine carré)

Soit

$$E(n_x,n_y,n_z) = \hbar\omega\left((n_x+n_y+1)\sqrt{1+\frac{2\alpha}{3}} + (n_z+1/2)\sqrt{1-\frac{4\alpha}{3}}\right)\hbar\omega$$

3) Energie état fondamental $\quad \alpha = 0 \Rightarrow E = \frac{3}{2}\hbar\omega$

$n_x = n_y = n_z = 0 \quad \alpha = 3/4 \Rightarrow E = \sqrt{\frac{3}{2}}\hbar\omega$

Variations : décroissante sur l'ensemble de l'intervalle $\alpha \in [0, 3/4]$

max pour $\alpha = 0$

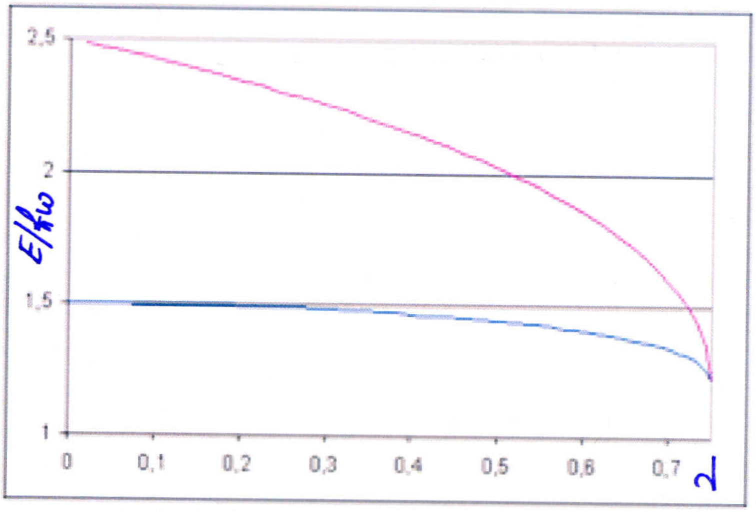
$$\left.\frac{dE}{d\alpha}\right|_{\alpha=0} = 0 \quad ; \quad \left.\frac{dE}{d\alpha}\right|_{\alpha=3/4} = -\infty$$

Energie 1er état excité $\qquad \alpha = 0 \Rightarrow E = \frac{5}{2}\hbar\omega$

$n_x = n_y = 0 \; ; \; n_z = 1 \qquad \alpha = 3/4 \Rightarrow E = \sqrt{\frac{3}{2}}\hbar\omega \Rightarrow$ dégénérescence avec le fondamental

Variations : { décroissante sur l'ensemble de l'intervalle $\alpha \in [0, 3/4]$
{ aucun extremum

$$\left.\frac{dE}{d\alpha}\right|_{\alpha=0} = -\frac{2}{3}\hbar\omega \quad ; \quad \left.\frac{dE}{d\alpha}\right|_{\alpha=3/4} = -\infty$$



<u>Moment cinétique</u> $\qquad |+1\rangle, |0\rangle$ et $|-1\rangle$

$$\hat{H}_0 = a\hat{J}_3 + \frac{b}{\hbar}\hat{J}_3^2$$

1) $\hat{H}_0|JM\rangle = a\hat{J}_3|JM\rangle + \frac{b}{\hbar}\hat{J}_3\hat{J}_3|JM\rangle = E_0|JM\rangle$

$$= a\hbar M|JM\rangle + \frac{b}{\hbar}\hbar^2 M^2|JM\rangle = E_0|JM\rangle$$

soit $(a\hbar M + b\hbar M^2) = E_0(M) \Rightarrow E_0(M) = \hbar(\underbrace{bM^2 + aM}_{})$

polynôme du 2nd degré en M

$|+1\rangle \Rightarrow E_0(+1) = \hbar(a+b)$

$|0\rangle \Rightarrow E_0(0) = 0$

$|-1\rangle = E_0(-1) = -\hbar(a-b)$

{ dég si $a = \pm b$; $a = 0$

soit $\frac{b}{a} = \pm 1$

2) $W = -\vec{M}\cdot\vec{B_0} = -\gamma \vec{J}\cdot\vec{B_0} = -\gamma B_0 \hat{J}_u = \omega_0 \hat{J}_u$

avec $\hat{J}_u = \hat{J}_x \sin\theta \cos\phi + \hat{J}_y \sin\theta \sin\phi + \hat{J}_3 \cos\theta$

$\hat{J}_x = \frac{\hat{J}_+ + \hat{J}_-}{2}$ et $\hat{J}_y = \frac{\hat{J}_+ - \hat{J}_-}{2i}$

Il faut évaluer

$$\begin{cases} J_+ |+1\rangle = 0 \\ J_+ |0\rangle = \hbar\sqrt{2}|1\rangle \\ J_+ |-1\rangle = \hbar\sqrt{2}|0\rangle \end{cases} \qquad \begin{cases} J_- |+1\rangle = \hbar\sqrt{2}|0\rangle \\ J_- |0\rangle = \hbar\sqrt{2}|-1\rangle \\ J_- |-1\rangle = 0 \end{cases}$$

Soit
$$\begin{cases} J_x |\pm1\rangle = \frac{\hbar}{\sqrt{2}}|0\rangle \\ J_x |0\rangle = \frac{\hbar}{\sqrt{2}}(|1\rangle + |-1\rangle) \\ J_x |-1\rangle = \frac{\hbar}{\sqrt{2}}|0\rangle \end{cases} \qquad \begin{cases} J_y |\pm1\rangle = \frac{i\hbar}{\sqrt{2}}|0\rangle \\ J_y |0\rangle = -\frac{i\hbar}{\sqrt{2}}(|1\rangle - |-1\rangle) \\ J_y |-1\rangle = -\frac{i\hbar}{\sqrt{2}}|0\rangle \end{cases}$$

et
$$\begin{cases} J_3 |+1\rangle = \hbar|1\rangle \\ J_3 |0\rangle = 0 \\ J_3 |-1\rangle = -\hbar|-1\rangle \end{cases}$$

$$J_u = \sin\theta\cos\phi \begin{pmatrix} 0 & \frac{\hbar}{\sqrt{2}} & 0 \\ \frac{\hbar}{\sqrt{2}} & 0 & \frac{\hbar}{\sqrt{2}} \\ 0 & \frac{\hbar}{\sqrt{2}} & 0 \end{pmatrix} \begin{matrix} |1\rangle \\ |0\rangle \\ |-1\rangle \end{matrix} + i\sin\theta\sin\phi \begin{pmatrix} 0 & -\frac{\hbar}{\sqrt{2}} & 0 \\ \frac{\hbar}{\sqrt{2}} & 0 & -\frac{\hbar}{\sqrt{2}} \\ 0 & \frac{\hbar}{\sqrt{2}} & 0 \end{pmatrix} + \cos\theta \begin{pmatrix} \hbar & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -\hbar \end{pmatrix}$$

$$= \begin{pmatrix} \hbar\cos\theta & \frac{\hbar}{\sqrt{2}}(\sin\theta\cos\phi - i\sin\theta\sin\phi) & 0 \\ \frac{\hbar}{\sqrt{2}}(\sin\theta\cos\phi + i\sin\theta\sin\phi) & 0 & \frac{\hbar}{\sqrt{2}}(\sin\theta\cos\phi - i\sin\theta\sin\phi) \\ 0 & \frac{\hbar}{\sqrt{2}}(\sin\theta\cos\phi + i\sin\theta\sin\phi) & -\hbar\cos\theta \end{pmatrix}$$

soit $W = \hbar\omega_0 \begin{pmatrix} \cos\theta & \frac{1}{\sqrt{2}}\sin\theta e^{-i\phi} & 0 \\ \frac{1}{\sqrt{2}}\sin\theta e^{i\phi} & 0 & \frac{1}{\sqrt{2}}\sin\theta e^{-i\phi} \\ 0 & \frac{1}{\sqrt{2}}\sin\theta e^{i\phi} & -\cos\theta \end{pmatrix} \begin{matrix} |1\rangle \\ |0\rangle \\ |-1\rangle \end{matrix}$ soit $\alpha = \frac{1}{\sqrt{2}}$

3) $a = b$ $\quad E_0(0) = E_0(-1)$ dégénérescence en $\hat{H}_0$

$\vec{u} // \vec{Ox}$: $\theta = \pi/2$, $\phi = 0$

$\omega_0 \ll a \rightarrow$ perturbation W

$$W = \hbar\omega_0 \begin{pmatrix} 0 & \frac{1}{\sqrt{2}} & 0 \\ \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \\ 0 & \frac{1}{\sqrt{2}} & 0 \end{pmatrix} \begin{matrix} |1\rangle \\ |0\rangle \\ |-1\rangle \end{matrix} = \frac{\hbar\omega_0}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \begin{matrix} \\ |0\rangle \\ |-1\rangle \end{matrix}$$

- Niveau non dégénéré $|+1\rangle$ $\qquad E_{|+1\rangle} = 2\hbar a + 0 = 2\hbar a$
- Niveaux dégénérés en $\hat{H}_0$ $\qquad$ Diagonaliser $\Pi = \frac{\hbar\omega_0}{\sqrt{2}} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$

$\Rightarrow$ 2 valeurs propres + 2 vecteurs propres

$$E_+^{(1)} = \frac{\hbar\omega_0}{\sqrt{2}} \Rightarrow |\psi_+\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |-1\rangle)$$

$$E_-^{(1)} = -\frac{\hbar\omega_0}{\sqrt{2}} \Rightarrow |\psi_-\rangle = \frac{1}{\sqrt{2}}(|0\rangle - |-1\rangle)$$

$\rightarrow$ levée de dégénérescence par $\hat{W}$

4) $b = 2a$

$$E_0(+1) = 3\hbar a = E_{+1}$$
$$E_0(0) = 0 = E_0$$
$$E_0(-1) = \hbar a = E_{-1}$$

$\Rightarrow$ plus de dégénérescence avec $E_0 - E_{-1} = -\hbar a$ et $E_0 - E_{+1} = -3\hbar a$

$$W = \hbar\omega_0 \begin{pmatrix} \cos\theta & \frac{1}{\sqrt{2}}\sin\theta e^{-i\phi} & 0 \\ \frac{1}{\sqrt{2}}\sin\theta e^{i\phi} & 0 & \frac{1}{\sqrt{2}}\sin\theta e^{-i\phi} \\ 0 & \frac{1}{\sqrt{2}}\sin\theta e^{i\phi} & -\cos\theta \end{pmatrix} \begin{matrix} |+1\rangle \\ |0\rangle \\ |-1\rangle \end{matrix}$$

Calcul de $\langle -1|W|0\rangle$ et $\langle +1|W|0\rangle$

- $\langle -1|W|0\rangle = \frac{\hbar\omega_0}{\sqrt{2}} \sin\theta e^{i\phi}$
- $\langle +1|W|0\rangle = \frac{\hbar\omega_0}{\sqrt{2}} \sin\theta e^{-i\phi}$

$$\Rightarrow |\psi_0\rangle = |0\rangle - \frac{\omega_0}{a\sqrt{2}} \sin\theta e^{i\phi} |-1\rangle - \frac{\omega_0}{3a\sqrt{2}} \sin\theta e^{-i\phi} |+1\rangle$$

5) $\langle \vec{M} \rangle \Rightarrow$ calculer $\langle \varphi_0 | \hat{M}_x | \varphi_0 \rangle = \gamma \langle \varphi_0 | \hat{J}_x | \varphi_0 \rangle$

$\langle \varphi_0 | \hat{M}_y | \varphi_0 \rangle = \gamma \langle \varphi_0 | \hat{J}_y | \varphi_0 \rangle$

$\langle \varphi_0 | \hat{M}_z | \varphi_0 \rangle = \gamma \langle \varphi_0 | \hat{J}_z | \varphi_0 \rangle$

$\longrightarrow$ $\hat{J}_x|\varphi_0\rangle = \hat{J}_x \left(|0\rangle - \frac{\omega_0}{a\sqrt{2}} \sin\theta e^{i\phi}|-1\rangle - \frac{\omega_0}{3a\sqrt{2}} \sin\theta e^{-i\phi}|+1\rangle \right)$

$= \frac{\hbar}{\sqrt{2}}(|1\rangle + |-1\rangle) - \frac{\omega_0}{a\sqrt{2}} \sin\theta e^{i\phi} \frac{\hbar}{\sqrt{2}}|0\rangle - \frac{\omega_0}{3a\sqrt{2}} \sin\theta e^{-i\phi} \frac{\hbar}{\sqrt{2}}|0\rangle$

$= \frac{\hbar}{\sqrt{2}}|1\rangle - \frac{\hbar\omega_0}{2a} \sin\theta \left(e^{i\phi} + \frac{e^{-i\phi}}{3}\right)|0\rangle + \frac{\hbar}{\sqrt{2}}|-1\rangle$

soit $\langle J_x \rangle_{|\varphi_0\rangle} = -\frac{\hbar\omega_0}{2a} \sin\theta \left(\cancel{e^{i\phi}} + \frac{e^{-i\phi}}{3}\right) - \cancel{\frac{\hbar\omega_0 \sin\theta e^{-i\phi}}{2a}} - \frac{\hbar\omega_0 \sin\theta e^{i\phi}}{2a \times 3}$

$= -\frac{3\hbar\omega_0 \sin\theta}{3a} \left(\frac{e^{i\phi} + e^{-i\phi}}{2}\right) - \frac{\hbar\omega_0 \sin\theta}{3a} \left(\frac{e^{i\phi} + e^{-i\phi}}{2}\right)$

$= -\frac{4\hbar\omega_0}{3a} \sin\theta \cos\phi$

$\longrightarrow$ $\hat{J}_y|\varphi_0\rangle = \hat{J}_y \left(|0\rangle - \frac{\omega_0}{a\sqrt{2}} \sin\theta e^{i\phi}|-1\rangle - \frac{\omega_0}{3a\sqrt{2}} \sin\theta e^{-i\phi}|+1\rangle \right)$

$= -\frac{i\hbar}{\sqrt{2}}(|1\rangle - |-1\rangle) - \frac{i\omega_0}{ia\sqrt{2}} \sin\theta e^{i\phi} \times -\frac{i\hbar}{\sqrt{2}}|0\rangle - \frac{i\omega_0}{i3a\sqrt{2}} \sin\theta e^{-i\phi} \times \frac{i\hbar}{\sqrt{2}}|0\rangle$

$= -\frac{i\hbar}{\sqrt{2}}|1\rangle - \frac{\hbar\omega_0 \sin\theta}{2ai} \left(e^{i\phi} - \frac{e^{-i\phi}}{3}\right)|0\rangle + \frac{i\hbar}{\sqrt{2}}|-1\rangle$

soit $\langle J_y \rangle_{|\varphi_0\rangle} = -\frac{\hbar\omega_0 \sin\theta}{2ai} \left(\cancel{e^{i\phi}} - \frac{e^{-i\phi}}{3}\right) + \cancel{\frac{\hbar\omega_0 \sin\theta e^{-i\phi}}{2ai}} - \frac{\hbar\omega_0 \sin\theta e^{i\phi}}{3 \times 2ai}$

$= -\frac{3\hbar\omega_0}{3a} \sin\theta \left(\frac{e^{i\phi} - e^{-i\phi}}{2i}\right) - \frac{\hbar\omega_0 \sin\theta}{3a} \left(\frac{e^{i\phi} - e^{-i\phi}}{2i}\right)$

$= -\frac{4\hbar}{3a}\omega_0 \sin\theta \sin\phi$

$\longrightarrow$ $\hat{J}_z|\varphi_0\rangle = \hat{J}_z \left(|0\rangle - \frac{\omega_0}{a\sqrt{2}} \sin\theta e^{i\phi}|-1\rangle - \frac{\omega_0}{3a\sqrt{2}} \sin\theta e^{-i\phi}|+1\rangle \right)$

$= +\frac{\hbar\omega_0}{a\sqrt{2}} \sin\theta e^{i\phi}|-1\rangle - \frac{\hbar\omega_0}{3a\sqrt{2}} \sin\theta e^{-i\phi}|+1\rangle$

soit $\langle J_z \rangle_{|\varphi_0\rangle} = \frac{-9\hbar\omega_0^2 \sin^2\theta}{9 \cdot 2a^2} + \frac{\hbar\omega_0^2 \sin^2\theta}{2 \times 9a^2} = \frac{-8\hbar\omega_0^2 \sin^2\theta}{18a^2}$ ordre 2

$= 0$ ordre 1.