# Degenerirane perturbacije V

Vito Plahuta

## Navodilo:

Obravnavaj lastna stanja dveh delcev s spinom 1/2 in Hamiltonianom:

$$\mathrm{H} = \mathrm{J}\mathbf{S}_1 \cdot \mathbf{S}_2 + \frac{g\mu_b}{\hbar}\mathbf{S}_1 \cdot \mathbf{B}$$

1. točno,
2. perturbativno v limiti, ko je sklopitev med spini J majhna.

## Točni izračun

Najprej pogledamo Hamiltonijan.

Malce poenostavimo ($\gamma = \frac{g\mu_B}{\hbar}B$), pravtako postavimo magnetno polje v z-smer

$$\frac{g\mu_b}{\hbar}\mathbf{S}_1 \cdot \mathbf{B} = \gamma S_{1z}$$

Sedaj nas zanima še

$$2\mathbf{S}_1 \cdot \mathbf{S}_2 = (\mathbf{S}_1 + \mathbf{S}_2)^2 - \mathbf{S}_1^2 - \mathbf{S}_2^2$$

Vemo, da lahko zapišemo $\mathbf{S} = \mathbf{S}_1 + \mathbf{S}_2$ in upoštevamo $\mathbf{S}_i^2 = \hbar^2 S_i\left(S_i + 1\right)$ter vrednosti spinov, dobimo:

$$\mathbf{S}_1 \cdot \mathbf{S}_2 = \frac{1}{2}\left(\mathrm{S}^2 - \frac{3}{2}\hbar^2\right)$$

Lastna stanja operatorja $\mathrm{S}^2$so $|l, m\rangle$, lastna stanja $\mathbf{S}_1$pa $|s_1, s_2\rangle$, rešujmo v bazi $|s_1, s_2\rangle$:

$$|\uparrow\downarrow\rangle = \frac{1}{\sqrt{2}}\left(|10\rangle + |10\rangle\right)$$

$$|\uparrow\uparrow\rangle = |11\rangle$$

$$\left|\downarrow\uparrow\right\rangle = \frac{1}{\sqrt{2}}\left(\left|10\right\rangle - \left|00\right\rangle\right)$$

$$\left|\downarrow\downarrow\right\rangle = \left|1-1\right\rangle$$

Sedaj izračunajmo še lastne energije - delujmo na funkcije z Hamiltonijanom $H\left|\psi\right\rangle = E\left|\psi\right\rangle$:

$$H\left|\uparrow\uparrow\right\rangle = \left(\frac{1}{4}J\hbar^2 + \frac{1}{2}\gamma\hbar\right)\left|\uparrow\uparrow\right\rangle$$

$$H\left|\downarrow\downarrow\right\rangle = \left(\frac{1}{4}J\hbar^2 - \frac{1}{2}\gamma\hbar\right)\left|\downarrow\downarrow\right\rangle$$

$$H\left|\uparrow\downarrow\right\rangle = \left(-\frac{1}{2}J\hbar^2 + \frac{1}{2}\gamma\hbar\right)\left|\uparrow\downarrow\right\rangle + \frac{1}{4}J\hbar^2\left|\downarrow\uparrow\right\rangle$$

$$H\left|\downarrow\uparrow\right\rangle = \left(-\frac{1}{2}J\hbar^2 - \frac{1}{2}\gamma\hbar\right)\left|\downarrow\uparrow\right\rangle + \frac{1}{4}J\hbar^2\left|\uparrow\downarrow\right\rangle$$

Pri zadnjih dveh je bazna funkcija sestavljena iz linearne kombinacije dveh funkcij, torej bo potrebno še malo računanja, da dobimo vse lastne vrednosti:

$$\begin{vmatrix} \left(-\frac{1}{2}J\hbar^2 + \frac{1}{2}\gamma\hbar\right) - E & \frac{1}{4}J\hbar^2 \\ \frac{1}{4}J\hbar^2 & \left(-\frac{1}{2}J\hbar^2 - \frac{1}{2}\gamma\hbar\right) - E \end{vmatrix} = 0$$

$$E = -\frac{1}{2}J\hbar^2 \pm \sqrt{\left(\frac{1}{4}J\hbar^2\right)^2 + \left(\gamma\frac{\hbar}{2}\right)^2} \sim -\frac{1}{2}J\hbar^2 \pm \frac{1}{2}\gamma\hbar$$

V našem primeru imamo majhen $J$ , zato lahko ustrezno razvijemo po Taylorju (do prvega reda).

# Perturbacija

Hamiltonijan lahko zapišemo kot:

$$H = H_0 + \lambda H_1$$

V našem primeru je $J$ majhen, ker perturbacija velja le za majhe motnje bo veljalo $\lambda = J$ in $H_0 = \frac{g\mu_b}{\hbar}\mathbf{S}_1 \cdot \mathbf{B}$ in $H_1 = \mathbf{S}_1 \cdot \mathbf{S}_2$. Najprej pogledamo neperturbiran primer $J = 0$:

Poglejmo energije stanj:

$$H_0 \left|\uparrow\uparrow\right\rangle = \gamma \frac{\hbar}{2} \left|\uparrow\uparrow\right\rangle$$

$$H_0 \left|\downarrow\downarrow\right\rangle = -\gamma \frac{\hbar}{2} \left|\downarrow\downarrow\right\rangle$$

$$H_0 \left|\uparrow\downarrow\right\rangle = \gamma \frac{\hbar}{2} \left|\uparrow\downarrow\right\rangle$$

$$H_0 \left|\downarrow\uparrow\right\rangle = -\gamma \frac{\hbar}{2} \left|\downarrow\uparrow\right\rangle$$

Vidimo, da bomo 2x uporabili perturbacijo za degenerirana stanja, to so popravki prvega reda:

$$\begin{vmatrix} \left\langle\uparrow\uparrow\right| J\mathbf{S}_1 \cdot \mathbf{S}_2 \left|\uparrow\uparrow\right\rangle - E & \left\langle\uparrow\uparrow\right| J\mathbf{S}_1 \cdot \mathbf{S}_2 \left|\uparrow\downarrow\right\rangle \\ \left\langle\uparrow\downarrow\right| J\mathbf{S}_1 \cdot \mathbf{S}_2 \left|\uparrow\uparrow\right\rangle & \left\langle\uparrow\downarrow\right| J\mathbf{S}_1 \cdot \mathbf{S}_2 \left|\uparrow\downarrow\right\rangle - E \end{vmatrix} = 0$$

$$\begin{vmatrix} \left(\frac{1}{4}J\hbar^2 + \frac{1}{2}\gamma\hbar\right) - E & 0 \\ 0 & \left(-\frac{1}{2}J\hbar^2 + \frac{1}{2}\gamma\hbar\right) - E \end{vmatrix} = 0$$

Še za drugi dve stanji:

$$\begin{vmatrix} \left\langle\downarrow\downarrow\right| J\mathbf{S}_1 \cdot \mathbf{S}_2 \left|\downarrow\downarrow\right\rangle - E & \left\langle\downarrow\downarrow\right| J\mathbf{S}_1 \cdot \mathbf{S}_2 \left|\downarrow\uparrow\right\rangle \\ \left\langle\downarrow\uparrow\right| J\mathbf{S}_1 \cdot \mathbf{S}_2 \left|\downarrow\downarrow\right\rangle & \left\langle\downarrow\uparrow\right| J\mathbf{S}_1 \cdot \mathbf{S}_2 \left|\downarrow\uparrow\right\rangle - E \end{vmatrix} = 0$$

$$\begin{vmatrix} \left(\frac{1}{4}J\hbar^2 - \frac{1}{2}\gamma\hbar\right) - E & 0 \\ 0 & \left(-\frac{1}{2}J\hbar^2 - \frac{1}{2}\gamma\hbar\right) - E \end{vmatrix} = 0$$

Zaradi ortonormiranosti nam ostanejo le diagonalni elementi, primerjava s točnimi izračuni energije se ujema.