

Problem lahko zapišemo tudi s Pavljevimi matrikami. Če imamo spin $S = 1/2$, lahko zapišemo:

$$\vec{\sigma} = \frac{\hbar}{2} \vec{\sigma}, \quad \vec{S} = (S_x, S_y, S_z)$$

kjer je \vec{S} vektor Pavljevih matrik:

$$\vec{\sigma} = \left(\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \right)$$

V bazi x, y, z komponente vektorja $\vec{\sigma}$ zapišemo kot (npr σ_y):

$$\sigma_y = \frac{2}{\hbar} \begin{bmatrix} \langle \uparrow | S_y | \uparrow \rangle & \langle \uparrow | S_y | \downarrow \rangle \\ \langle \downarrow | S_y | \uparrow \rangle & \langle \downarrow | S_y | \downarrow \rangle \end{bmatrix}$$

Če spin opišemo z linearno kombinacijo $\alpha |\uparrow\rangle + \beta |\downarrow\rangle$, lahko v tej bazi to zapišemo kot vektor, imenovan spinor:

$$\alpha |\uparrow\rangle + \beta |\downarrow\rangle = \begin{pmatrix} \alpha \\ \beta \end{pmatrix}$$

Primer:

$$\begin{aligned} H &= \frac{p^2}{2m} + \lambda \left(p_x \frac{\hbar}{2} \sigma_y - p_y \frac{\hbar}{2} \sigma_x \right) \\ H \left[e^{i \vec{k} \cdot \vec{r}} \right] &= \frac{\hbar^2 k^2}{2m} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} e^{-i \vec{k} \cdot \vec{r}} + \lambda \left(\frac{\hbar^2 k_x}{2} \begin{bmatrix} -i \\ i \end{bmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} - \frac{\hbar^2 k_y}{2} \begin{bmatrix} 1 \\ -1 \end{bmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} \right) e^{i \vec{k} \cdot \vec{r}} \\ &= \begin{bmatrix} \frac{\hbar^2 k_x^2}{2m} & \frac{\lambda \hbar^2}{2} (-ik_x - k_y) \\ \frac{\lambda \hbar^2}{2} (ik_x - k_y) & \frac{\hbar^2 k_y^2}{2m} \end{bmatrix} e^{i \vec{k} \cdot \vec{r}} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} \end{aligned}$$

Sipanje delca na δ potencialu Bodí $S_1 = 1/2$ ($|\uparrow\rangle$), $S_2 = 1$ ($|1, 0\rangle$). Delec (2) stoji pri $x = 0$, ¹ delec (1) pa leti mimo njega. Imamo Hamiltonian:

$$H = \frac{p_1^2}{2m} - \frac{\lambda}{\hbar^2} \delta(x_1) \vec{S}_1 \cdot \vec{S}_2$$

Zanima nas, kakšen je spin delca (1) po sipanju in s kakšno verjetnostjo se pri sisanju spremeni.

Za delta potencial vemo:

$$\psi_0(x) = \sqrt{\kappa_0} e^{-\kappa_0|x|}$$

Tu je $\kappa_0 = m\lambda/\hbar^2$. Lastna energija tega stanja je

$$E_0 = \frac{\hbar^2 \kappa_0^2}{2m}$$

Zapišemo tudi

$$S = \begin{pmatrix} r & t' \\ t & r' \end{pmatrix} = \frac{1}{k + i\kappa_0} \begin{pmatrix} -i\kappa_0 & k \\ k & -i\kappa_0 \end{pmatrix}, \quad k = \sqrt{\frac{2mE}{\hbar^2}}$$

Problem moramo opisati v nekakšni bazi: imamo dve možnosti. Produktno bazo določajo vektorji

$$\begin{array}{ll} |\uparrow\rangle |1, 1\rangle & |\downarrow\rangle |1, 1\rangle \\ |\uparrow\rangle |1, 0\rangle & |\downarrow\rangle |1, 0\rangle \\ |\uparrow\rangle |1, -1\rangle & |\downarrow\rangle |1, -1\rangle \end{array}$$

V tej bazi imajo operatorji $S_1^2, S_{1z}, S_2^2, S_{2z}$ skupne lastne vrednosti.

Baza z dobrim skupnim spinom je baza vektorja

$$\vec{S} = \vec{S}_1 + \vec{S}_2$$

¹Privzamemo, da se odmika dovolj malo, da na naš problem to ne vpliva - sicer bi kršili Heisenbergovo nedoločenost.

V njej imajo operatorji S^2, S_1^2, S_2^2, S_z iste lastne vrednosti.

Izbira baze na rešitev ne bo vplivala, lahko pa nam poenostavi računanje.

Clebsch-Gordanovi koeficienti za spina 1 in 1/2 nam omogočajo prehod med bazama:

$$|\downarrow\rangle|1,1\rangle = \sqrt{\frac{1}{3}}\left|\frac{3}{2}, \frac{1}{2}\right\rangle + \sqrt{\frac{2}{3}}\left|\frac{1}{2}, \frac{1}{2}\right\rangle$$

$$|\downarrow\rangle|1,0\rangle = \sqrt{\frac{2}{3}}\left|\frac{3}{2}, \frac{1}{2}\right\rangle - \sqrt{\frac{1}{3}}\left|\frac{1}{2}, \frac{1}{2}\right\rangle$$

Ali obratno:

$$\left|\frac{3}{2}, \frac{1}{2}\right\rangle = \sqrt{\frac{1}{3}}|\downarrow\rangle|1,1\rangle + \sqrt{\frac{2}{3}}|\uparrow\rangle|1,0\rangle$$

$$\left|\frac{1}{2}, \frac{1}{2}\right\rangle = \sqrt{\frac{2}{3}}|\downarrow\rangle|1,1\rangle - \sqrt{\frac{1}{3}}|\uparrow\rangle|1,0\rangle$$

Kaj lahko ugotovimo na podlagi simetrije problema? Vemo:

$$\vec{S}_1 \cdot \vec{S}_2 = S^2 - S_1^2 - S_2^2$$

$$H = \frac{p_1^2}{2m} - \frac{\lambda}{2\hbar^2}(S^2 - S_1^2 - S_2^2)$$

Velja, da operatorji S^2, S_1^2, S_2^2, S_z , in tudi H , saj je linearna kombinacija prvih štirih, komutirajo. To pomeni, da lahko celotno valovno funkcijo zapišemo kot

$$|\Psi\rangle = |\psi\rangle|sm\rangle$$

Če uporabimo bazo z dobrim skupnim spinom, si torej iskanje valovne funkcije lahko poenostavimo z zgornjim nastavkom.

$$\left(\frac{p_1^2}{2m}|\psi\rangle\right)|sm\rangle - \frac{\lambda}{2\hbar^2}\delta(x)|\psi\rangle(S^2|sm\rangle - S_1^2|sm\rangle - S_2^2|sm\rangle) = E|\psi\rangle|sm\rangle$$

Ker so S^2, S_1^2, S_2^2 lastna stanja ψ , jih lahko nadomestimo z njihovimi lastnimi vrednostmi, nakar na $|sm\rangle$ ne deluje noben operator več - se pravi lahko računamo samo krajevni del:

$$\frac{p_1^2}{2m}|\psi\rangle|sm\rangle - \frac{\lambda}{2\hbar^2}\delta(x)|\psi\rangle(\hbar^2 s(s+1) - \hbar^2 s_1(s_1+1) - \hbar^2 s_2(s_2+1))|sm\rangle = E|\psi\rangle|sm\rangle$$

$$\frac{p_1^2}{2m}|\psi\rangle + \frac{\lambda}{2\hbar^2}(\hbar^2 s(s+1) - \hbar^2 s_1(s_1+1) - \hbar^2 s_2(s_2+1))\delta(x)|\psi\rangle = E|\psi\rangle$$

Seveda je $s_1 = 1/2$ in $s_2 = 1$. Vprašanje je le, kakšen je skupni spin:

$$s = \frac{3}{2} : \quad \frac{p_1^2}{2m}|\psi\rangle - \frac{\lambda}{2}\delta(x)|\psi\rangle = E|\psi\rangle$$

$$s = \frac{1}{2} : \quad \frac{p_1^2}{2m}|\psi\rangle + \lambda\delta(x)|\psi\rangle = E|\psi\rangle$$

Ta dva primera nam data dve možni spialni matriki: $S(\lambda/2)$ za $s = 3/2$ in $S(-\lambda)$ za $s = 1/2$.

$$S(\lambda/2) = \begin{pmatrix} r_{3/2} & t'_{3/2} \\ t_{3/2} & r_{3/2} \end{pmatrix}$$

$$S(-\lambda) = \begin{pmatrix} r_{1/2} & t'_{1/2} \\ t_{1/2} & r_{1/2} \end{pmatrix}$$

$$\psi_{3/2, 1/2}(x < 0) = (e^{ikx} + r_{3/2}e^{-ikx})\left|\frac{3}{2}, \frac{1}{2}\right\rangle$$

$$\psi_{3/2, 1/2}(x > 0) = t_{3/2}e^{ikx}\left|\frac{3}{2}, \frac{1}{2}\right\rangle$$

$$\begin{aligned}\psi_{1/2, 1/2}(x < 0) &= (e^{ikx} + r_{1/2}e^{-ikx}) \left| \frac{1}{2}, \frac{1}{2} \right\rangle \\ \psi_{1/2, 1/2}(x > 0) &= t_{1/2}e^{ikx} \left| \frac{1}{2}, \frac{1}{2} \right\rangle\end{aligned}$$

Sestavimo $\psi(x)$ tako, da se ujema z začetnim stanjem:

$$\psi(x) = \sqrt{\frac{2}{3}}\psi_{3/2, 1/2}(x) - \sqrt{\frac{1}{3}}\psi_{1/2, 1/2}(x)$$

Preostane nam le, da rešitev izrazimo v primerni bazi:

$$\begin{aligned}\psi(x > 0) &= e^{ikx} |\uparrow\rangle |1, 0\rangle + e^{-ikx} \left[|\downarrow\rangle |1, 1\rangle \left(\frac{\sqrt{2}}{3}r_{3/2} - \frac{\sqrt{2}}{3}r_{1/2} \right) + |\uparrow\rangle |1, 0\rangle \left(\frac{2}{3}r_{3/2} + \frac{1}{3}r_{1/2} \right) \right] \\ \psi(x > 0) &= e^{ikx} \left[|\downarrow\rangle |1, 1\rangle \left(\frac{\sqrt{2}}{3}t_{3/2} - \frac{\sqrt{2}}{3}t_{1/2} \right) + |\uparrow\rangle |1, 0\rangle \left(\frac{2}{3}t_{3/2} + \frac{1}{3}t_{1/2} \right) \right]\end{aligned}$$

Označimo:

$$\begin{aligned}r_{\downarrow\uparrow} &= \frac{\sqrt{2}}{3}r_{3/2} - \frac{\sqrt{2}}{3}r_{1/2} \\ r_{\uparrow\uparrow} &= \frac{2}{3}r_{3/2} + \frac{2}{3}r_{1/2} \\ r_{\downarrow\uparrow} &= \frac{\sqrt{2}}{3}t_{3/2} - \frac{\sqrt{2}}{3}t_{1/2} \\ r_{\uparrow\uparrow} &= \frac{2}{3}t_{3/2} + \frac{2}{3}t_{1/2}\end{aligned}$$

Tako smo dobili rešitev:

$$\begin{aligned}R_{\downarrow\uparrow} &= |r_{\downarrow\uparrow}|^2 \\ R_{\uparrow\uparrow} &= |r_{\uparrow\uparrow}|^2 \\ T_{\downarrow\uparrow} &= |t_{\downarrow\uparrow}|^2 \\ T_{\uparrow\uparrow} &= |t_{\uparrow\uparrow}|^2\end{aligned}$$

Nazadnje lahko preverimo, da je $R_{\downarrow\uparrow} + R_{\uparrow\uparrow} + T_{\downarrow\uparrow} + T_{\uparrow\uparrow} = 1$. Večina členov se med sabo odšteje, ostane

$$R_{\downarrow\uparrow} + R_{\uparrow\uparrow} + T_{\downarrow\uparrow} + T_{\uparrow\uparrow} = \frac{2}{9}|r_{3/2}|^2 + \frac{2}{9}|r_{1/2}|^2 + \frac{4}{9}|r_{3/2}|^2 + \frac{1}{9}|r_{1/2}|^2 + \frac{2}{9}|t_{3/2}|^2 + \frac{2}{9}|t_{1/2}|^2 + \frac{4}{9}|t_{3/2}|^2 + \frac{1}{9}|t_{1/2}|^2$$

Upoštevamo: $|r_i|^2 + |t_i|^2 = 1$.

$$R_{\downarrow\uparrow} + R_{\uparrow\uparrow} + T_{\downarrow\uparrow} + T_{\uparrow\uparrow} = \frac{2}{9} + \frac{4}{9} + \frac{2}{9} + \frac{1}{9} = 1$$