VRTILNA KOLIČINA II

Peter Gregorčič

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1 Naloga

V simetričen 3D harmonski oscilator ($V(x) = 1/2kr^2$) postavim elektron. Kako se razcepi 2. vzbujeno stanje v prisotnosti magnetnega polja?

2 Rešitev

Zapišem potencial v kartezičnih koordinatah:

$$V(x) = 1/2k(x^2 + y^2 + z^2) \tag{1}$$

Ker lahko potencial zapišem tako, da v vsakem členu nastopa svoja koordinata, lahko tudi valovno funkcijo zapišem kot produkt 1D valovnih funkcij:

$$\Psi(x, y, z) = X(x)Y(y)Z(z) \tag{2}$$

$$E = E(x) + E(y) + E(z) \tag{3}$$

$$E = \hbar\omega(n_x + n_y + n_z + 3/2) \tag{4}$$

To, da je elektron v 2. vzbujenem stanju, pomeni, da n = 2:

$$n = n_x + n_y + n_z \tag{5}$$

Imam torej 6 možnosti:

n_x	n_y	n_z
1	1	0
1	0	1
0	1	1
2	0	0
0	2	0
0	0	2

Še Hamiltonova funkcija za elektron v magnetnem polju:

$$H = \frac{p^2}{2m} + 1/2kr^2 - \vec{p_m}\vec{B} \tag{6}$$

Ker je vse simetrično, si lahko izberem polje B v smeri z:

$$H = \frac{p^2}{2m} + 1/2kr^2 + \frac{\mu_b}{\hbar}L_zB_z \tag{7}$$

Torej:

$$H|R > |lm >= (\hbar\omega 7/2 + \mu_b B_z\omega)|R > |lm > \tag{8}$$

Oglejmo si vseh 6 možnih stanj:

$$\Psi_{ijk}(x, y, z) = |ijk >= \Psi_i(X)\Psi_j(Y)\Psi_k(Z) \tag{9}$$

Ψ_0, Ψ_1 in Ψ_2 poznam:

$$\Psi_0 = \frac{1}{\sqrt[4]{\pi x_0^2}} \exp - \frac{x^2}{2x_0^2} \tag{10}$$

$$\Psi_1 = \Psi_0 \sqrt{2} x / x_0 \tag{11}$$

$$\Psi_2 = \Psi_0 (\sqrt{2}(x/x_0)^2 - \frac{1}{\sqrt{2}}) \tag{12}$$

Kartezične koordinate pa niso preveč ugodne za računanje, saj se izkaže, da moram računati s sfernimi harmoniki. Zato grem v sferične koordinate:

$$x = r \cos\phi \sin\theta \tag{13}$$

$$y = r \sin\phi \sin\theta \tag{14}$$

$$z = r \cos\theta \tag{15}$$

Dobim:

$$|110 >= (\pi r_0^2)^{-3/4} \exp\Big(- \frac{r^2}{2r_0^2}\Big) \frac{2}{r_0^2} r^2 \cos\phi \sin\phi \sin^2\theta \tag{16}$$

$$|101 >= (\pi r_0^2)^{-3/4} \exp\Big(- \frac{r^2}{2r_0^2}\Big) \frac{2}{r_0^2} r^2 \cos\phi \sin\theta \cos\theta \tag{17}$$

$$|011 >= (\pi r_0^2)^{-3/4} \exp\Big(- \frac{r^2}{2r_0^2}\Big) \frac{2}{r_0^2} r^2 \sin\phi \sin\theta \cos\theta \tag{18}$$

$$|200 >= (\pi r_0^2)^{-3/4} \exp\Big(- \frac{r^2}{2r_0^2}\Big) \frac{2\Big(\frac{r\cos\phi\sin\theta}{r_0}\Big)^2 - 1}{\sqrt{2}} \tag{19}$$

$$|020 >= (\pi r_0^2)^{-3/4} \exp\Big(- \frac{r^2}{2r_0^2}\Big) \frac{2\Big(\frac{r\sin\phi\sin\theta}{r_0}\Big)^2 - 1}{\sqrt{2}} \tag{20}$$

$$|002 >= (\pi r_0^2)^{-3/4} \exp\Big(- \frac{r^2}{2r_0^2}\Big) \frac{2\Big(\frac{r\cos\theta}{r_0}\Big)^2 - 1}{\sqrt{2}} \tag{21}$$

Razcep v homogenem magnetnem polju je odvisen od obhodnega kvantnega števila m_l, imam torej 5 možnosti:

$$m_l = \{-2, -1, 0, 1, 2\} \tag{22}$$

Žal funkcije (16)-(21) niso lastne za razcepljena stanja. Lastne funkcije za ta stanja so sferni harmoniki $Y_{lm} = |lm >$. Zato poskušam gornje funkcije izraziti s pomočjo |lm>. To storim tako, da najprej zapišem |ijk> kot linearno kombinacijo |lm>:

$$|ijk >= a_{00} \cdot |l_0 m_0 > \ldots a_{uv} \cdot |l_u m_v >, \tag{23}$$

kjer a_{pq} izračunam po formuli:

$$\int_0^\pi \int_0^{2\pi} < ijk | l_p m_q > sin\theta d\phi \, d\theta \tag{24}$$

Če gornjemu integralu odstranim radialni del, dobim ravno a_{pq}.

Za 2. vzbujeno stanje se izkaže, da so od nič različni koeficienti pred sfernimi harmoniki: Y_{00}, Y_{22}, Y_{21}, Y_{20}, Y_{2-1}, Y_{2-2}. Kako se posamezni sferni harmonik eksplicitno zapiše, si lahko pogleda vsak sam tako, da v Mathematici napiše ukaz $SphericalHarmonicY[l, m, \theta, \phi]$.
2. vzbujeno stanje elektrona v takem potencialu se torej razcepi v 6 novih stanj:

$|L^2, L_z >$
|2,2>
|2,1>
|2,0> in |0,0>
|2,-1>
|2,-2>

2.1 Izračun lastnih funkcij

Kot sem že napisal, funkcije (16-21) niso lastne funkcije za razcepljena stanja. Za lastne funkcije mora veljati:

$$L_z|lm >= \hbar m|lm > \tag{25}$$

Koeficiente, ki sem jih izračunal s pomočjo enačbe (24), zapišem v matriko in tako dobim sistem 6x6. Paziti moram, da so funkcije normirane:

$$\begin{pmatrix} \Psi_{011} \\ \Psi_{101} \\ \Psi_{110} \\ \Psi_{200} \\ \Psi_{020} \\ \Psi_{002} \end{pmatrix} = \begin{pmatrix} 0 & 0 & -2i\sqrt{\frac{2}{15}} & 0 & -2i\sqrt{\frac{2}{15}} & 0 \\ 0 & 0 & -2\sqrt{\frac{2}{15}} & 0 & 2i\sqrt{\frac{2}{15}} & 0 \\ 0 & 2i\sqrt{\frac{2}{15}} & 0 & 0 & 0 & -2i\sqrt{\frac{2}{15}} \\ \frac{2\sqrt{2}}{3} & \frac{2}{\sqrt{15}} & 0 & -\frac{2\sqrt{\frac{2}{5}}}{3} & 0 & \frac{2}{\sqrt{15}} \\ \frac{2\sqrt{2}}{3} & -\frac{2}{\sqrt{15}} & 0 & -\frac{2\sqrt{\frac{2}{5}}}{3} & 0 & -\frac{2}{\sqrt{15}} \\ \frac{2\sqrt{2}}{3} & 0 & 0 & \frac{4\sqrt{\frac{2}{5}}}{3} & 0 & 0 \end{pmatrix} \cdot \begin{pmatrix} Y_{00} \\ Y_{22} \\ Y_{21} \\ Y_{20} \\ Y_{2-1} \\ Y_{2-2} \end{pmatrix} \tag{26}$$

Sedaj sferne harmonike izrazim s pomočjo valovnih funkcij Ψ_{ijk}:

$$\begin{pmatrix} Y_{00} \\ Y_{22} \\ Y_{21} \\ Y_{20} \\ Y_{2-2} \\ Y_{2-1} \end{pmatrix} = A^{-1} \cdot \begin{pmatrix} \Psi_{011} \\ \Psi_{101} \\ \Psi_{110} \\ \Psi_{200} \\ \Psi_{020} \\ \Psi_{002} \end{pmatrix} \tag{27}$$

In končno dobim lastne funkcije za nova stanja:

$$\begin{pmatrix} Y_{00} \\ Y_{22} \\ Y_{21} \\ Y_{20} \\ Y_{2-1} \\ Y_{2-2} \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 & \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} \\ 0 & 0 & -\frac{i}{\sqrt{2}} & \frac{1}{2} & -\frac{1}{2} & 0 \\ \frac{i}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{1}{\sqrt{6}} & -\frac{1}{\sqrt{6}} & -\sqrt{\frac{2}{3}} \\ \frac{i}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{i}{\sqrt{2}} & \frac{1}{2} & -\frac{1}{2} & 0 \end{pmatrix} \cdot \begin{pmatrix} \Psi_{011} \\ \Psi_{101} \\ \Psi_{110} \\ \Psi_{200} \\ \Psi_{020} \\ \Psi_{002} \end{pmatrix} \tag{28}$$

3 Kako se razcepi 3. vzbujeno stanje

Za 3. vzbujeno stanje velja:

$$n = n_x +_y +_n z = 3 \tag{29}$$

Imam torej 10 možnosti:

n_x	n_y	n_z
1	1	1
2	1	0
0	2	1
1	0	2
2	0	1
1	2	0
0	1	2
3	0	0
0	3	0
0	0	3

Podobno kot za 2. vzbujeno stanje lahko izračunam:

$$\Psi_{111} = \Psi_1(X)\Psi_1(Y)\Psi_1(Z) \tag{30}$$
$$\Psi_{210} = \Psi_2(X)\Psi_1(Y)\Psi_0(Z) \tag{31}$$
$$\Psi_{021} = \Psi_0(X)\Psi_2(Y)\Psi_1(Z) \tag{32}$$
$$\Psi_{102} = \Psi_1(X)\Psi_0(Y)\Psi_2(Z) \tag{33}$$
$$\Psi_{201} = \Psi_2(X)\Psi_0(Y)\Psi_1(Z) \tag{34}$$
$$\Psi_{120} = \Psi_1(X)\Psi_2(Y)\Psi_0(Z) \tag{35}$$
$$\Psi_{012} = \Psi_0(X)\Psi_1(Y)\Psi_2(Z) \tag{36}$$
$$\Psi_{300} = \Psi_3(X)\Psi_0(Y)\Psi_0(Z) \tag{37}$$
$$\Psi_{030} = \Psi_0(X)\Psi_3(Y)\Psi_0(Z) \tag{38}$$
$$\Psi_{003} = \Psi_0(X)\Psi_0(Y)\Psi_3(Z) \tag{39}$$

V sferičnih koordinatah:

$$|111>= \frac{\sqrt{2}\exp{(\frac{-r^2}{2x_0^2})}r^3(x_0^2)^{9/4}\cos\theta\sin^2\theta\sin 2\phi}{\pi^{3/4}x_0^9} \tag{40}$$

$$|210>= -\frac{2\exp{(\frac{-r^2}{2x_0^2})}rx_0^{2/4}\sin\theta(x_0^2-r^2\cos^2\phi\sin^2\theta)\sin\phi}{\pi^{3/4}x_0^5} \tag{41}$$

$$|021>= -\frac{2\exp{(\frac{-r^2}{2x_0^2})}rx_0^{2/4}\cos\theta(x_0^2-r^2\sin^2\phi\sin^2\theta)}{\pi^{3/4}x_0^5} \tag{42}$$

$$|102>= -\frac{2\exp{(\frac{-r^2}{2x_0^2})}rx_0^{2/4}(x_0^2-r^2\cos^2\theta)\cos\phi\sin\phi}{\pi^{3/4}x_0^5} \tag{43}$$

$$|201>= -\frac{2\exp{(\frac{-r^2}{2x_0^2})}rx_0^{2/4}\cos\theta(x_0^2-r^2\cos^2\phi\sin^2\theta)}{\pi^{3/4}x_0^5} \tag{44}$$

$$|120>= -\frac{2\exp{(\frac{-r^2}{2x_0^2})}rx_0^{2/4}\cos\phi\sin\theta(x_0^2-r^2\sin^2\theta\sin^2\phi)}{\pi^{3/4}x_0^5} \tag{45}$$

$$|012>= -\frac{2\exp{(\frac{-r^2}{2x_0^2})}rx_0^{2/4}(x_0^2-r^2\cos^2\theta)\sin\theta\sin\phi}{\pi^{3/4}x_0^5} \tag{46}$$

$$|300>= \frac{\exp{(\frac{-r^2}{2x_0^2})}rx_0^{2/4}\cos\phi\sin\theta(-3x_0^2+2r^2\cos^2\phi\sin^2\theta)}{\sqrt{3}\pi^{3/4}x_0^5} \tag{47}$$

$$|030>= \frac{\exp{(\frac{-r^2}{2x_0^2})}rx_0^{2/4}\sin\phi\sin\theta(-3x_0^2+2r^2\sin^2\phi\sin^2\theta)}{\sqrt{3}\pi^{3/4}x_0^5} \tag{48}$$

$$|003>= \frac{\exp{(\frac{-r^2}{2x_0^2})}rx_0^{2/4}\cos\theta(-3x_0^2+2r^2\cos^2\theta)}{\sqrt{3}\pi^{3/4}x_0^5} \tag{49}$$

Sedaj velja:

$$H|R>|lm>=(\hbar\omega 9/2+\mu_b B_z\omega)|R>|lm> \tag{50}$$

Za obhodno kvantno število m_l, imam sedaj 7 možnosti:

$$m_l=\{-3,-2,-1,0,1,2,3\} \tag{51}$$

Razcepljena stanja in lastne funkcije izračunam enako kot pri 2. vzbujenem stanju: Valovne funkcije (40-49) izrazim s pomočjo sfernih harmoinikov. Izkaže se, da za to potrebujem: $Y_{11}, Y_{10}, Y_{1-1}, Y_{33}, Y_{32}, Y_{31}, Y_{30}, Y_{3-1}, Y_{3-2}, Y_{3-3}$. Torej se 3. vzbujeno stanje v magnetnem polju razcepi - kot smo pričakovali - na 10 novih stanj:

$|L^2, L_z>$
|3,3>
|3,2>
|3,1> in |1,1>
|3,0> in |1,0>
|3,-1> in |1,-1>
|3,-2>
|3,-3>

3.1 Izračun lastnih funkcij

Najprej valovne funkcije (40-49) izrazim s pomočjo sfernih harmonikov. Sistem 10x10 zapišem v matrični obliki:

$$\begin{pmatrix} \Psi_{111} \\ \Psi_{210} \\ \Psi_{021} \\ \Psi_{102} \\ \Psi_{201} \\ \Psi_{120} \\ \Psi_{012} \\ \Psi_{300} \\ \Psi_{030} \\ \Psi_{003} \end{pmatrix} = A \cdot \begin{pmatrix} Y_{11} \\ Y_{10} \\ Y_{1-1} \\ Y_{33} \\ Y_{32} \\ Y_{31} \\ Y_{30} \\ Y_{3-1} \\ Y_{3-2} \\ Y_{3-3} \end{pmatrix} \tag{52}$$

$$A = \begin{pmatrix}
0 & 0 & 0 & 0 & \frac{4i}{\sqrt{105}} & 0 & 0 & 0 & -\frac{4i}{\sqrt{105}} & 0 \\
-\frac{2}{5}i\sqrt{\frac{2}{3}} & 0 & -\frac{2}{5}i\sqrt{\frac{2}{3}} & -\frac{2i}{\sqrt{35}} & 0 & \frac{2i}{5sqrt21} & 0 & \frac{2i}{5\sqrt{21}} & 0 & -\frac{2i}{\sqrt{35}} \\
0 & \frac{4}{5\sqrt{3}} & 0 & 0 & -2\sqrt{\frac{2}{105}} & 0 & -\frac{4}{5\sqrt{7}} & 0 & -2\sqrt{\frac{2}{105}} & 0 \\
-\frac{2\sqrt{\frac{2}{3}}}{5} & 0 & \frac{2\sqrt{\frac{2}{3}}}{5} & 0 & 0 & -\frac{8}{5\sqrt{21}} & 0 & \frac{8}{5\sqrt{21}} & 0 & 0 \\
0 & \frac{4}{5\sqrt{3}} & 0 & 0 & 2\sqrt{\frac{2}{105}} & 0 & -\frac{4}{5\sqrt{7}} & 0 & 2\sqrt{\frac{2}{105}} & 0 \\
-\frac{2\sqrt{\frac{2}{3}}}{5} & 0 & \frac{2\sqrt{\frac{2}{3}}}{5} & \frac{2}{\sqrt{35}} & 0 & \frac{2}{5\sqrt{21}} & 0 & -\frac{2}{5\sqrt{21}} & 0 & -\frac{2}{\sqrt{35}} \\
-\frac{2}{5}i\sqrt{\frac{2}{3}} & 0 & -\frac{2}{5}i\sqrt{\frac{2}{3}} & 0 & 0 & -\frac{8}{5\sqrt{21}} & 0 & -\frac{8}{5\sqrt{21}} & 0 & 0 \\
\frac{\sqrt{2}}{5} & 0 & \frac{\sqrt{2}}{5} & -\frac{2}{\sqrt{105}} & 0 & \frac{2}{5\sqrt{7}} & 0 & -\frac{2}{5\sqrt{7}} & 0 & \frac{2}{\sqrt{105}} \\
\frac{i\sqrt{2}}{5} & 0 & \frac{i\sqrt{2}}{5} & \frac{2i}{\sqrt{105}} & 0 & \frac{2i}{5\sqrt{7}} & 0 & \frac{2i}{5\sqrt{7}} & 0 & \frac{2i}{\sqrt{105}} \\
0 & 1 & 0 & 0 & 0 & 0 & \frac{8}{5\sqrt{21}} & 0 & 0 & 0
\end{pmatrix} \tag{53}$$

Obrnem matriko A in že dobim lastne funkcije za nova stanja:

$$\begin{pmatrix} Y_{11} \\ Y_{10} \\ Y_{1-1} \\ Y_{33} \\ Y_{32} \\ Y_{31} \\ Y_{30} \\ Y_{3-1} \\ Y_{3-2} \\ Y_{3-3} \end{pmatrix} = A^{-1} \cdot \begin{pmatrix} \Psi_{111} \\ \Psi_{210} \\ \Psi_{021} \\ \Psi_{102} \\ \Psi_{201} \\ \Psi_{120} \\ \Psi_{012} \\ \Psi_{300} \\ \Psi_{030} \\ \Psi_{003} \end{pmatrix} \tag{54}$$

$$A^{-1} = \begin{pmatrix} 0 & \frac{7i}{5\sqrt{10}} & 0 & -\frac{1}{5\sqrt{10}} & 0 & -\frac{1}{5\sqrt{10}} & \frac{7i}{5\sqrt{10}} & \frac{\sqrt{\frac{3}{10}}}{5} & \frac{7}{5}i\sqrt{\frac{3}{10}} & 0 \\ 0 & 0 & \frac{1}{\sqrt{5}} & 0 & \frac{1}{\sqrt{5}} & 0 & 0 & 0 & 0 & \sqrt{\frac{3}{5}} \\ 0 & \frac{i}{\sqrt{10}} & 0 & \frac{1}{\sqrt{10}} & 0 & \frac{1}{\sqrt{10}} & \frac{i}{\sqrt{10}} & \sqrt{\frac{3}{10}} & i\sqrt{\frac{3}{10}} & 0 \\ 0 & i\sqrt{\frac{3}{62}} & 0 & i\sqrt{\frac{3}{62}} & 0 & sqrt\frac{3}{62} & -i\sqrt{\frac{3}{62}} & \frac{-5}{\sqrt{62}} & \frac{-5i}{\sqrt{62}} & 0 \\ -\frac{i}{\sqrt{2}} & 0 & -\frac{1}{2} & 0 & \frac{1}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{-7i}{\sqrt{226}} & 0 & \frac{-1}{\sqrt{226}} & 0 & \frac{1}{\sqrt{226}} & \frac{-5i}{\sqrt{226}} & \sqrt{\frac{3}{226}} & -7i\sqrt{\frac{3}{226}} & 0 \\ 0 & 0 & -5\sqrt{\frac{3}{214}} & 0 & 5\sqrt{\frac{3}{214}} & 0 & 0 & 0 & 0 & 4\sqrt{\frac{2}{107}} \\ 0 & -\frac{i}{\sqrt{10}} & 0 & \frac{1}{\sqrt{10}} & 0 & -\frac{1}{\sqrt{10}} & \frac{i}{\sqrt{10}} & -\sqrt{\frac{3}{10}} & -i\sqrt{\frac{3}{10}} & 0 \\ \frac{i}{\sqrt{2}} & 0 & -\frac{1}{2} & 0 & \frac{1}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{9}{7}i\sqrt{\frac{3}{38}} & 0 & \frac{\sqrt{\frac{3}{38}}}{7} & 0 & -\frac{\sqrt{\frac{3}{38}}}{7} & -\frac{11}{7}i\sqrt{\frac{3}{38}} & \frac{5}{7\sqrt{38}} & -i\frac{5}{7\sqrt{38}} & 0 \end{pmatrix} \tag{55}$$