Kvantna mehanika I

Spin V

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Delca s spinoma $S_1 = 1$ in $S_2 = 1/2$ sta slopljena z anziotropno Heissenbergovo interakcijo $H = -J\mathbf{S_1} \cdot \mathbf{S_2} + hS_{1z}S_{2z}$. Poišči lastna stanja sistema tako, da obravnavaš h kot parameter motnje. Ta rezultat primerjaj s točnim izračunom.

$$\begin{array}{lllll} |s\,m\rangle & & & & \\ \frac{1}{2} & -\frac{1}{2} & \frac{1}{2} & & \\ \frac{3}{2} & -\frac{3}{2} & -\frac{1}{2} & \frac{1}{2} & \frac{3}{2} \end{array} \tag{1}$$

Prvo zračunajmo energije nezmotenega sistema $H_0 = -J\mathbf{S_1} \cdot \mathbf{S_2}$. Upoštevamo:

$$S^2 = (\mathbf{S_1} + \mathbf{S_2})^2 = S_1^2 + 2\mathbf{S_1} \cdot \mathbf{S_2} + S_2^2 \tag{2}$$

$$\mathbf{S_1} \cdot \mathbf{S_2} = \frac{1}{2}(S^2 - S_1^2 - S_2^2) \tag{3}$$

$$H_0 = J\frac{1}{2}(S_1^2 + S_2^2 - S^2) \tag{4}$$

$$H_0|s\,m\rangle = E^0|s\,m\rangle \tag{5}$$

Tako zapišemo energije:

$$E^0 = \frac{J\hbar^2}{2}\big(S_1(S_1+1) + S_2(S_2+1) - S(S+1)\big) \tag{6}$$

$$E^0 = \frac{J\hbar^2}{2}\big(\frac{11}{4} - S(S+1)\big) \tag{7}$$

Za spin 1/2 dobimo:

$$E^0_{1/2} = \frac{J\hbar^2}{2} \cdot 2 = J\hbar^2 \ , \quad \text{2x deg.} \tag{8}$$

in za spin 3/2:

$$E^0_{3/2} = \frac{J\hbar^2}{2} \cdot (-\frac{4}{4}) = -\frac{J\hbar^2}{2} \ , \quad \text{4x deg.} \tag{9}$$

S pomočjo Clebsch–Gordan koeficientov zapišemo produktno bazo za spina $S_1 = 1$ in $S_2 = 1/2$, kjer za lažjo pisavo upoštevamo:

$$|s\,m\rangle = |s_1\,m_1\rangle|s_2\,m_2\rangle = |m_1\,m_2\rangle \tag{10}$$

$$|\frac{3}{2}\frac{3}{2}\rangle = |11\rangle|\frac{1}{2}\frac{1}{2}\rangle = |1\,\frac{1}{2}\rangle \tag{11}$$

$$|\frac{3}{2}\frac{1}{2}\rangle = \frac{1}{\sqrt{3}}|1\,-\frac{1}{2}\rangle + \sqrt{\frac{2}{3}}|0\,\frac{1}{2}\rangle \tag{12}$$

$$|\frac{1}{2}\,\frac{1}{2}\rangle = \sqrt{\frac{2}{3}}|1\,-\frac{1}{2}\rangle - \sqrt{\frac{1}{3}}|0\,\frac{1}{2}\rangle \tag{13}$$

$$|\frac{3}{2}\,-\frac{1}{2}\rangle = \sqrt{\frac{2}{3}}|0\,-\frac{1}{2}\rangle + \sqrt{\frac{1}{3}}|-1\,\frac{1}{2}\rangle \tag{14}$$

$$|\frac{1}{2}\,-\frac{1}{2}\rangle = \sqrt{\frac{1}{3}}|0\,-\frac{1}{2}\rangle - \sqrt{\frac{2}{3}}|-1\,\frac{1}{2}\rangle \tag{15}$$

$$|\frac{3}{2}\,-\frac{3}{2}\rangle = |-1\,-\frac{1}{2}\rangle \tag{16}$$

Motnja je $H' = hS_{z1}S_{z2}$. Element matrike, katere lastne vrednosti nam predstavljajo popravke k energijam nemotenega sistema, zapišemo:

$$\langle s\,m|H'|s'\,m'\rangle = \langle s\,m|hS_{z1}S_{z2}|s'\,m'\rangle \tag{17}$$

Pri tem uporabimo

$$S_z|s\,m\rangle = \hbar m|s\,m\rangle \tag{18}$$

in zvezo, ki smo jo izpeljali tudi na vajah:

$$\langle s\,m|H'|s'\,m'\rangle(m'-m)\hbar = 0 \tag{19}$$

Od tu vidimo, da morajo biti vsi matrični elementi, ki imajo različna m in m' enaki nič. Ostale pa poračunamo takole:

$$\langle\frac{3}{2}\frac{3}{2}|H'|\frac{3}{2}\frac{3}{2}\rangle = h\langle 1\frac{1}{2}|S_{z1}S_{z2}|1\frac{1}{2}\rangle = h\,\hbar\,1\,\hbar\frac{1}{2} = h\,\hbar^2\frac{1}{2} \tag{20}$$

kjer smo upoštevali računali v produktni bazi. Za lažjo orientacijo v spodnjih matrikah pišemo celoten spin in njegovo projekcijo. Za spin 1/2 je perturbacijska matrika:

$$h\,\hbar^2\,\cdot \begin{bmatrix} & |\frac{1}{2}\,\frac{1}{2}\rangle & |\frac{1}{2}\,-\frac{1}{2}\rangle \\ |\frac{1}{2}\,\frac{1}{2}\rangle & -1/3 & 0 \\ |\frac{1}{2}\,-\frac{1}{2}\rangle & 0 & -1/3 \end{bmatrix} \tag{21}$$

Z lastnimi vrednostmi:

$$\varepsilon_{1,2} = -\frac{h\,\hbar^2}{3} \tag{22}$$

Popravljeni energiji:

$$E_{1,2} = E^0_{1/2} + \varepsilon_{1,2} = \hbar^2(J - \frac{h}{3})\,, \quad \text{2x deg.} \tag{23}$$

Za spin 3/2 je perturbacijska matrika:

$$h\,\hbar^2\,\cdot \begin{bmatrix} & |\frac{3}{2}\,\frac{3}{2}\rangle & |\frac{3}{2}\,\frac{1}{2}\rangle & |\frac{3}{2}\,-\frac{1}{2}\rangle & |\frac{3}{2}\,-\frac{3}{2}\rangle \\ |\frac{3}{2}\,\frac{3}{2}\rangle & 1/2 & 0 & 0 & 0 \\ |\frac{3}{2}\,\frac{1}{2}\rangle & 0 & -1/6 & 0 & 0 \\ |\frac{3}{2}\,-\frac{1}{2}\rangle & 0 & 0 & -1/6 & 0 \\ |\frac{3}{2}\,-\frac{3}{2}\rangle & 0 & 0 & 0 & 1/2 \end{bmatrix} \tag{24}$$

Z lastnimi vrednostmi:

$$\varepsilon_{3,4} = \frac{h\,\hbar^2}{2} \quad \text{in} \quad \varepsilon_{5,6} = -\frac{h\,\hbar^2}{6} \tag{25}$$

Popravljene energije:

$$E_{3,4} = E^0_{3/2} + \varepsilon_{3,4} = \frac{\hbar^2}{2}(h - J)\ , \quad \text{2x deg.} \tag{26}$$

$$E_{5,6} = E^0_{3/2} + \varepsilon_{5,6} = -\frac{\hbar^2}{2}(J + \frac{h}{3})\ , \quad \text{2x deg.} \tag{27}$$

Pri točnem računu pa poiščemo lastne vrednosti matrike katere lastne vrednosti predstavljajo elementi:

$$\langle s\, m|H|s'\, m'\rangle = \langle s\, m|H_0|s\, m\rangle + \langle s\, m|H'|s'\, m'\rangle \tag{28}$$

Tokrat zapišemo za vse spine skupaj.

$$\begin{array}{cccccc}
|\frac{3}{2}\,\frac{3}{2}\rangle & |\frac{3}{2}\,\frac{1}{2}\rangle & |\frac{1}{2}\,\frac{1}{2}\rangle & |\frac{3}{2}\,-\frac{1}{2}\rangle & |\frac{1}{2}\,-\frac{1}{2}\rangle & |\frac{3}{2}\,-\frac{3}{2}\rangle
\end{array}$$

$$\begin{bmatrix}
\frac{h\hbar^2}{2} - \frac{J\hbar^2}{2} & 0 & 0 & 0 & 0 & 0 \\
0 & -\frac{h\hbar^2}{6} - \frac{J\hbar^2}{2} & -\frac{\sqrt{2}h\hbar^2}{6} & 0 & 0 & 0 \\
0 & -\frac{\sqrt{2}h\hbar^2}{6} & -\frac{h\hbar^2}{3} + J\hbar^2 & 0 & 0 & 0 \\
0 & 0 & 0 & -\frac{h\hbar^2}{6} - \frac{J\hbar^2}{2} & \frac{\sqrt{2}h\hbar^2}{6} & 0 \\
0 & 0 & 0 & \frac{\sqrt{2}h\hbar^2}{6} & -\frac{h\hbar^2}{3} + J\hbar^2 & 0 \\
0 & 0 & 0 & 0 & 0 & \frac{h\hbar^2}{2} - \frac{J\hbar^2}{2}
\end{bmatrix} \tag{29}$$

Karakteristični polinom je tokrat:

$$\left(\frac{\hbar^2}{2}(h - J) - \lambda\right)^2 \left(\lambda^2 + \lambda\frac{\hbar^2}{2}(h - J) - \frac{J^2\hbar^4}{2}\right)^2 = 0 \tag{30}$$

Rešitve drugega oklepaja so

$$\lambda = \frac{1}{2}\left(\frac{\hbar^2}{2}(J - h) \pm \sqrt{\frac{\hbar^4}{4}(h - J)^2 + 2J^2\hbar^4}\right) \tag{31}$$

Tako dobimo energije:

$$E_{1,2} = \frac{\hbar^2}{4}\left((J - h) + \sqrt{(h - J)^2 + 8J^2}\right)\ , \quad \text{2x deg.} \tag{32}$$

$$E_{3,4} = \frac{\hbar^2}{2}(h - J)\ , \quad \text{2x deg.} \tag{33}$$

$$E_{5,6} = \frac{\hbar^2}{4}\left((J - h) - \sqrt{(h - J)^2 + 8J^2}\right)\ , \quad \text{2x deg.} \tag{34}$$

Vidimo, da je točna vrednost energije $E_{3,4}$ enaka tisti dobljeni z perturbacijo. Preverimo še za ostala dva para energiji tako, da koren razvijemo okoli motnje do prvega reda:

$$\sqrt{(h - J)^2 + 8J^2} = 3J\sqrt{1 - \frac{2h}{9J} + \frac{h^2}{9J^2}} \approx 3J\left(1 - \frac{h}{9J}\right) = 3J - \frac{h}{3} \tag{35}$$

$$E_{1,2} \approx \frac{\hbar^2}{4}\left((J - h) + (3J - \frac{h}{3})\right) = \hbar^2(J - \frac{h}{3}) \tag{36}$$

$$E_{5,6} \approx \frac{\hbar^2}{4}\left((J - h) - (3J - \frac{h}{3}\right) = -\frac{\hbar^2}{2}(J + \frac{h}{3}) \tag{37}$$