Implementació del camp magnètic arbitràriament orientat en QDs II. Incloent acció de bandes remotes en el terme Zeeman

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1 de març de 2016

L'Hamiltonià d'un sistema en presència de camp magnètic el qual presenta la massa anisòtropa i depenent de la posició és, com indica l'eq. (10) en JPCM,[1]

$$\mathcal{H} = \sum_i^{x,y,z} (p_i - q\,A_i)\frac{1}{2m_i}(p_i - q\,A_i) - \frac{q\hbar}{2}\,\bar{\boldsymbol{\sigma}} \cdot \mathbf{B} \tag{1}$$

on $\bar{\sigma}_i = \frac{\sigma_i}{\sqrt{m_j\,m_k}}$, $i \neq j \neq k$.

1 El terme cinètic

Considerem ara el primer terme de l'eq. (1):

$$(p_i - q\,A_i)\,\frac{1}{2m_i}\,(p_i - q\,A_i) = p_i\,\frac{1}{2m_i}\,p_i + \frac{qA_i^2}{2m_i} - \frac{q}{2}\left(\frac{A_i}{m_i}\,p_i + p_i\,\frac{A_i}{m_i}\right) \tag{2}$$

El primer sumand és l'energia cinètica, i.e. l'Hamiltonià en absència de camp magnètic –a falta del terme d'energia potencial. El segon sumand és purament multiplicatiu, de manera que:

$$\langle u_j|\frac{qA_i^2}{2m_i}\,(|u_k\rangle|f_k\rangle) = \delta_{jk}\,\frac{qA_i^2}{2m_i}\,|f_k\rangle \tag{3}$$

El tercer sumand, que representem per H_3, conté derivades. Escrivim doncs,

$$\langle u_j|H_3\,(|u_k\rangle|f_k\rangle) = |f_k\rangle\langle u_j|H_3|u_k\rangle + \delta_{jk}\,H_3\,|f_k\rangle \tag{4}$$

Aquest tercer sumand fa aparèixer, per tant, un terme diagonal que actual sobre les envolupants,

$$\sum_i^{x,y,z} -\frac{q}{2}\left(\frac{A_i}{m_i}\,\hat{p}_i + \hat{p}_i\,\frac{A_i}{m_i}\right)\,|f_k\rangle, \tag{5}$$

més un terme no diagonal, $\langle u_j|H_3|u_k\rangle$, que multiplica les envolupants. Terme que, com indica la fórmula anterior, cal calcular integrant H_3 en la cel·la unitat entre dues funcions de Bloch. La massa, que pot ser anisòtropa ($m_x \neq m_y \neq m_z$), és però constant dins de la cel·la unitat (no depèn de la posició, i.e. $m_i(\mathbf{r}) = m_i^0$ en tota la cel·la unitat). A més, triarem el gauge de Coulomb per al potencial vector de manera que $\hat{p}_i(A_i) = 0$. En conseqüència, sols hem de calcular la integral del terme $\sum_i -\frac{q\,A_i}{m_i}\,\hat{p}_i$.

Considerarem un camp arbitrari $\mathbf{B} = (B_x^0, B_y^0, B_z^0) = B_0(\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$ que el generem a partir del potencial vector $\mathbf{A} = \frac{1}{2}(zB_y^0 - yB_z^0, xB_z^0 - zB_x^0, yB_x^0 - xB_y^0)$, per al qual és immediat comprovar que $\nabla \cdot \mathbf{A} = 0$. Assumim d'ara en avant que $m_x = m_y = m_\perp \neq m_z$. Amb tot açò tenim que:

$$
\begin{aligned}
-q\sum_i^{x,y,z}\frac{A_i}{m_i}\,\hat{p}_i &= -\frac{q}{2}\left\{\frac{z\,B_y^0-y\,B_z^0}{m_\perp}\,\hat{p}_x+\frac{x\,B_z^0-z\,B_x^0}{m_\perp}\,\hat{p}_y+\frac{y\,B_x^0-x\,B_y^0}{m_z}\,\hat{p}_z\right\}\\
&= (-q)\left\{\frac{B_z^0}{2m_\perp}\,\hat{L}_z+\frac{B_y^0}{2m_\perp}\,z\,\hat{p}_x-\frac{B_y^0}{2m_z}\,x\,\hat{p}_z+\frac{B_x^0}{2m_z}\,y\,\hat{p}_z-\frac{B_x^0}{2m_\perp}\,z\,\hat{p}_y\right\} \qquad (6)\\
&= (-q)\left\{\frac{B_z^0}{2m_\perp}\,\hat{L}_z+\frac{B_y^0}{2m_\perp}\,\hat{L}_y+\frac{B_x^0}{2m_\perp}\,\hat{L}_x+\left(\frac{1}{m_\perp}-\frac{1}{m_z}\right)\left[\frac{B_y^0}{2}\,x\,\hat{p}_z-\frac{B_x^0}{2}\,y\,\hat{p}_z\right]\right\}
\end{aligned}
$$

per tant,

$$
\langle u_j|(-q)\sum_i^{x,y,z}\frac{A_i\,\hat{p}_i}{m_i}|u_k\rangle=(-q)\left\{\frac{1}{2m_\perp}\mathbf{B}\cdot\mathbf{L}+\frac{1}{2}\frac{m_z-m_\perp}{m_z m_\perp}\left(B_y^0\,\langle u_j|x\hat{p}_z|u_k\rangle-B_x^0\,\langle u_j|y\hat{p}_z|u_k\rangle\right)\right\} \qquad (7)
$$

A l'apèndix 1 demostrarem que en la base $\{|Y_{11}\rangle,|Y_{10}\rangle,|Y_{1,-1}\rangle\}$:

$$
\langle u_j|x\hat{p}_z|u_k\rangle = -\frac{1}{2}\,\langle u_j|\hat{L}_y|u_k\rangle \qquad (8)
$$

$$
\langle u_j|y\hat{p}_z|u_k\rangle = \frac{1}{2}\,\langle u_j|\hat{L}_x|u_k\rangle \qquad (9)
$$

Amb la qual cosa:[1]

$$
\boxed{\langle u_j|(-q)\sum_i^{x,y,z}\frac{A_i\,\hat{p}_i}{m_i}|u_k\rangle=-\frac{q\hbar}{2m_\perp}\mathbf{B}\cdot\mathbb{L}_{jk}-\frac{q}{4}\frac{m_\perp-m_z}{m_z m_\perp}\left(B_y^0\,(\mathbb{L}_y)_{jk}+B_x^0\,(\mathbb{L}_x)_{jk}\right) \qquad (10)}
$$

2 El terme Zeeman

Considerem ara el terme Zeeman,

$$
H_Z=-\frac{q\hbar}{2}\,\bar{\boldsymbol{\sigma}}\cdot\mathbf{B} \qquad (11)
$$

Si considerem que $m_x=m_y=m_\perp\neq m_z$ tenim que

$$
\bar{\sigma}_x = \frac{\sigma_x}{\sqrt{m_z m_\perp}}=\frac{\sigma_x}{m_\perp}+\frac{\sigma_x}{m_\perp}\left(\sqrt{\frac{m_\perp}{m_z}}-1\right) \qquad (12)
$$

$$
\bar{\sigma}_y = \frac{\sigma_y}{\sqrt{m_z m_\perp}}=\frac{\sigma_y}{m_\perp}+\frac{\sigma_y}{m_\perp}\left(\sqrt{\frac{m_\perp}{m_z}}-1\right) \qquad (13)
$$

$$
\bar{\sigma}_z = \frac{\sigma_z}{m_\perp} \qquad (14)
$$

Aleshores,

$$
\boxed{H_Z=-\frac{q\hbar}{2m_\perp}\,\boldsymbol{\sigma}\cdot\mathbf{B}-\frac{q\hbar}{2m_\perp}\,\frac{\sqrt{m_\perp}-\sqrt{m_z}}{\sqrt{m_z}}\,\left(B_y^0\,\sigma_y+B_x^0\,\sigma_x\right) \qquad (15)}
$$

[1] Cal tenir en compte que el moment angular $\mathbb{L}$ inclou la constant $\hbar$ que li dona unitats, mentre que les matrius de Pauli no tenen unitats i, per tant, no inclouen $\hbar$. Si considerem que $\mathbf{L}$ és adimensional com $\boldsymbol{\sigma}$, aleshores hem d'afegir $\hbar$.

3 La suma dels dos termes

$$
\begin{aligned}
\langle u_j|(-q)\sum_i \tfrac{A_i\,\hat{p}_i}{m_i} + \tfrac{(-q)\hbar}{2m_\perp}\boldsymbol{\sigma}\cdot\mathbf{B}|u_k\rangle \quad &= \\
&\tfrac{(-q)\hbar}{2m_\perp}\mathbf{B}\cdot(\mathbb{L}_{jk}+\sigma_{jk})+ \\
&\tfrac{(-q)\hbar}{2m_\perp}\left(B_y^0\left[\tfrac{m_\perp-m_z}{2m_z}(\mathbb{L}_y)_{jk}+\tfrac{\sqrt{m_\perp}-\sqrt{m_z}}{\sqrt{m_z}}(\sigma_y)_{jk}\right]+B_x^0\left[\tfrac{m_\perp-m_z}{2m_z}(\mathbb{L}_x)_{jk}+\tfrac{\sqrt{m_\perp}-\sqrt{m_z}}{\sqrt{m_z}}(\sigma_x)_{jk}\right]\right)
\end{aligned}
\tag{16}
$$

Si en la expressió anterior fem que $m_\perp = m_z = m_0$ la convertim en:

$$
\langle u_j|(-q)\sum_i \frac{A_i\,\hat{p}_i}{m_i} + \frac{(-q)\hbar}{2m_\perp}\boldsymbol{\sigma}\cdot\mathbf{B}|u_k\rangle = \frac{(-q)\hbar}{2m_0}\mathbf{B}\cdot(\mathbb{L}+\boldsymbol{\sigma})_{jk} \tag{17}
$$

que en el cas de forats, amb $q=|e|$, $\mu_B = \frac{|e|\hbar}{2m_0}$ és redueix al terme $-\mu_B\mathbf{B}\cdot(\mathbb{L}+\boldsymbol{\sigma})_{jk}$ que és el resultat que trobarem en els apunts *Implementació del camp magnètic arbitràriament orientat en QDs* de 17 de febrer de 2016, on consideràvem un *quenching* total de l'acció de les bandes remotes en el terme multiplicatiu no diagonal $\langle u_j|H_3+H_Z|u_k\rangle$.[2]

A efectes pràctics, cal únicament modificar el fitxer Mathematica canviant $-\mu_B\mathbf{B}\cdot(\mathbb{L}+\boldsymbol{\sigma})$ pel terme deduït abans, eq. (16). En l'esmentada equació podem afegir coeficients per modular el pes de l'acció de les bandes remotes (que, segons Bree et. al.,[2] sofreix un *quenching* complet en QDs). Veure detalls de la implementació en l'apèndix 3.

Pot ser un tractament semblant per a ZnBl amb factors ajustables com s'indica en l'apèndix 3 permetria la perfecta reproducció dels resultats experimentals de Dotty en JPCM.[1]

4 Apèndix 1: Representació matricial dels operadors $x\hat{p}_z$ i $y\hat{p}_z$ en la base $|11\,|10\rangle, |1,-1\rangle$.

En primer lloc escrivim aquesta base en termes del les funcions reals $|X\rangle, |Y\rangle, |Z\rangle$, tenint molt en compte les fases d'acord amb la definició de creadors i anihiladors (fase de Condon-Shortley):

$$
|11\rangle = -(|X\rangle + i|Y\rangle) \quad, |10\rangle = |Z\rangle \quad, |1,-1\rangle = |X\rangle - i|Y\rangle \tag{18}
$$

4.1 Elements de matriu de $x\hat{p}_z$ que són zero per simetria

$$
\begin{aligned}
\langle 11|x\hat{p}_z|11\rangle &= (\langle X|-i\langle Y|)|x\hat{p}_z(|X\rangle+i|Y\rangle) = \langle X|x\hat{p}_z|X\rangle + i\langle Y|x\hat{p}_z|X\rangle + i\langle X|x\hat{p}_z|Y\rangle - \langle Y|x\hat{p}_z|Y\rangle \\
&= 0+0+0+0=0 \\
\\
\langle 11|x\hat{p}_z|1,-1\rangle &= -(\langle X|+i\langle Y|)|x\hat{p}_z(|X\rangle-i|Y\rangle) = 0+0+0+0=0
\end{aligned}
\tag{19}
$$

Per idèntiques raons $\langle 1,-1|x\hat{p}_z|11\rangle = 0$ i en conseqüència també $\langle 1,-1|x\hat{p}_z|1,-1\rangle = 0$. Finalment, $\langle 10|x\hat{p}_z|10\rangle = \langle Z|x\hat{p}_z|Z\rangle = 0$.

[2] En els esmentats apunts escrivíem $\mathbb{L}/\hbar$ perquè consideràvem $\mathbb{L}$ amb dimensions, i.e. que $\mathbb{L}$ incloïa $\hbar$.

4.2 Elements de matriu de $x\hat{p}_z$ no nuls

$$\begin{aligned}
\langle 11|x\hat{p}_z|10\rangle &= -(\langle X| - i\langle Y|)|x\hat{p}_z|Z\rangle = -\langle X|x\hat{p}_z|Z\rangle \\
\langle 10|x\hat{p}_z|11\rangle &= -\langle Z|x\hat{p}_z(|X\rangle + i|Y\rangle) = -\langle Z|x\hat{p}_z|X\rangle \\
\langle 10|x\hat{p}_z|1,-1\rangle &= \langle Z|x\hat{p}_z(|X\rangle - i|Y\rangle) = \langle Z|x\hat{p}_z|X\rangle \\
\langle 1,-1|x\hat{p}_z|10\rangle &= (\langle X| + i\langle Y|)|x\hat{p}_z|Z\rangle = \langle X|x\hat{p}_z|Z\rangle
\end{aligned} \tag{20}$$

Com l'operador $x\hat{p}_z$ és hermític, aleshores, $\langle X|x\hat{p}_z|Z\rangle = \langle Z|x\hat{p}_z|X\rangle^*$. Per tant, si anomenem $a = -\langle X|x\hat{p}_z|Z\rangle$ tenim que:

$$\langle x\hat{p}_z\rangle = \begin{bmatrix} 0 & a & 0 \\ a^* & 0 & -a^* \\ 0 & -a & 0 \end{bmatrix} \tag{21}$$

Per tal de determinar a calcularem $\langle z\hat{p}_x\rangle$ i tindrem en compte que $\langle L_y\rangle = \langle z\hat{p}_x - x\hat{p}_z\rangle$. A l'hora de calcular $\langle z\hat{p}_x\rangle$ tenim que els elements de matriu no nuls han de ser els mateixos, per motius de simetria. Ens centrem en els elements no nuls:

$$\begin{aligned}
\langle 11|z\hat{p}_x|10\rangle &= -(\langle X| - i\langle Y|)|z\hat{p}_x|Z\rangle = -\langle X|z\hat{p}_x|Z\rangle \\
\langle 10|z\hat{p}_x|11\rangle &= -\langle Z|z\hat{p}_x|X\rangle \\
\langle 10|z\hat{p}_x|1,-1\rangle &= \langle Z|z\hat{p}_x|X\rangle \\
\langle 1,-1|z\hat{p}_x|10\rangle &= \langle X|z\hat{p}_x|Z\rangle
\end{aligned} \tag{22}$$

Com en el càlcul de la integral els índexs són muts, tenim que $\langle X|x\hat{p}_z|Z\rangle$ i $\langle Z|z\hat{p}_x|X\rangle$, que suposa canviar la coordenada x per z, són iguals. Per tant, $\langle Z|z\hat{p}_x|X\rangle = -a$. Amb la qual cosa, atès que $\langle X|z\hat{p}_x|Z\rangle = \langle Z|z\hat{p}_x|X\rangle^*$, trobem que:

$$\langle z\hat{p}_x\rangle = \begin{bmatrix} 0 & a^* & 0 \\ a & 0 & -a \\ 0 & -a^* & 0 \end{bmatrix} \tag{23}$$

Aleshores si comparem

$$\langle z\hat{p}_x - x\hat{p}_z\rangle = \begin{bmatrix} 0 & a^* - a & 0 \\ a - a^* & 0 & a^* - a \\ 0 & a - a^* & 0 \end{bmatrix} \tag{24}$$

amb

$$\langle \hat{L}_y\rangle = \frac{i}{\sqrt{2}} \begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & -1 \\ 0 & 1 & 0 \end{bmatrix} \tag{25}$$

concloem que $a - a^* = i/\sqrt{2}$. Finalment, com les integrals $\langle X|z\hat{p}_x|Z\rangle$ han de ser imaginàries pures (atès que $|X\rangle, |Y\rangle, |Z\rangle$ són reals, z és real, i $\hat{p}_x = -id/dx$ és imaginari pur), trobem que $a - a^* = 2a = i/\sqrt{2} \rightarrow a = i/2\sqrt{2}$, cosa que dóna lloc a:

$$\langle x\hat{p}_z\rangle = \frac{i}{2\sqrt{2}} \begin{bmatrix} 0 & 1 & 0 \\ -1 & 0 & 1 \\ 0 & -1 & 0 \end{bmatrix} = -\frac{1}{2}\langle \hat{L}_y\rangle \tag{26}$$

Hem comprovat aquesta relació general integrant $x\hat{p}_z$ en la base d'orbitals atòmics $2p$ de l'hidrogen.

4.3 Elements de matriu de $y\hat{p}_z$

Les mateixes raons de simetria fan també que els elements de matriu $m_{11}, m_{13}, m_{22}, m_{31}, m_{33}$ siguen zero. Cal parar atenció als no nuls $m_{12}, m_{21}, m_{23}, m_{32}$. Abans però farem una consideració que ens estalviarà treball: l'operador $x\hat{p}_z$ es transforma en $-y\hat{p}_z$ en efectuar una rotació $\pi/2$ al voltant del l'eix z. Tanmateix, les integrals són escalars, invariants doncs sota rotacions. Aleshores, considerem per exemple:

$$\langle 10|x\hat{p}_z|1,-1\rangle = \langle Z|x\hat{p}_z(|X\rangle - i|Y\rangle) = \langle Z|x\hat{p}_z|X\rangle = -a^* = \frac{i}{2\sqrt{2}}$$

Per tant,

$$\frac{i}{2\sqrt{2}} = \langle 10|x\hat{p}_z|1,-1\rangle = \mathcal{R}_z^{(\pi/2)}\langle Z|x\hat{p}_z(|X\rangle - i|Y\rangle) = \langle Z|y\hat{p}_z(|Y\rangle + i|X\rangle) = \langle Z|x\hat{p}_z|Y\rangle$$

Amb la qual cosa hem determinat que $\langle Z|x\hat{p}_z|Y\rangle = \frac{i}{2\sqrt{2}}$.

Procedim ara al càlcul de les integrals:

$$\begin{aligned}
\langle 11|y\hat{p}_z|10\rangle &= -(\langle X| - i\langle Y|)|y\hat{p}_z|Z\rangle = i\,\langle Y|y\hat{p}_z|Z\rangle = i\,(\frac{i}{2\sqrt{2}})^* = \frac{1}{2\sqrt{2}} \\
\langle 10|y\hat{p}_z|11\rangle &= -\langle Z|y\hat{p}_z(|X\rangle + i|Y\rangle) = -i\,\langle Z|y\hat{p}_z|Y\rangle = -i\,\frac{i}{2\sqrt{2}} = \frac{1}{2\sqrt{2}} \\
\langle 10|y\hat{p}_z|1,-1\rangle &= \langle Z|y\hat{p}_z(|X\rangle - i|Y\rangle) = -i\langle Z|y\hat{p}_z|Y\rangle = -i\frac{i}{2\sqrt{2}} = \frac{1}{2\sqrt{2}} \\
\langle 1,-1|y\hat{p}_z|10\rangle &= (\langle X| + i\langle Y|)y\hat{p}_z|Z\rangle = i\langle Y|y\hat{p}_z|Z\rangle = i(\frac{i}{2\sqrt{2}})^* = \frac{1}{2\sqrt{2}}
\end{aligned} \tag{27}$$

Aleshores,

$$\langle y\hat{p}_z\rangle = \frac{1}{2\sqrt{2}}\begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix} = \frac{1}{2}\langle \hat{L}_x\rangle \tag{28}$$

Hem comprovat també aquesta relació general integrant $y\hat{p}_z$ en la base d'orbitals atòmics $2p$ de l'hidrogen.

4.4 Comprovacions amb la base $2p$ de l'hidrogen

Per a fer-ho (amb Mathematica) tenim en compte que:

$$\frac{\partial}{\partial x} = \sin\theta\cos\phi\frac{\partial}{\partial r} + \frac{\cos\theta\cos\phi}{r}\frac{\partial}{\partial\theta} - \frac{\sin\phi}{r\sin\theta}\frac{\partial}{\partial\phi} \tag{29}$$

$$\frac{\partial}{\partial y} = \sin\theta\sin\phi\frac{\partial}{\partial r} + \frac{\cos\theta\sin\phi}{r}\frac{\partial}{\partial\theta} + \frac{\cos\phi}{r\sin\theta}\frac{\partial}{\partial\phi} \tag{30}$$

$$\frac{\partial}{\partial z} = \cos\theta\frac{\partial}{\partial r} - \frac{\sin\theta}{r}\frac{\partial}{\partial\theta} \tag{31}$$

$$R(r) = 2e^{-r} \tag{32}$$

$$Y_{11}(\theta,\phi) = -\sqrt{\frac{3}{8\pi}}\sin\theta e^{i\phi} \tag{33}$$

$$Y_{1,-1}(\theta,\phi) = \sqrt{\frac{3}{8\pi}}\sin\theta e^{-i\phi} \tag{34}$$

$$Y_{10}(\theta,\phi) = \sqrt{\frac{3}{4\pi}}\cos\theta \tag{35}$$

5 Apèndix 2: Els factors màssics.

En el cas dels termes diagonals, agafem la massa m_z que inclou el terme en p_z^2 i la massa $m_\perp$ de p_x^2 i p_y^2. Hi ha termes extradiagonals que deriven de la representació matricial de $\hat{L}_x, \hat{L}_y$ en la base WZ (elements m_{13}, m_{23}, m_{31} i m_{32}) que corresponen a interaccions entre bandes A (o B que té les mateixes masses) i la banda C. També hi ha els que deriven de la representació matricial de σ_x, σ_y en la base WZ (elements $m_{15}, m_{24}, m_{16}, m_{42}, m_{51}$ i m_{61}) que corresponen a interaccions entre bandes A amb B i C amb C. Per tant, per al cas dels termes que deriven de σ el factor màssic està perfectament definit. Per al cas $\hat{L}_i$ una opció seria agafar la massa (tant $m_\perp$ com m_z) com $m = \sqrt{m_A}\sqrt{m_C}$, on m_A indica la massa ($m_\perp$ o m_z) de la banda A i m_C les de la banda C. Cal para atenció a que les masses poden ser negatives, però tant mathematica com comsol saben calcular arrels de números negatius.

6 Apèndix 3: Implementació dels coeficients dels factors màssics.

Les masses dels elements diagonals són $m_\perp^{-1} = A_2 + A_4$, $m_z^{-1} = A_1 + A_3$ per a les bandes A i B i $m_\perp^{-1} = A_2$, $m_z^{-1} = A_1$ per a la banda C. Per als elements de matriu extradiagonals que connecten les bandes A i B li assignem la massa que tenen aquestes bandes. Finalment, per als elements extradiagonals que connecten les bandes A i C o B i C assignem el producte de arrels quadrades de les masses de les bandes connectades, és a dir, $m_\perp^{-1} = \sqrt{A_2 + A_4}\sqrt{A_2}$ i $m_z^{-1} = \sqrt{A_1 + A_2}\sqrt{A_1}$. Com les masses són negatives cada arrel quadrada genera un número imaginari i, de manera que com $i^2 = -1$ la massa resultant és també, com cal, negativa.

Per tal de modular el valor d'aquestes masses entre el valor que assignen la interacció amb les bandes i el límit de *quenching* total incloem sis coeficients $c_i \in [1, m_i]$ que fem variar de manera síncrona entre els límits dels corresponents intervals. Per a implementar la sincronia definim un factor $0 < f < 1$. Aleshores, multipliquem els termes on estan les masses (les quals apareixen sempre dividint) pels coeficients $c_i = 1 + f(m_i - 1)$. Cosa que vol dir que $f = 1$ ($c_i = m_i$) representa el *quenching* total de l'acció de les bandes que fa que les masses siguen la unitat (i.e. la massa de l'electró lliure m_e), mentre que $f = 0$ ($c_i = 1$) representa el *quenching* nul, que vol dir plena acció de les bandes modificant les masses.

Referències

[1] J. Planelles and J.I. Climente 2013 *J. Phys.: Condens. Matt.* **25** 485801.

[2] van Bree J, Silov A Y, Koenraad P M, Flatté M E and Pryor C E 2012 *Phys Rev. B* **85** 165323.

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ClearAll["Global`*"]
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$$2p_z \qquad \frac{(Z/a_0)^{5/2}}{4\sqrt{2\pi}}\, r e^{-Zr/2a_0} \cos\theta$$

$$2p_x \qquad \frac{(Z/a_0)^{5/2}}{4\sqrt{2\pi}}\, r e^{-Zr/2a_0} \sin\theta \cos\varphi$$

$$2p_y \qquad \frac{(Z/a_0)^{5/2}}{4\sqrt{2\pi}}\, r e^{-Zr/2a_0} \sin\theta \sin\varphi$$

```
(*

                                                                  *)
```

$$\texttt{Y11}[\theta\_,\ \phi\_] = -\sqrt{\frac{3}{8\,\pi}}\ \texttt{Sin}[\theta]\ e^{i\,\phi};\ \texttt{Y1m1}[\theta\_,\ \phi\_] = \sqrt{\frac{3}{8\,\pi}}\ \texttt{Sin}[\theta]\ e^{-i\,\phi};\ \texttt{(* conjY11=Y1m1;}$$

$$\texttt{conY1m1= Y11*)}\ \texttt{Y10}[\theta\_,\ \phi\_] = \sqrt{\frac{3}{4\,\pi}}\ \texttt{Cos}[\theta];\ \texttt{R}[r\_] = \frac{\sqrt{6}}{12}\ r * e^{-r/2};$$

```
x[r_, θ_, ϕ_] = r Sin[θ] Cos[ϕ]; y[r_, θ_, ϕ_] = r Sin[θ] Sin[ϕ]; z[r_, θ_, ϕ_] = r Cos[θ]; (* kz=i Sin[θ] D[F,θ] *)
```

```
(*************************************  Comprove normes  **************************************************)
```

$$\texttt{Print}\left[\texttt{"r -> "},\ \int_0^\infty \texttt{R}[r]\texttt{\^{}2}\ r^2\, dr,\ \texttt{"   angles -> "},\ \int_0^{2\pi}\left(\int_0^\pi \texttt{Y1m1}[\theta,\ \phi]\ \texttt{Y11}[\theta,\ \phi] * \texttt{Sin}[\theta]\, d\theta\right) d\phi\right]$$

```
r -> 1    angles -> -1
```

```
(*************************************  Comprove valors de Lz en aquesta base R[r]  *************************************)
```

$$\int_0^\infty \texttt{R}[r]\left(\int_0^{2\pi}\left(\int_0^\pi (-\texttt{Y1m1}[\theta,\ \phi]) * (-i\,\texttt{R}[r]\ \texttt{D}[\texttt{Y11}[\theta,\ \phi],\ \phi]) * \texttt{Sin}[\theta]\, d\theta\right) d\phi\right) r^2\, dr$$

1

$$\int_0^\infty \texttt{R}[r]\left(\int_0^{2\pi}\left(\int_0^\pi (-\texttt{Y11}[\theta,\ \phi]) * (-i\,\texttt{R}[r]\ \texttt{D}[\texttt{Y1m1}[\theta,\ \phi],\ \phi]) * \texttt{Sin}[\theta]\, d\theta\right) d\phi\right) r^2\, dr$$

-1

$$\int_0^\infty R[r]\left(\int_0^{2\pi}\left(\int_0^\pi Y10[\theta,\phi]*(-i\,R[r]\,D[Y10[\theta,\phi],\phi])*Sin[\theta]\,d\theta\right)d\phi\right)r^2\,dr$$

0

(*************************************** x kz **)

$$\int_0^\infty R[r]\left(\int_0^{2\pi}\left(\int_0^\pi(-Y1m1[\theta,\phi])*x[r,\theta,\phi]*\left(-i\,Cos[\theta]\,Y11[\theta,\phi]\,D[R[r],r]+i\,\frac{Sin[\theta]}{r}\,R[r]\,D[Y11[\theta,\phi],\theta]\right)*Sin[\theta]\,d\theta\right)d\phi\right)r^2\,dr$$

0

$$\int_0^\infty R[r]\left(\int_0^{2\pi}\left(\int_0^\pi(-Y1m1[\theta,\phi])*x[r,\theta,\phi]*\left(-i\,Cos[\theta]\,Y1m1[\theta,\phi]\,D[R[r],r]+i\,\frac{Sin[\theta]}{r}\,R[r]\,D[Y1m1[\theta,\phi],\theta]\right)*Sin[\theta]\,d\theta\right)d\phi\right)r^2\,dr$$

0

$$\int_0^\infty R[r]\left(\int_0^{2\pi}\left(\int_0^\pi(-Y1m1[\theta,\phi])*x[r,\theta,\phi]*\left(-i\,Cos[\theta]\,Y10[\theta,\phi]\,D[R[r],r]+i\,\frac{Sin[\theta]}{r}\,R[r]\,D[Y10[\theta,\phi],\theta]\right)*Sin[\theta]\,d\theta\right)d\phi\right)r^2\,dr$$

$$\frac{i}{2\sqrt{2}}$$

$$\int_0^\infty R[r]\left(\int_0^{2\pi}\left(\int_0^\pi(-Y11[\theta,\phi])*x[r,\theta,\phi]*\left(-i\,Cos[\theta]\,Y11[\theta,\phi]\,D[R[r],r]+i\,\frac{Sin[\theta]}{r}\,R[r]\,D[Y11[\theta,\phi],\theta]\right)*Sin[\theta]\,d\theta\right)d\phi\right)r^2\,dr$$

0

$$\int_0^\infty R[r]\left(\int_0^{2\pi}\left(\int_0^\pi(-Y11[\theta,\phi])*x[r,\theta,\phi]*\left(-i\,Cos[\theta]\,Y1m1[\theta,\phi]\,D[R[r],r]+i\,\frac{Sin[\theta]}{r}\,R[r]\,D[Y1m1[\theta,\phi],\theta]\right)*Sin[\theta]\,d\theta\right)d\phi\right)r^2\,dr$$

0

$$\int_0^\infty R[r]\left(\int_0^{2\pi}\left(\int_0^\pi(-Y11[\theta,\phi])*x[r,\theta,\phi]*\left(-i\,Cos[\theta]\,Y10[\theta,\phi]\,D[R[r],r]+i\,\frac{Sin[\theta]}{r}\,R[r]\,D[Y10[\theta,\phi],\theta]\right)*Sin[\theta]\,d\theta\right)d\phi\right)r^2\,dr$$

$$-\frac{i}{2\sqrt{2}}$$

$$\int_0^\infty R[r]\left(\int_0^{2\pi}\left(\int_0^\pi Y10[\theta,\phi]*x[r,\theta,\phi]*\left(-i\,Cos[\theta]\,Y11[\theta,\phi]\,D[R[r],r]+i\,\frac{Sin[\theta]}{r}\,R[r]\,D[Y11[\theta,\phi],\theta]\right)*Sin[\theta]\,d\theta\right)d\phi\right)r^2\,dr$$

$$-\frac{i}{2\sqrt{2}}$$

$$\int_0^\infty R[r]\left(\int_0^{2\pi}\left(\int_0^\pi Y10[\theta,\phi]*x[r,\theta,\phi]*\left(-i\,Cos[\theta]\,Y1m1[\theta,\phi]\,D[R[r],r]+i\,\frac{Sin[\theta]}{r}\,R[r]\,D[Y1m1[\theta,\phi],\theta]\right)*Sin[\theta]\,d\theta\right)d\phi\right)r^2\,dr$$

$$\frac{i}{2\sqrt{2}}$$

$$\int_0^\infty R[r]\left(\int_0^{2\pi}\left(\int_0^\pi Y10[\theta,\phi]*x[r,\theta,\phi]*\left(-i\,Cos[\theta]\,Y10[\theta,\phi]\,D[R[r],r]+i\,\frac{Sin[\theta]}{r}\,R[r]\,D[Y10[\theta,\phi],\theta]\right)*Sin[\theta]\,d\theta\right)d\phi\right)r^2\,dr$$

0

$$mxz=\left\{\left\{0,0,-\frac{i}{2\sqrt{2}}\right\},\left\{0,0,-\frac{i}{2\sqrt{2}}\right\},\left\{\frac{i}{2\sqrt{2}},\frac{i}{2\sqrt{2}},0\right\}\right\};\ Eigensystem[mxz]$$

$$\left\{\left\{-\frac{1}{2},\frac{1}{2},0\right\},\left\{\left\{\frac{i}{\sqrt{2}},\frac{i}{\sqrt{2}},1\right\},\left\{-\frac{i}{\sqrt{2}},-\frac{i}{\sqrt{2}},1\right\},\{-1,1,0\}\right\}\right\}$$

(*************************************   y kz   **)

$$\int_0^\infty R[r]\left(\int_0^{2\pi}\left(\int_0^\pi (-Y1m1[\theta,\phi])*y[r,\theta,\phi]*\left(-i\,Cos[\theta]\,Y11[\theta,\phi]\,D[R[r],r]+i\,\frac{Sin[\theta]}{r}\,R[r]\,D[Y11[\theta,\phi],\theta]\right)*Sin[\theta]\,d\theta\right)d\phi\right)r^2\,dr$$

0

$$\int_0^\infty R[r]\left(\int_0^{2\pi}\left(\int_0^\pi (-Y1m1[\theta,\phi])*y[r,\theta,\phi]*\left(-i\,Cos[\theta]\,Y1m1[\theta,\phi]\,D[R[r],r]+i\,\frac{Sin[\theta]}{r}\,R[r]\,D[Y1m1[\theta,\phi],\theta]\right)*Sin[\theta]\,d\theta\right)d\phi\right)r^2\,dr$$

0

$$\int_0^\infty R[r]\left(\int_0^{2\pi}\left(\int_0^\pi (-Y1m1[\theta,\phi])*y[r,\theta,\phi]*\left(-i\,Cos[\theta]\,Y10[\theta,\phi]\,D[R[r],r]+i\,\frac{Sin[\theta]}{r}\,R[r]\,D[Y10[\theta,\phi],\theta]\right)*Sin[\theta]\,d\theta\right)d\phi\right)r^2\,dr$$

$$\frac{1}{2\sqrt{2}}$$

$$\int_0^\infty R[r]\left(\int_0^{2\pi}\left(\int_0^\pi (-Y11[\theta,\phi])*y[r,\theta,\phi]*\left(-i\,Cos[\theta]\,Y11[\theta,\phi]\,D[R[r],r]+i\,\frac{Sin[\theta]}{r}\,R[r]\,D[Y11[\theta,\phi],\theta]\right)*Sin[\theta]\,d\theta\right)d\phi\right)r^2\,dr$$

0

$$\int_0^{\infty} R[r] \left(\int_0^{2\pi}\left(\int_0^{\pi}(-Y11[\theta,\phi]) * y[r,\theta,\phi] * \left(-i\, Cos[\theta]\, Y1m1[\theta,\phi]\, D[R[r],r] + i\, \frac{Sin[\theta]}{r} R[r]\, D[Y1m1[\theta,\phi],\theta]\right) * Sin[\theta]\, d\theta\right) d\phi\right) r^2\, dr$$

0

$$\int_0^{\infty} R[r] \left(\int_0^{2\pi}\left(\int_0^{\pi}(-Y11[\theta,\phi]) * y[r,\theta,\phi] * \left(-i\, Cos[\theta]\, Y10[\theta,\phi]\, D[R[r],r] + i\, \frac{Sin[\theta]}{r} R[r]\, D[Y10[\theta,\phi],\theta]\right) * Sin[\theta]\, d\theta\right) d\phi\right) r^2\, dr$$

$$\frac{1}{2\sqrt{2}}$$

$$\int_0^{\infty} R[r] \left(\int_0^{2\pi}\left(\int_0^{\pi}Y10[\theta,\phi] * y[r,\theta,\phi] * \left(-i\, Cos[\theta]\, Y11[\theta,\phi]\, D[R[r],r] + i\, \frac{Sin[\theta]}{r} R[r]\, D[Y11[\theta,\phi],\theta]\right) * Sin[\theta]\, d\theta\right) d\phi\right) r^2\, dr$$

$$\frac{1}{2\sqrt{2}}$$

$$\int_0^{\infty} R[r] \left(\int_0^{2\pi}\left(\int_0^{\pi}Y10[\theta,\phi] * y[r,\theta,\phi] * \left(-i\, Cos[\theta]\, Y1m1[\theta,\phi]\, D[R[r],r] + i\, \frac{Sin[\theta]}{r} R[r]\, D[Y1m1[\theta,\phi],\theta]\right) * Sin[\theta]\, d\theta\right) d\phi\right) r^2\, dr$$

$$\frac{1}{2\sqrt{2}}$$

$$\int_0^{\infty} R[r] \left(\int_0^{2\pi}\left(\int_0^{\pi}Y10[\theta,\phi] * y[r,\theta,\phi] * \left(-i\, Cos[\theta]\, Y10[\theta,\phi]\, D[R[r],r] + i\, \frac{Sin[\theta]}{r} R[r]\, D[Y10[\theta,\phi],\theta]\right) * Sin[\theta]\, d\theta\right) d\phi\right) r^2\, dr$$

0

$$myz = \left\{\left\{0, 0, -\frac{1}{2\sqrt{2}}\right\}, \left\{0, 0, \frac{1}{2\sqrt{2}}\right\}, \left\{-\frac{1}{2\sqrt{2}}, \frac{1}{2\sqrt{2}}, 0\right\}\right\}; Eigensystem[myz]$$

$$\left\{\left\{-\frac{1}{2}, \frac{1}{2}, 0\right\}, \left\{\left\{\frac{1}{\sqrt{2}}, -\frac{1}{\sqrt{2}}, 1\right\}, \left\{-\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}, 1\right\}, \{1, 1, 0\}\right\}\right\}$$

```
(****************************************   z  kx    ********************************************************)
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$$\int_0^{\infty} R[r] \left(\int_0^{2\pi}\left(\int_0^{\pi}(-Y1m1[\theta,\phi]) * z[r,\theta,\phi] * \left(-i\, Sin[\theta]\, Cos[\phi]\, Y11[\theta,\phi]\, D[R[r],r] - i\, \frac{Cos[\theta]\, Cos[\phi]}{r} R[r]\, D[Y11[\theta,\phi],\theta] + i\, \frac{Sin[\phi]}{r\, Sin[\theta]} R[r]\, D[Y11[\theta,\phi],\phi]\right) * Sin[\theta]\, d\theta\right) d\phi\right) r^2\, dr$$

0

$$\int_0^\infty R[r]\left(\int_0^{2\pi}\left(\int_0^\pi(-Y1m1[\theta,\phi]) * z[r,\theta,\phi] * \left(-i\,Sin[\theta]\,Cos[\phi]\,Y1m1[\theta,\phi]\,D[R[r],r] - i\,\frac{Cos[\theta]\,Cos[\phi]}{r}\,R[r]\,D[Y1m1[\theta,\phi],\theta] + i\,\frac{Sin[\phi]}{r\,Sin[\theta]}\,R[r]\,D[Y1m1[\theta,\phi],\phi]\right) * Sin[\theta]\,d\theta\right)d\phi\right)r^2\,dr$$

0

$$\int_0^\infty R[r]\left(\int_0^{2\pi}\left(\int_0^\pi(-Y1m1[\theta,\phi]) * z[r,\theta,\phi] * \left(-i\,Sin[\theta]\,Cos[\phi]\,Y10[\theta,\phi]\,D[R[r],r] - i\,\frac{Cos[\theta]\,Cos[\phi]}{r}\,R[r]\,D[Y10[\theta,\phi],\theta] + i\,\frac{Sin[\phi]}{r\,Sin[\theta]}\,R[r]\,D[Y10[\theta,\phi],\phi]\right) * Sin[\theta]\,d\theta\right)d\phi\right)r^2\,dr$$

$$-\frac{i}{2\sqrt{2}}$$

$$\int_0^\infty R[r]\left(\int_0^{2\pi}\left(\int_0^\pi(-Y11[\theta,\phi]) * z[r,\theta,\phi] * \left(-i\,Sin[\theta]\,Cos[\phi]\,Y11[\theta,\phi]\,D[R[r],r] - i\,\frac{Cos[\theta]\,Cos[\phi]}{r}\,R[r]\,D[Y11[\theta,\phi],\theta] + i\,\frac{Sin[\phi]}{r\,Sin[\theta]}\,R[r]\,D[Y11[\theta,\phi],\phi]\right) * Sin[\theta]\,d\theta\right)d\phi\right)r^2\,dr$$

0

$$\int_0^\infty R[r]\left(\int_0^{2\pi}\left(\int_0^\pi(-Y11[\theta,\phi]) * z[r,\theta,\phi] * \left(-i\,Sin[\theta]\,Cos[\phi]\,Y1m1[\theta,\phi]\,D[R[r],r] - i\,\frac{Cos[\theta]\,Cos[\phi]}{r}\,R[r]\,D[Y1m1[\theta,\phi],\theta] + i\,\frac{Sin[\phi]}{r\,Sin[\theta]}\,R[r]\,D[Y1m1[\theta,\phi],\phi]\right) * Sin[\theta]\,d\theta\right)d\phi\right)r^2\,dr$$

0

$$\int_0^\infty R[r]\left(\int_0^{2\pi}\left(\int_0^\pi(-Y11[\theta,\phi]) * z[r,\theta,\phi] * \left(-i\,Sin[\theta]\,Cos[\phi]\,Y10[\theta,\phi]\,D[R[r],r] - i\,\frac{Cos[\theta]\,Cos[\phi]}{r}\,R[r]\,D[Y10[\theta,\phi],\theta] + i\,\frac{Sin[\phi]}{r\,Sin[\theta]}\,R[r]\,D[Y10[\theta,\phi],\phi]\right) * Sin[\theta]\,d\theta\right)d\phi\right)r^2\,dr$$

$$\frac{i}{2\sqrt{2}}$$

$$\int_0^\infty R[r]\left(\int_0^{2\pi}\left(\int_0^\pi Y10[\theta,\phi]*z[r,\theta,\phi]*\left(-i\,Sin[\theta]\,Cos[\phi]\,Y11[\theta,\phi]\,D[R[r],r]-i\,\frac{Cos[\theta]\,Cos[\phi]}{r}\,R[r]\,D[Y11[\theta,\phi],\theta]+i\,\frac{Sin[\phi]}{r\,Sin[\theta]}\,R[r]\,D[Y11[\theta,\phi],\phi]\right)*Sin[\theta]\,d\theta\right)d\phi\right)r^2\,dr$$

$$\frac{i}{2\sqrt{2}}$$

$$\int_0^\infty R[r]\left(\int_0^{2\pi}\left(\int_0^\pi Y10[\theta,\phi]*z[r,\theta,\phi]*\left(-i\,Sin[\theta]\,Cos[\phi]\,Y1m1[\theta,\phi]\,D[R[r],r]-i\,\frac{Cos[\theta]\,Cos[\phi]}{r}\,R[r]\,D[Y1m1[\theta,\phi],\theta]+i\,\frac{Sin[\phi]}{r\,Sin[\theta]}\,R[r]\,D[Y1m1[\theta,\phi],\phi]\right)*Sin[\theta]\,d\theta\right)d\phi\right)r^2\,dr$$

$$-\frac{i}{2\sqrt{2}}$$

$$\int_0^\infty R[r]\left(\int_0^{2\pi}\left(\int_0^\pi Y10[\theta,\phi]*z[r,\theta,\phi]*\left(-i\,Sin[\theta]\,Cos[\phi]\,Y10[\theta,\phi]\,D[R[r],r]-i\,\frac{Cos[\theta]\,Cos[\phi]}{r}\,R[r]\,D[Y10[\theta,\phi],\theta]+i\,\frac{Sin[\phi]}{r\,Sin[\theta]}\,R[r]\,D[Y10[\theta,\phi],\phi]\right)*Sin[\theta]\,d\theta\right)d\phi\right)r^2\,dr$$

0

$$mzx=\left\{\left\{0,0,\frac{i}{2\sqrt{2}}\right\},\left\{0,0,\frac{i}{2\sqrt{2}}\right\},\left\{-\frac{i}{2\sqrt{2}},-\frac{i}{2\sqrt{2}},0\right\}\right\};\ Eigensystem[mzx]$$

$$\left\{\left\{-\frac{1}{2},\frac{1}{2},0\right\},\left\{\left\{-\frac{i}{\sqrt{2}},-\frac{i}{\sqrt{2}},1\right\},\left\{\frac{i}{\sqrt{2}},\frac{i}{\sqrt{2}},1\right\},\{-1,1,0\}\right\}\right\}$$

(** z ky **)

$$\int_0^\infty R[r]\left(\int_0^{2\pi}\left(\int_0^\pi (-Y1m1[\theta,\phi])*z[r,\theta,\phi]*\left(-i\,Sin[\theta]\,Sin[\phi]\,Y11[\theta,\phi]\,D[R[r],r]-i\,\frac{Cos[\theta]\,Sin[\phi]}{r}\,R[r]\,D[Y11[\theta,\phi],\theta]-i\,\frac{Cos[\phi]}{r\,Sin[\theta]}\,R[r]\,D[Y11[\theta,\phi],\phi]\right)*Sin[\theta]\,d\theta\right)d\phi\right)r^2\,dr$$

0

$$\int_0^{\infty} \mathbf{R[r]} \left(\int_0^{2\pi} \left(\int_0^{\pi} (-\mathbf{Y1m1}[\theta,\phi]) * \mathbf{z}[\mathbf{r},\theta,\phi] * \left(-i\,\mathbf{Sin}[\theta]\,\mathbf{Sin}[\phi]\,\mathbf{Y1m1}[\theta,\phi]\,\mathbf{D}[\mathbf{R[r]},\mathbf{r}] - i\,\frac{\mathbf{Cos}[\theta]\,\mathbf{Sin}[\phi]}{\mathbf{r}}\,\mathbf{R[r]}\,\mathbf{D}[\mathbf{Y1m1}[\theta,\phi],\theta] - i\,\frac{\mathbf{Cos}[\phi]}{\mathbf{r}\,\mathbf{Sin}[\theta]}\,\mathbf{R[r]}\,\mathbf{D}[\mathbf{Y1m1}[\theta,\phi],\phi]\right) * \mathbf{Sin}[\theta]\,d\theta\right) d\phi\right) \mathbf{r}^2\,d\mathbf{r}$$

0

$$\int_0^{\infty} \mathbf{R[r]} \left(\int_0^{2\pi} \left(\int_0^{\pi} (-\mathbf{Y1m1}[\theta,\phi]) * \mathbf{z}[\mathbf{r},\theta,\phi] * \left(-i\,\mathbf{Sin}[\theta]\,\mathbf{Sin}[\phi]\,\mathbf{Y10}[\theta,\phi]\,\mathbf{D}[\mathbf{R[r]},\mathbf{r}] - i\,\frac{\mathbf{Cos}[\theta]\,\mathbf{Sin}[\phi]}{\mathbf{r}}\,\mathbf{R[r]}\,\mathbf{D}[\mathbf{Y10}[\theta,\phi],\theta] - i\,\frac{\mathbf{Cos}[\phi]}{\mathbf{r}\,\mathbf{Sin}[\theta]}\,\mathbf{R[r]}\,\mathbf{D}[\mathbf{Y10}[\theta,\phi],\phi]\right) * \mathbf{Sin}[\theta]\,d\theta\right) d\phi\right) \mathbf{r}^2\,d\mathbf{r}$$

$$-\frac{1}{2\sqrt{2}}$$

$$\int_0^{\infty} \mathbf{R[r]} \left(\int_0^{2\pi} \left(\int_0^{\pi} (-\mathbf{Y11}[\theta,\phi]) * \mathbf{z}[\mathbf{r},\theta,\phi] * \left(-i\,\mathbf{Sin}[\theta]\,\mathbf{Sin}[\phi]\,\mathbf{Y11}[\theta,\phi]\,\mathbf{D}[\mathbf{R[r]},\mathbf{r}] - i\,\frac{\mathbf{Cos}[\theta]\,\mathbf{Sin}[\phi]}{\mathbf{r}}\,\mathbf{R[r]}\,\mathbf{D}[\mathbf{Y11}[\theta,\phi],\theta] - i\,\frac{\mathbf{Cos}[\phi]}{\mathbf{r}\,\mathbf{Sin}[\theta]}\,\mathbf{R[r]}\,\mathbf{D}[\mathbf{Y11}[\theta,\phi],\phi]\right) * \mathbf{Sin}[\theta]\,d\theta\right) d\phi\right) \mathbf{r}^2\,d\mathbf{r}$$

0

$$\int_0^{\infty} \mathbf{R[r]} \left(\int_0^{2\pi} \left(\int_0^{\pi} (-\mathbf{Y11}[\theta,\phi]) * \mathbf{z}[\mathbf{r},\theta,\phi] * \left(-i\,\mathbf{Sin}[\theta]\,\mathbf{Sin}[\phi]\,\mathbf{Y1m1}[\theta,\phi]\,\mathbf{D}[\mathbf{R[r]},\mathbf{r}] - i\,\frac{\mathbf{Cos}[\theta]\,\mathbf{Sin}[\phi]}{\mathbf{r}}\,\mathbf{R[r]}\,\mathbf{D}[\mathbf{Y1m1}[\theta,\phi],\theta] - i\,\frac{\mathbf{Cos}[\phi]}{\mathbf{r}\,\mathbf{Sin}[\theta]}\,\mathbf{R[r]}\,\mathbf{D}[\mathbf{Y1m1}[\theta,\phi],\phi]\right) * \mathbf{Sin}[\theta]\,d\theta\right) d\phi\right) \mathbf{r}^2\,d\mathbf{r}$$

0

$$\int_0^{\infty} \mathbf{R[r]} \left(\int_0^{2\pi} \left(\int_0^{\pi} (-\mathbf{Y11}[\theta,\phi]) * \mathbf{z}[\mathbf{r},\theta,\phi] * \left(-i\,\mathbf{Sin}[\theta]\,\mathbf{Sin}[\phi]\,\mathbf{Y10}[\theta,\phi]\,\mathbf{D}[\mathbf{R[r]},\mathbf{r}] - i\,\frac{\mathbf{Cos}[\theta]\,\mathbf{Sin}[\phi]}{\mathbf{r}}\,\mathbf{R[r]}\,\mathbf{D}[\mathbf{Y10}[\theta,\phi],\theta] - i\,\frac{\mathbf{Cos}[\phi]}{\mathbf{r}\,\mathbf{Sin}[\theta]}\,\mathbf{R[r]}\,\mathbf{D}[\mathbf{Y10}[\theta,\phi],\phi]\right) * \mathbf{Sin}[\theta]\,d\theta\right) d\phi\right) \mathbf{r}^2\,d\mathbf{r}$$

$$-\frac{1}{2\sqrt{2}}$$

$$\int_0^\infty R[r]\left(\int_0^{2\pi}\left(\int_0^\pi Y10[\theta,\phi]*z[r,\theta,\phi]*\left(-i\,Sin[\theta]\,Sin[\phi]\,Y11[\theta,\phi]\,D[R[r],r]-i\,\frac{Cos[\theta]\,Sin[\phi]}{r}\,R[r]\,D[Y11[\theta,\phi],\theta]-i\,\frac{Cos[\phi]}{r\,Sin[\theta]}\,R[r]\,D[Y11[\theta,\phi],\phi]\right)*Sin[\theta]\,d\theta\right)d\phi\right)r^2\,dr$$

$$-\frac{1}{2\sqrt{2}}$$

$$\int_0^\infty R[r]\left(\int_0^{2\pi}\left(\int_0^\pi Y10[\theta,\phi]*z[r,\theta,\phi]*\left(-i\,Sin[\theta]\,Sin[\phi]\,Y1m1[\theta,\phi]\,D[R[r],r]-i\,\frac{Cos[\theta]\,Sin[\phi]}{r}\,R[r]\,D[Y1m1[\theta,\phi],\theta]-i\,\frac{Cos[\phi]}{r\,Sin[\theta]}\,R[r]\,D[Y1m1[\theta,\phi],\phi]\right)*Sin[\theta]\,d\theta\right)d\phi\right)r^2\,dr$$

$$-\frac{1}{2\sqrt{2}}$$

$$\int_0^\infty R[r]\left(\int_0^{2\pi}\left(\int_0^\pi Y10[\theta,\phi]*z[r,\theta,\phi]*\left(-i\,Sin[\theta]\,Sin[\phi]\,Y10[\theta,\phi]\,D[R[r],r]-i\,\frac{Cos[\theta]\,Sin[\phi]}{r}\,R[r]\,D[Y10[\theta,\phi],\theta]-i\,\frac{Cos[\phi]}{r\,Sin[\theta]}\,R[r]\,D[Y10[\theta,\phi],\phi]\right)*Sin[\theta]\,d\theta\right)d\phi\right)r^2\,dr$$

0

$$mzy=\left\{\left\{0,0,\frac{1}{2\sqrt{2}}\right\},\left\{0,0,-\frac{1}{2\sqrt{2}}\right\},\left\{\frac{1}{2\sqrt{2}},-\frac{1}{2\sqrt{2}},0\right\}\right\};\ Eigensystem[mzy]$$

$$\left\{\left\{-\frac{1}{2},\frac{1}{2},0\right\},\left\{\left\{-\frac{1}{\sqrt{2}},\frac{1}{\sqrt{2}},1\right\},\left\{\frac{1}{\sqrt{2}},-\frac{1}{\sqrt{2}},1\right\},\{1,1,0\}\right\}\right\}$$

(*************************************** y kx **)

$$\int_0^\infty R[r]\left(\int_0^{2\pi}\left(\int_0^\pi(-Y1m1[\theta,\phi])*y[r,\theta,\phi]*\left(-i\,Sin[\theta]\,Cos[\phi]\,Y11[\theta,\phi]\,D[R[r],r]-i\,\frac{Cos[\theta]\,Cos[\phi]}{r}\,R[r]\,D[Y11[\theta,\phi],\theta]+i\,\frac{Sin[\phi]}{r\,Sin[\theta]}\,R[r]\,D[Y11[\theta,\phi],\phi]\right)*Sin[\theta]\,d\theta\right)d\phi\right)r^2\,dr$$

$$-\frac{1}{2}$$

$$\int_0^\infty R[r]\left(\int_0^{2\pi}\left(\int_0^\pi(-Y1m1[\theta,\phi]) * y[r,\theta,\phi] * \left(-i\,Sin[\theta]\,Cos[\phi]\,Y1m1[\theta,\phi]\,D[R[r],r] - i\,\frac{Cos[\theta]\,Cos[\phi]}{r}\,R[r]\,D[Y1m1[\theta,\phi],\theta] + i\,\frac{Sin[\phi]}{r\,Sin[\theta]}\,R[r]\,D[Y1m1[\theta,\phi],\phi]\right) * Sin[\theta]\,d\theta\right)d\phi\right)r^2\,dr$$

0

$$\int_0^\infty R[r]\left(\int_0^{2\pi}\left(\int_0^\pi(-Y1m1[\theta,\phi]) * y[r,\theta,\phi] * \left(-i\,Sin[\theta]\,Cos[\phi]\,Y10[\theta,\phi]\,D[R[r],r] - i\,\frac{Cos[\theta]\,Cos[\phi]}{r}\,R[r]\,D[Y10[\theta,\phi],\theta] + i\,\frac{Sin[\phi]}{r\,Sin[\theta]}\,R[r]\,D[Y10[\theta,\phi],\phi]\right) * Sin[\theta]\,d\theta\right)d\phi\right)r^2\,dr$$

0

$$\int_0^\infty R[r]\left(\int_0^{2\pi}\left(\int_0^\pi(-Y11[\theta,\phi]) * y[r,\theta,\phi] * \left(-i\,Sin[\theta]\,Cos[\phi]\,Y11[\theta,\phi]\,D[R[r],r] - i\,\frac{Cos[\theta]\,Cos[\phi]}{r}\,R[r]\,D[Y11[\theta,\phi],\theta] + i\,\frac{Sin[\phi]}{r\,Sin[\theta]}\,R[r]\,D[Y11[\theta,\phi],\phi]\right) * Sin[\theta]\,d\theta\right)d\phi\right)r^2\,dr$$

0

$$\int_0^\infty R[r]\left(\int_0^{2\pi}\left(\int_0^\pi(-Y11[\theta,\phi]) * y[r,\theta,\phi] * \left(-i\,Sin[\theta]\,Cos[\phi]\,Y1m1[\theta,\phi]\,D[R[r],r] - i\,\frac{Cos[\theta]\,Cos[\phi]}{r}\,R[r]\,D[Y1m1[\theta,\phi],\theta] + i\,\frac{Sin[\phi]}{r\,Sin[\theta]}\,R[r]\,D[Y1m1[\theta,\phi],\phi]\right) * Sin[\theta]\,d\theta\right)d\phi\right)r^2\,dr$$

$$\frac{1}{2}$$

$$\int_0^\infty R[r]\left(\int_0^{2\pi}\left(\int_0^\pi(-Y11[\theta,\phi]) * y[r,\theta,\phi] * \left(-i\,Sin[\theta]\,Cos[\phi]\,Y10[\theta,\phi]\,D[R[r],r] - i\,\frac{Cos[\theta]\,Cos[\phi]}{r}\,R[r]\,D[Y10[\theta,\phi],\theta] + i\,\frac{Sin[\phi]}{r\,Sin[\theta]}\,R[r]\,D[Y10[\theta,\phi],\phi]\right) * Sin[\theta]\,d\theta\right)d\phi\right)r^2\,dr$$

0

$$\int_0^\infty R[r]\left(\int_0^{2\pi}\left(\int_0^\pi Y10[\theta,\phi]*y[r,\theta,\phi]*\left(-i\,Sin[\theta]\,Cos[\phi]\,Y11[\theta,\phi]\,D[R[r],r]-i\,\frac{Cos[\theta]\,Cos[\phi]}{r}\,R[r]\,D[Y11[\theta,\phi],\theta]+i\,\frac{Sin[\phi]}{r\,Sin[\theta]}\,R[r]\,D[Y11[\theta,\phi],\phi]\right)*Sin[\theta]\,d\theta\right)d\phi\right)r^2\,dr$$

0

$$\int_0^\infty R[r]\left(\int_0^{2\pi}\left(\int_0^\pi Y10[\theta,\phi]*y[r,\theta,\phi]*\left(-i\,Sin[\theta]\,Cos[\phi]\,Y1m1[\theta,\phi]\,D[R[r],r]-i\,\frac{Cos[\theta]\,Cos[\phi]}{r}\,R[r]\,D[Y1m1[\theta,\phi],\theta]+i\,\frac{Sin[\phi]}{r\,Sin[\theta]}\,R[r]\,D[Y1m1[\theta,\phi],\phi]\right)*Sin[\theta]\,d\theta\right)d\phi\right)r^2\,dr$$

0

$$\int_0^\infty R[r]\left(\int_0^{2\pi}\left(\int_0^\pi Y10[\theta,\phi]*y[r,\theta,\phi]*\left(-i\,Sin[\theta]\,Cos[\phi]\,Y10[\theta,\phi]\,D[R[r],r]-i\,\frac{Cos[\theta]\,Cos[\phi]}{r}\,R[r]\,D[Y10[\theta,\phi],\theta]+i\,\frac{Sin[\phi]}{r\,Sin[\theta]}\,R[r]\,D[Y10[\theta,\phi],\phi]\right)*Sin[\theta]\,d\theta\right)d\phi\right)r^2\,dr$$

0

$$myx=\left\{\left\{-\frac{1}{2},0,0\right\},\left\{0,\frac{1}{2},0\right\},\{0,0,0\}\right\};\ Eigensystem[myx]$$

$$\left\{\left\{-\frac{1}{2},\frac{1}{2},0\right\},\{\{1,0,0\},\{0,1,0\},\{0,0,1\}\}\right\}$$

(*************************************** x ky **)

$$\int_0^\infty R[r]\left(\int_0^{2\pi}\left(\int_0^\pi (-Y1m1[\theta,\phi])*x[r,\theta,\phi]*\left(-i\,Sin[\theta]\,Sin[\phi]\,Y11[\theta,\phi]\,D[R[r],r]-i\,\frac{Cos[\theta]\,Sin[\phi]}{r}\,R[r]\,D[Y11[\theta,\phi],\theta]-i\,\frac{Cos[\phi]}{r\,Sin[\theta]}\,R[r]\,D[Y11[\theta,\phi],\phi]\right)*Sin[\theta]\,d\theta\right)d\phi\right)r^2\,dr$$

$$\frac{1}{2}$$

$$\int_0^\infty R[r]\left(\int_0^{2\pi}\left(\int_0^\pi (-Y1m1[\theta,\phi]) * x[r,\theta,\phi] * \left(-i\,Sin[\theta]\,Sin[\phi]\,Y1m1[\theta,\phi]\,D[R[r],r] - i\,\frac{Cos[\theta]\,Sin[\phi]}{r}\,R[r]\,D[Y1m1[\theta,\phi],\theta] - i\,\frac{Cos[\phi]}{r\,Sin[\theta]}\,R[r]\,D[Y1m1[\theta,\phi],\phi]\right) * Sin[\theta]\,d\theta\right) d\phi\right) r^2\,dr$$

0

$$\int_0^\infty R[r]\left(\int_0^{2\pi}\left(\int_0^\pi (-Y1m1[\theta,\phi]) * x[r,\theta,\phi] * \left(-i\,Sin[\theta]\,Sin[\phi]\,Y10[\theta,\phi]\,D[R[r],r] - i\,\frac{Cos[\theta]\,Sin[\phi]}{r}\,R[r]\,D[Y10[\theta,\phi],\theta] - i\,\frac{Cos[\phi]}{r\,Sin[\theta]}\,R[r]\,D[Y10[\theta,\phi],\phi]\right) * Sin[\theta]\,d\theta\right) d\phi\right) r^2\,dr$$

0

$$\int_0^\infty R[r]\left(\int_0^{2\pi}\left(\int_0^\pi (-Y11[\theta,\phi]) * x[r,\theta,\phi] * \left(-i\,Sin[\theta]\,Sin[\phi]\,Y11[\theta,\phi]\,D[R[r],r] - i\,\frac{Cos[\theta]\,Sin[\phi]}{r}\,R[r]\,D[Y11[\theta,\phi],\theta] - i\,\frac{Cos[\phi]}{r\,Sin[\theta]}\,R[r]\,D[Y11[\theta,\phi],\phi]\right) * Sin[\theta]\,d\theta\right) d\phi\right) r^2\,dr$$

0

$$\int_0^\infty R[r]\left(\int_0^{2\pi}\left(\int_0^\pi (-Y11[\theta,\phi]) * x[r,\theta,\phi] * \left(-i\,Sin[\theta]\,Sin[\phi]\,Y1m1[\theta,\phi]\,D[R[r],r] - i\,\frac{Cos[\theta]\,Sin[\phi]}{r}\,R[r]\,D[Y1m1[\theta,\phi],\theta] - i\,\frac{Cos[\phi]}{r\,Sin[\theta]}\,R[r]\,D[Y1m1[\theta,\phi],\phi]\right) * Sin[\theta]\,d\theta\right) d\phi\right) r^2\,dr$$

$$-\frac{1}{2}$$

$$\int_0^\infty R[r]\left(\int_0^{2\pi}\left(\int_0^\pi (-Y11[\theta,\phi]) * x[r,\theta,\phi] * \left(-i\,Sin[\theta]\,Sin[\phi]\,Y10[\theta,\phi]\,D[R[r],r] - i\,\frac{Cos[\theta]\,Sin[\phi]}{r}\,R[r]\,D[Y10[\theta,\phi],\theta] - i\,\frac{Cos[\phi]}{r\,Sin[\theta]}\,R[r]\,D[Y10[\theta,\phi],\phi]\right) * Sin[\theta]\,d\theta\right) d\phi\right) r^2\,dr$$

0

$$\int_0^\infty R[r]\left(\int_0^{2\pi}\left(\int_0^{\pi} Y10[\theta,\phi] * x[r,\theta,\phi] * \left(-i\,Sin[\theta]\,Sin[\phi]\,Y11[\theta,\phi]\,D[R[r],r] - i\,\frac{Cos[\theta]\,Sin[\phi]}{r}\,R[r]\,D[Y11[\theta,\phi],\theta] - i\,\frac{Cos[\phi]}{r\,Sin[\theta]}\,R[r]\,D[Y11[\theta,\phi],\phi]\right) * Sin[\theta]\,d\theta\right)d\phi\right) r^2\,dr$$

0

$$\int_0^\infty R[r]\left(\int_0^{2\pi}\left(\int_0^{\pi} Y10[\theta,\phi] * x[r,\theta,\phi] * \left(-i\,Sin[\theta]\,Sin[\phi]\,Y1m1[\theta,\phi]\,D[R[r],r] - i\,\frac{Cos[\theta]\,Sin[\phi]}{r}\,R[r]\,D[Y1m1[\theta,\phi],\theta] - i\,\frac{Cos[\phi]}{r\,Sin[\theta]}\,R[r]\,D[Y1m1[\theta,\phi],\phi]\right) * Sin[\theta]\,d\theta\right)d\phi\right) r^2\,dr$$

0

$$\int_0^\infty R[r]\left(\int_0^{2\pi}\left(\int_0^{\pi} Y10[\theta,\phi] * x[r,\theta,\phi] * \left(-i\,Sin[\theta]\,Sin[\phi]\,Y10[\theta,\phi]\,D[R[r],r] - i\,\frac{Cos[\theta]\,Sin[\phi]}{r}\,R[r]\,D[Y10[\theta,\phi],\theta] - i\,\frac{Cos[\phi]}{r\,Sin[\theta]}\,R[r]\,D[Y10[\theta,\phi],\phi]\right) * Sin[\theta]\,d\theta\right)d\phi\right) r^2\,dr$$

0

$$mxy = \left\{\left\{\frac{1}{2}, 0, 0\right\}, \left\{0, -\frac{1}{2}, 0\right\}, \{0, 0, 0\}\right\};\ Eigensystem[mxy]$$

$$\left\{\left\{-\frac{1}{2}, \frac{1}{2}, 0\right\}, \{\{0, 1, 0\}, \{1, 0, 0\}, \{0, 0, 1\}\}\right\}$$

(comprovacions addicionals **)**

Eigensystem[mzy - myz]

$$\left\{\{-1, 1, 0\}, \left\{\left\{-\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}, 1\right\}, \left\{\frac{1}{\sqrt{2}}, -\frac{1}{\sqrt{2}}, 1\right\}, \{1, 1, 0\}\right\}\right\}$$

Eigensystem[mzx - mxz]

$$\left\{\{-1, 1, 0\}, \left\{\left\{-\frac{i}{\sqrt{2}}, -\frac{i}{\sqrt{2}}, 1\right\}, \left\{\frac{i}{\sqrt{2}}, \frac{i}{\sqrt{2}}, 1\right\}, \{-1, 1, 0\}\right\}\right\}$$

Eigensystem[mxy - myx]

$$\{\{-1, 1, 0\}, \{\{0, 1, 0\}, \{1, 0, 0\}, \{0, 0, 1\}\}\}$$