(1)

Hverfiþungi

$\mathbb{L}$: brautarhverfiþungi einnar agnar — klassísk hliðstæða

$\mathbb{S}$: spuni — engin kl. hliðst.

$\mathbb{J}$: heildar hverfiþ. kerfis

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nota klassíska skilgr.

$$\vec{L} = \vec{R} \times \vec{P}$$

$\rightarrow$ $L_x = yP_z - zP_y$

y og P_z , z og P_y víxlast

$\rightarrow$ ekki þarf að gera L_x samhverfann

(2)

$\rightarrow$ skammta virkinn

$$\hat{L}_x = \hat{y}\hat{p}_z - \hat{z}\hat{p}_y$$

$$\hat{L}_y = \hat{z}\hat{p}_x - \hat{x}\hat{p}_z$$

athuga

$$[\hat{L}_x, \hat{L}_y] = [\hat{y}\hat{p}_z - \hat{z}\hat{p}_y, \hat{z}\hat{p}_x - \hat{x}\hat{p}_z]$$

$$= [\hat{y}\hat{p}_z, \hat{z}\hat{p}_x] + [\hat{z}\hat{p}_y, \hat{x}\hat{p}_z]$$

$$= \hat{y}[\hat{p}_z, \hat{z}]\hat{p}_x + \hat{x}[\hat{z}, \hat{p}_z]\hat{p}_y$$

$$= -i\hbar\,\hat{y}\hat{p}_x + i\hbar\,\hat{x}\hat{p}_y$$

$$= i\hbar L_z$$

$$\left.\begin{aligned} [L_x, L_y] &= i\hbar L_z \\ [L_y, L_z] &= i\hbar L_x \\ [L_z, L_x] &= i\hbar L_y \end{aligned}\right\} \quad [L_i, L_j] = \epsilon_{ijk} L_k i\hbar$$

$\epsilon_{iik} = 0$

$\epsilon_{ijk} = -\epsilon_{jik}$

$\epsilon_{123} = 1$

$\epsilon_{ijk} = \epsilon_{kij} = \epsilon_{jki}$

hverfiþungi er hvaða 3 mælistærðir sem uppfylla

$$[\hat{J}_i, \hat{J}_j] = i\hbar\epsilon_{ijk}\hat{J}_k$$

p.s. í raun verða „víxlin" til vegna eiginleika snúnings í 3D

$$\hat{J}^2 \equiv \hat{J}_x^2 + \hat{J}_y^2 + \hat{J}_z^2$$

$$\longrightarrow [\hat{J}^2, \hat{J}] = 0$$

$[\hat{J}^2, J_i]$ $i = x, y, z$

Ef ögn er í miðjumætti

$$\longrightarrow \underbrace{[\hat{H}, \hat{J}]}_{[\hat{H}, \hat{J}_i]=0} = 0$$

$\hat{J}$ er Hermite virki $\to$ $\hat{J}^2$ er einnig

En þar sem L_i víxlast ekki er ekki hægt að mæla þau öll samtímis

fullkomið mengi víxlandi mælistærða er því

$$\boxed{\hat{H}, \hat{J}^2, \hat{J}_z}$$

Skilgreina

Allir eiginleikar hverfiþunga koma frá $[J_i, J_j] \simeq \epsilon_{ijk} J_k$

$$\left.\begin{aligned} J_+ &\equiv J_x + iJ_y \\ J_- &\equiv J_x - iJ_y \end{aligned}\right\} \to J_+^{+} = J_-$$

ekki Hermite virkjar, svipar til a, a^+ í H.O.

þá fæst

$$[J_z, J_+] = \hbar J_+$$

$$[J_z, J_-] = -\hbar J_-$$

$$[J_+, J_-] = 2\hbar J_z$$

$$[J^2, J_+] = [J^2, J_-] = [J^2, J_z] = 0$$

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$$J_+ J_- = J^2 - J_z^2 + \hbar J_z$$
$$J_- J_+ = J^2 - J_z^2 - \hbar J_z$$

$J^2 = \frac{1}{2}(J_+J_- + J_-J_+) + J_z^2$

Eigingildi $\hat{J}^2$ og J_z

$\langle\psi|J^2|\psi\rangle = \langle\psi|J_x^2|\psi\rangle + \cdots$
$= \| J_x|\psi\rangle\|^2 + \cdots$

Öll eigingildi $\hat{J}^2$ eru ≥ 0

Eigingildin eru á forminu $\lambda\hbar^2$

veljum
$$\lambda = j(j+1)$$
með $j \geq 0$

er hægt því $j(j+1) = \lambda$ hefur aðeins eina (enga aðra) lausn með $j \geq 0$

fyrir J_z eru eigingildin valin sem
$$m\hbar$$

6

Eiginvektorar $\hat{J}^2$ og $\hat{J}_z$ eru því merktir með j og m, sem nægja ekki til að tilgreina ástand (J^2 og J_z eru ekki fullkomið mengi víxlandi virkja)

$$\rightarrow \quad J^2|k,j,m\rangle = j(j+1)\hbar^2|k,j,m\rangle$$
$$J_z|k,j,m\rangle = m\hbar|k,j,m\rangle$$

(i) fyrir m má sanna

$$-j \leq m \leq j$$

athuga

$$\| J_+|k,j,m\rangle\|^2 = \langle k,j,m|J_-J_+|k,j,m\rangle \geq 0$$
$$\| J_-|k,j,m\rangle\|^2 = \langle k,j,m|J_+J_-|k,j,m\rangle \geq 0$$

og

$$\langle k,j,m|J_-J_+|k,j,m\rangle = j(j+1)\hbar^2 - m^2\hbar^2 - m\hbar^2 \geq 0$$
$$\langle k,j,m|J_+J_-|k,j,m\rangle = j(j+1)\hbar^2 - m^2\hbar^2 + m\hbar^2 \geq 0$$

$\longrightarrow$

(7)

$$j(j+1)-m(m+1) = (j-m)(j+m+1) \geq 0$$
$$j(j+1)-m(m-1) = (j-m+1)(j+m) \geq 0$$

$$-(j+1) \leq m \leq j$$

$$-j \leq m \leq j+1$$

$$\longrightarrow \quad -j \leq m \leq j$$

(ii)

vanrida untl

Ef $m=-j \Leftrightarrow J_-|k,j,-j\rangle = 0$

$m>-j$ $\quad J_-|k,j,m\rangle$ er eiginvektor J^2 og J_z ~~með~~ eigingildi $j(j+1)\hbar^2$ og $(m-1)\hbar$

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höfum séð

$$\|J_-|k,j,m\rangle\|^2 = j(j+1)\hbar^2 - m^2\hbar^2 + m\hbar^2 \geq 0$$
$$= 0 \quad \text{ef} \quad m=-j$$

$$\longrightarrow J_-|k,j,m\rangle = 0$$

og öfugt

(8)

ef $m>-j$

$$\|J_-|k,j,m\rangle\|^2 \neq 0 \quad \longrightarrow J_-|k,j,m\rangle \neq 0.$$

$$[J^2, J_\pm] = 0$$

sama $J_-|kjm\rangle$ er eiginv. J^2 og J_z með $j(j+1)\hbar^2$ og $(m-1)\hbar$

$$\hookrightarrow [J^2, J_-]|k,j,m\rangle = 0$$

$$\rightarrow J^2 J_-|kjm\rangle = J_- J^2 |kjm\rangle$$
$$= j(j+1)\hbar^2 J_-|kjm\rangle$$

$\longrightarrow J_-|kjm\rangle$ er eiginvektor J^2 með $j(j+1)\hbar^2$

$$[J_z, J_-] = -\hbar J_-$$

$$\hookrightarrow J_z J_-|kjm\rangle = J_- J_z|kjm\rangle - \hbar J_-|kjm\rangle$$
$$= m\hbar J_-|kjm\rangle - \hbar J_-|kjm\rangle$$
$$= (m-1)\hbar J_-|kjm\rangle$$

$\longrightarrow J_-|kjm\rangle$ er eiginv. J_z með $(m-1)\hbar$

Samskonar fyrir J_+

(iii) ef $m=j$ $J_+|kjj\rangle = 0$

ef $m<j$ $J_+|kjm\rangle \neq 0$ eiginvektor

J^2 og J_z með eigingildi

$j(j+1)$ og $(m+1)\hbar$

$$\langle k_2jm|J_\mp J_\pm|k_1jm\rangle$$

$$= \langle k_2jm|(J^2 - J_z^2 \mp \hbar J_z)|k_1jm\rangle$$

$$= \{j(j+1) - m(m\pm 1)\}\hbar^2 \langle k_2jm|k_1jm\rangle$$

Nú má nota þrepun til að sýna að

einu möguleikar á gildum fyrir

j eru $0, 1/2, 1, 3/2, 2, 5/2, 3 \ldots$

og $m = -j, j+1, \ldots j-1, j$

En þessi gildi þurfa ekki að koma

öll fyrir í sama kerfinu.

$|k,j,m\rangle$ – grunnur (staðal grunnur)

fylkisstök $\bar{J}$

höfum

$$J_z|kjm\rangle = m\hbar|kjm\rangle$$

$$J_+|kjm\rangle = \hbar\sqrt{j(j+1)-m(m+1)}\,|kj\,m+1\rangle$$

$$J_-|kjm\rangle = \hbar\sqrt{j(j+1)-m(m-1)}\,|kj\,m-1\rangle$$

$$\langle kjm|J_z|k'j'm'\rangle = m\hbar\,\delta_{kk'}\delta_{jj'}\delta_{mm'}$$

$$\longrightarrow \quad \langle kjm|J_\pm|k'j'm'\rangle = \hbar\sqrt{j(j+1)-m'(m'\pm1)}\,\delta_{kk'}\delta_{jj'}\delta_{m,m'\pm1}$$

$$j=\tfrac{1}{2} \rightarrow \left\{ \begin{array}{ll} (J_z)^{1/2} = \frac{\hbar}{2}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}, & (J_+)^{1/2} = \hbar\begin{pmatrix}0 & 1\\ 0 & 0\end{pmatrix} \\ (J_-)^{1/2} = \hbar\begin{pmatrix}0 & 0\\ 1 & 0\end{pmatrix}, & (J_x)^{1/2} = \frac{\hbar}{2}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix} \\ (J_y)^{1/2} = \frac{\hbar^2}{2}\begin{pmatrix}0 & -i\\ i & 0\end{pmatrix}, & (J^2)^{1/2} = \frac{3}{4}\hbar^2\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix} \end{array} \right.$$

j = 1

$$(J)_z = \hbar\begin{pmatrix}1 & 0 & 0\\ 0 & 0 & 0\\ 0 & 0 & -1\end{pmatrix}$$

$$(J_+) = \hbar\begin{pmatrix}0 & \sqrt{2} & 0\\ 0 & 0 & \sqrt{2}\\ 0 & 0 & 0\end{pmatrix} \qquad (J_-) = \hbar\begin{pmatrix}0 & 0 & 0\\ \sqrt{2} & 0 & 0\\ 0 & \sqrt{2} & 0\end{pmatrix}$$

$$(J_x) = \frac{\hbar}{\sqrt{2}}\begin{pmatrix}0 & 1 & 0\\ 1 & 0 & 1\\ 0 & 1 & 0\end{pmatrix} \qquad (J_y) = \frac{\hbar}{\sqrt{2}}\begin{pmatrix}0 & -i & 0\\ i & 0 & -i\\ 0 & i & 0\end{pmatrix}$$

$$(J^2) = 2\hbar^2\begin{pmatrix}1 & 0 & 0\\ 0 & 1 & 0\\ 0 & 0 & 1\end{pmatrix}$$

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fylkin uppfylla einnig víxlin

$$[J_i, J_j] = i\hbar\,\epsilon_{ijk}J_k$$

spunalaus ögn

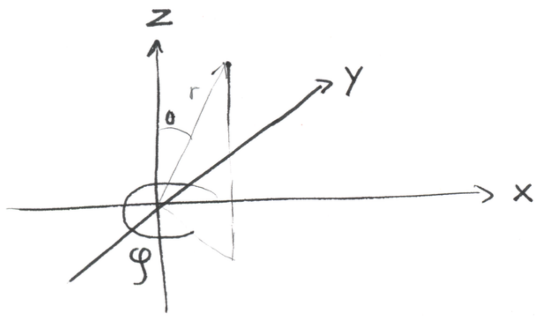
Brautarhverfiþungi í $\{|r\rangle\}$ framsetningu

$$\bar{L} = \bar{R} \times \bar{P} \qquad \langle \bar{r}|\bar{R}|\psi\rangle = \bar{r}\,\psi(\bar{r})$$

$$\langle \bar{r}|\bar{P}|\psi\rangle = -i\hbar\bar{\nabla}\psi(\bar{r})$$

$$\longrightarrow \begin{cases} L_x = -i\hbar\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right) \\ L_y = -i\hbar\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right) \\ L_z = -i\hbar\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right) \end{cases}$$

skipta um hnit
$$\begin{cases} x = r\sin\theta\cos\varphi \\ y = r\sin\theta\sin\varphi \\ z = r\cos\theta \end{cases}$$
Kúluhnit



$$\begin{cases} L_x = i\hbar\left(\sin\varphi\frac{\partial}{\partial\theta} + \frac{\cos\varphi}{\tan\theta}\frac{\partial}{\partial\varphi}\right) \\ L_y = i\hbar\left(-\cos\varphi\frac{\partial}{\partial\theta} + \frac{\sin\varphi}{\tan\theta}\frac{\partial}{\partial\varphi}\right) \\ L_z = -i\hbar\frac{\partial}{\partial\varphi} \end{cases}$$

$$\begin{cases} \bar{L}^2 = -\hbar^2\left(\frac{\partial^2}{\partial\theta^2} + \frac{1}{\tan\theta}\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right) \\ L_+ = \hbar e^{i\varphi}\left(\frac{\partial}{\partial\theta} + i\cot\theta\frac{\partial}{\partial\varphi}\right) \\ L_- = \hbar e^{-i\varphi}\left(-\frac{\partial}{\partial\theta} + i\cot\theta\frac{\partial}{\partial\varphi}\right) \end{cases}$$

höfðum séð

$$\hat{L}^2|klm\rangle = \hbar^2 l(l+1)|klm\rangle$$

$$L_z|klm\rangle = \hbar m|klm\rangle$$

$$\langle\bar{r}|\cdot \longrightarrow \boxed{\begin{aligned} \bar{L}^2\psi &= \hbar^2 l(l+1)\psi \\ L_z\psi &= \hbar m\psi \end{aligned}}$$

↗ leysa þessar diffurjöfnur

Lausnin verður

$$\psi_{lm}(r,\theta,\varphi) = f(r)\, Y_{lm}(\theta,\varphi)$$

$f(r)$: frjálst fall hér $\to$ L^2 og L_z
mynda ekki FSVM

Veljum normun $\int_0^\infty r^2 dr\, |f(r)|^2 = 1$

$$\int d\Omega\, |Y_{lm}|^2 = \int_0^{2\pi} d\varphi \int_0^{\pi} \sin\theta d\theta\, |Y_{lm}(\theta,\varphi)|^2 = 1$$

Í ljós mun koma að visst val á L og m er ódeins ein lausn Y_{lm}

Eiginleitar lausna

$$-i\hbar\partial_\varphi Y_{lm} = m\hbar Y_{lm}$$

$$\to Y_{lm}(\theta,\varphi) = F_{lm}(\theta)\, e^{im\varphi}$$

Samfelldni

$$\to Y_{lm}(\theta,0) = Y_{lm}(\theta,2\pi)$$

$$\to e^{2\pi i m} = 1 \to m \in \mathbb{Z}$$ $\to$ frá fyrri síðum $l \in \mathbb{N}_0$

$$L^2 Y_{lm} = \hbar^2 l(l+1) Y_{lm}$$

$$\to -\left\{\frac{\partial^2}{\partial\theta^2} + \frac{1}{\tan\theta}\frac{\partial}{\partial\theta} - \frac{m^2}{\sin^2\theta}\right\} F_{lm}(\theta) = l(l+1) F_{lm}(\theta)$$

$$\to Y_{lm}(\theta,\varphi) = \sqrt{\left(\frac{2l+1}{4\pi}\frac{(l-m)!}{(l+m)!}\right)}\, P_l^m(\cos\theta)\, e^{im\varphi}$$

{hin óháða lausnin $Q_l^m(\cos\theta)$ hefur sérstöðupunkta við $x=\pm1$}

þar sem

$$P_l^m(x) = \frac{(-1)^m}{2^l l!}(1-x^2)^{m/2}\frac{d^{l+m}}{dx^{l+m}}(x^2-1)^l$$

eru Legendre fleirliður skilgreindar á bilinu $[-1,1]$

t.d.

$$P_\ell^{-m}(x) = (-1)^m \frac{(\ell-m)!}{(\ell+m)!} P_\ell^m(x)$$

Lausnir einungis til fyrir

$$\ell \geq 0$$
$$-\ell \leq m \leq \ell$$

$$Y_{00} = \frac{1}{\sqrt{4\pi}}$$

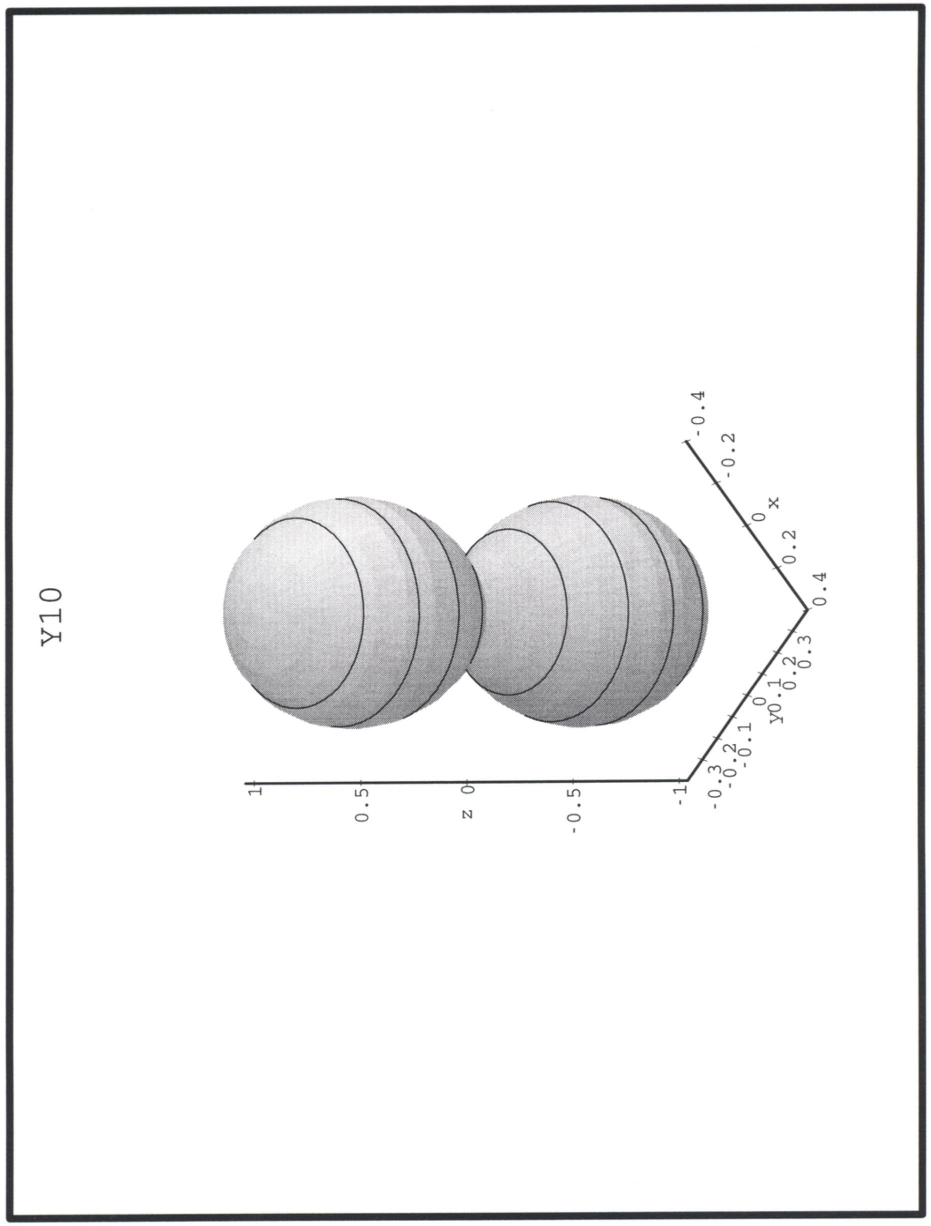
$$Y_{1,1} = -\sqrt{\frac{3}{8\pi}} \sin\theta \, e^{i\varphi}$$

$$Y_{1,0} = \sqrt{\frac{3}{4\pi}} \cos\theta$$

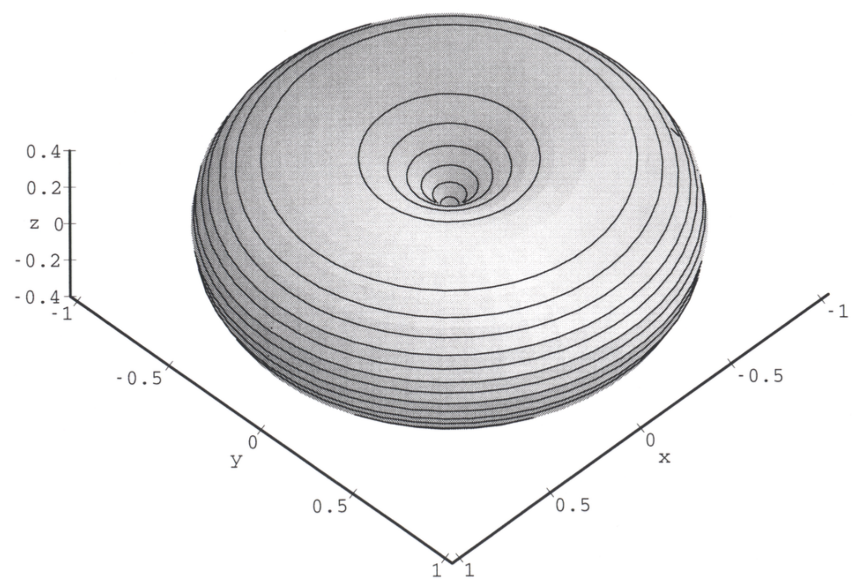
$$\vdots$$

$$\int d\Omega \, Y_{\ell m}^* Y_{\ell' m'} = \delta_{\ell,\ell'} \delta_{m,m'}$$ hornrétt og normuð

$$Y_{\ell,-m} = (-1)^m Y_{\ell,m}^*$$



Y11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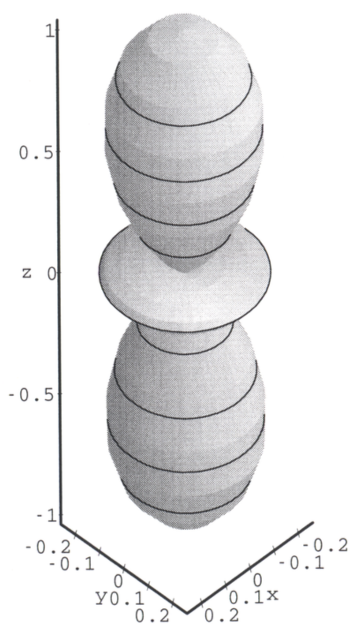
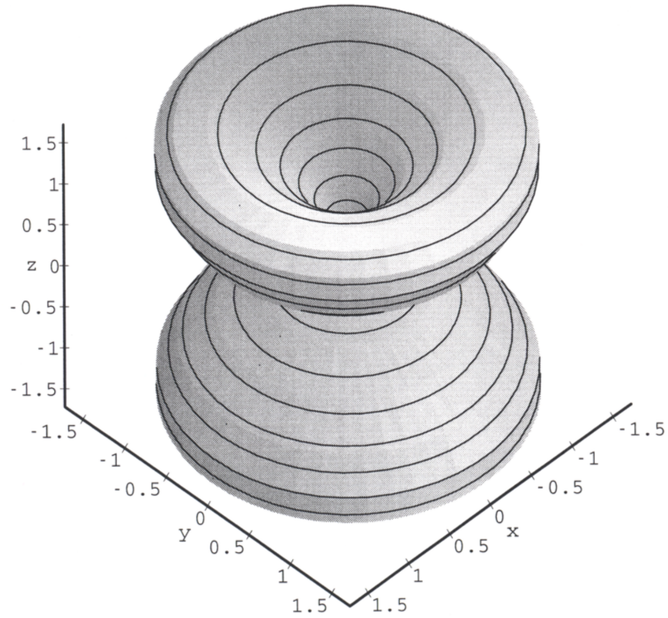
0.2
z 0
-0.2
-0.4
-1
-0.5
y 0
0.5
1
1
0.5
0 x
-0.5
-1

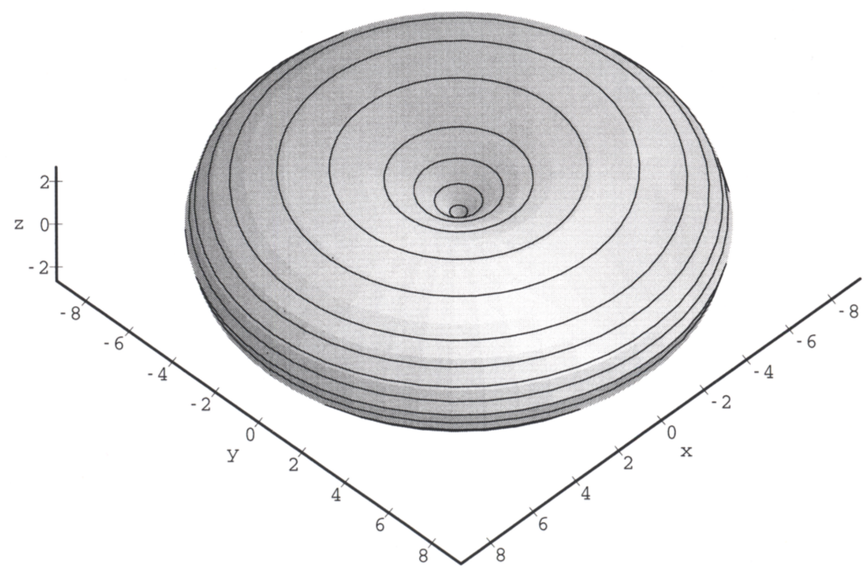
Y20

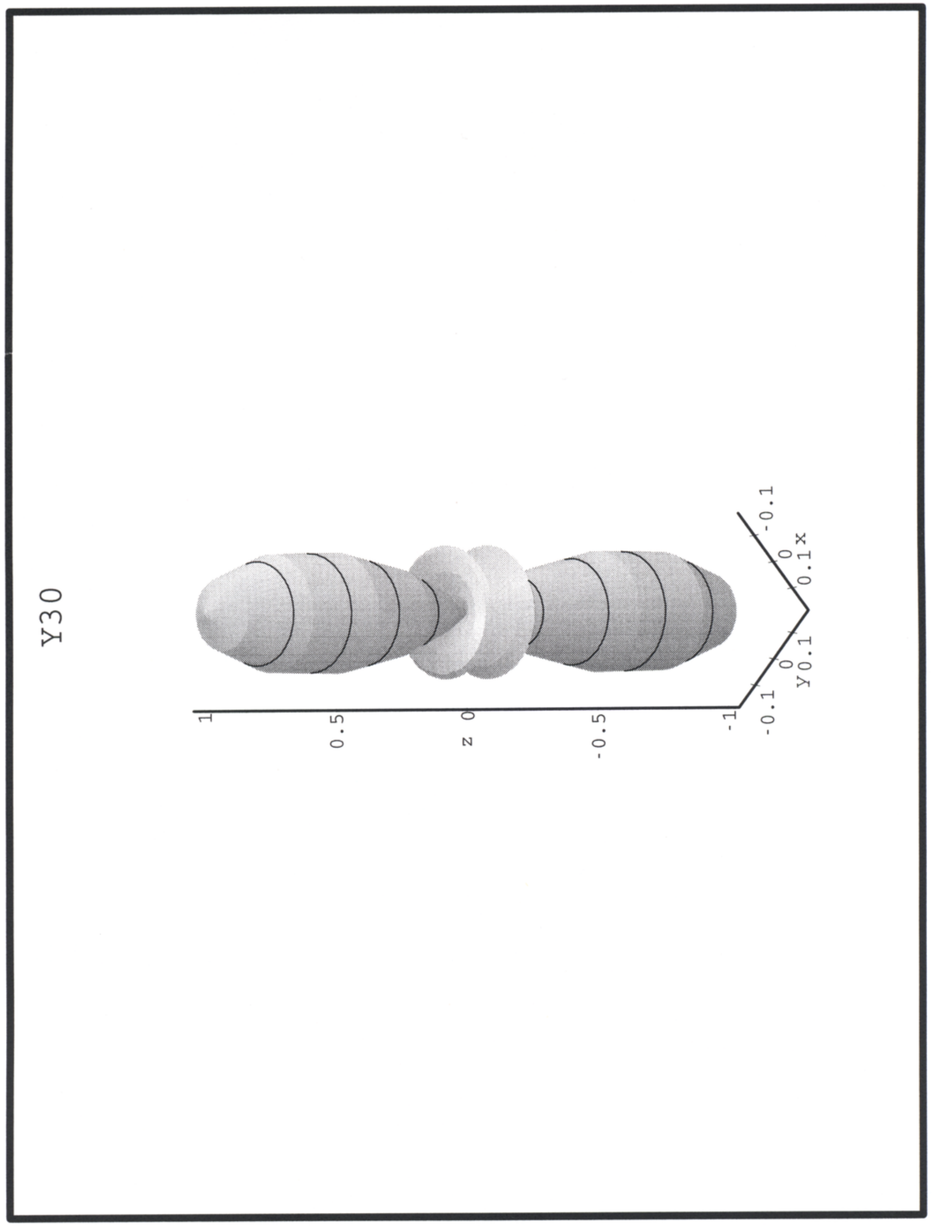

1
0.5
z 0
-0.5
-1
-0.2
-0.1
0
y0.1
0.2
0.2
0.1x
0
-0.1
-0.2

Y21



Y22





hægt að liða föll

$$f(\theta,\varphi) = \sum_{l=0}^{\infty} \sum_{m=-l}^{+l} C_{lm} Y_{lm}(\theta,\varphi)$$

$$C_{lm} = \int d\Omega \, Y_{lm}^{*}(\theta,\varphi) f(\theta,\varphi)$$

fullkomið mengi

$$\sum_{l=0}^{\infty} \sum_{m=-l}^{l} Y_{lm}(\theta,\varphi) Y_{lm}^{*}(\theta',\varphi')$$

$$= \delta(\cos\theta - \cos\theta')\delta(\varphi-\varphi')$$

$$= \frac{1}{\sin\theta} \delta(\theta-\theta')\delta(\varphi-\varphi')$$

summuregla

$$\frac{2l+1}{4\pi} P_l(\cos\alpha) = \sum_{m=-l}^{+l} Y_{lm}^{*}(\theta',\varphi') Y_{lm}(\theta,\varphi)$$

$$\cos\alpha = \cos\theta\cos\theta' + \sin\theta\sin\theta'\cos(\varphi-\varphi')$$

→

$$\sum_{m=-l}^{l} |Y_{lm}(\theta,\varphi)|^2 = \frac{2l+1}{4\pi}$$

þægileg jafna

$$\frac{1}{|\bar{x}-\bar{x}'|} = 4\pi \sum_{l=0}^{\infty} \sum_{m=-l}^{+l} \frac{1}{2l+1}\left(\frac{r_<^{l}}{r_>^{l+1}}\right) Y^{*}_{lm}(\theta',\varphi')\, Y_{lm}(\theta,\varphi)$$

$$r_< = \min(r,r')$$

$$r_> = \max(r,r')$$

Líkindin fyrir því að mæla samtímis $l(l+1)\hbar^2$ og $m\hbar$ fyrir L^2 og L_z

ástandi lýst með $\Psi(r,\theta,\varphi)$

liða

$$\Psi(r,\theta,\varphi) = \sum_{l}\sum_{m} a_{lm}(r)\, Y_{lm}(\theta,\varphi)$$

$$a_{lm}(r) = \int d\Omega\, Y^{*}_{lm}(\theta,\varphi)\,\Psi(r,\theta,\varphi)$$

→

$$\mathcal{P}_{L^2,L_z}(l,m) = \int_0^{\infty} r^2 dr\, |a_{lm}(r)|^2$$

$$\mathcal{P}_{L^2}(l) = \sum_{m=-l}^{+l} \int_0^{\infty} r^2 dr\, |a_{lm}(r)|^2$$

$$\mathcal{P}_{L_z}(m) = \sum_{l\geq|m|} \int_0^{\infty} r^2 dr\, |a_{lm}(r)|^2$$