KT1 4. 10. 2022 OPAKOVÁNÍ

⓪ JEDNOTKY

① LHO

(I) klasicky $H = T + V = \frac{p^2}{2m} + \frac{1}{2} m\omega^2 x^2$

$\Downarrow$

kvantově $\hat{H} = \hat{T} + \hat{V} = \frac{\hat{p}^2}{2m} + \frac{1}{2} m\omega^2 \hat{x}^2$

a platí $[\hat{x}, \hat{p}] = i\hbar$

$\Downarrow$

přeškálování $\Rightarrow$ $\underline{\underline{\hat{H} = \frac{\hat{p}^2}{2} + \frac{\hat{x}^2}{2}}}$ $[\hat{x}, \hat{p}] = i$

(II) $E_n = n + \frac{1}{2}$

$\left(E_n = \hbar\omega \left(n + \frac{1}{2}\right) \right)$

(III) $\hat{a} = \frac{1}{\sqrt{2}}(\hat{x} + i\hat{p})$ snižující op.

$\hat{a}^+ = \frac{1}{\sqrt{2}}(\hat{x} - i\hat{p})$ zvyšující op.

$[a, a^+] = 1$

(IV) $H = a^+a + \frac{1}{2}$

(V) $\underline{\underline{[a, a^+]}} = \left[\frac{1}{\sqrt{2}}(x + ip), \frac{1}{\sqrt{2}}(x - ip)\right] =$

$= \frac{1}{2}\left\{\underbrace{[x, x]}_{=0} + i\underbrace{[p, x]}_{=-i} - i\underbrace{[x, p]}_{=i} + \underbrace{[p, p]}_{=0}\right\} =$

$$= \frac{1}{2}\{1+1\} =$$

$$= \underline{\underline{1}}$$

$$\underline{\underline{[H, a]}} = [a^+a + \tfrac{1}{2}, a] =$$

$$= [a^+a, a] + \underbrace{[\tfrac{1}{2}, a]}_{=0} =$$

$$= a^+\underbrace{[a, a]}_{=0} + \underbrace{[a^+, a]}_{=-1}a =$$

$$= \underline{\underline{-a}}$$

$$\underline{\underline{[H, a^+]}} = [a^+a + \tfrac{1}{2}, a^+] =$$

$$= a^+\underbrace{[a, a^+]}_{=1} =$$

$$= \underline{\underline{a^+}}$$

(VI) $a|n\rangle = \sqrt{n}\,|n-1\rangle$

$a^+|n\rangle = \sqrt{n+1}\,|n+1\rangle$

(VII) $|\Psi\rangle = N(\,|0\rangle + 3|1\rangle + |2\rangle)$

normalizace:

$$\langle\Psi|\Psi\rangle = N^2\left(\langle 0| + 3\langle 1| + \langle 2|\right)\left(|0\rangle + 3|1\rangle + |2\rangle\right) =$$

$$= N^2\Big(\underbrace{\langle 0|0\rangle}_{=1} + 9\overbrace{\langle 1|1\rangle}^{=1} + \overbrace{\langle 2|2\rangle}^{=1} + \text{ ostatní členy } = 0\Big)$$

$$= N^2(1+9+1)$$

$$= 11N^2 \doteq 1$$

$$\Rightarrow N = \frac{1}{\sqrt{11}}$$

$\sim \quad \frac{1}{11}$

(VIII) $P_0 = |\langle 0|\Psi\rangle|^2 = \underline{\frac{1}{11}}$

$P_1 = |\langle 1|\Psi\rangle|^2 = \frac{9}{11}$

$P_2 = |\langle 2|\Psi\rangle|^2 = \underline{\underline{\frac{1}{11}}}$

$P_0 + P_1 + P_2 = 1 \qquad \underline{P_{\text{jiné}} = 0}$

(IX) $\langle H\rangle_\Psi = ?$

$$\underline{\underline{\langle H\rangle_\Psi}} = \langle\Psi|H|\Psi\rangle =$$

$$= N^2\left(\langle 0| + 3\langle 1| + \langle 2|\right) H \left(|0\rangle + 3|1\rangle + |2\rangle\right) =$$

$$= N^2\left(\langle 0| + 3\langle 1| + \langle 2|\right) \times$$

$$\times \left((0+\tfrac{1}{2})|0\rangle + 3(1+\tfrac{1}{2})|1\rangle + (2+\tfrac{1}{2})|2\rangle\right) =$$

$$= N^2\left(\tfrac{1}{2} + 9\cdot\tfrac{3}{2} + \tfrac{5}{2}\right)$$

$$= N^2\,\frac{33}{2}$$

$$= \underline{\underline{\frac{3}{2}}}$$

(X) $\hat{N} = a^+ a$

$$\langle\hat{N}\rangle_\Psi = \langle\Psi|\hat{N}|\Psi\rangle =$$

$$N|0\rangle = a^+a|0\rangle = 0\,|0\rangle$$

$$N|1\rangle = a^+a|1\rangle = 1\,|1\rangle$$

$$N|2\rangle = 2\,|2\rangle$$

$$\underline{\underline{\langle \hat{N} \rangle_\psi}} = \frac{1}{11}\cdot 0 + \frac{9}{11}\cdot 1 + \frac{1}{11}\cdot 2 =$$

$$= \underline{\underline{1}}$$

② HÜCKELOVA METODA

$$H_2\overset{1}{C}=\overset{2}{C}=\overset{3}{C}H_2$$

(I)
$$H = \begin{pmatrix} \alpha & \beta & 0 \\ \beta & \alpha & \beta \\ 0 & \beta & \alpha \end{pmatrix} \qquad \alpha < 0,\ \beta < 0$$

(II) $H|\psi\rangle = E|\psi\rangle \Rightarrow (H-E)|\psi\rangle = 0$

$$\det\begin{pmatrix} \alpha-E & \beta & 0 \\ \beta & \alpha-E & \beta \\ 0 & \beta & \alpha-E \end{pmatrix} \overset{!}{=} 0$$

$$\det\begin{pmatrix} x & 1 & 0 \\ 1 & x & 1 \\ 0 & 1 & x \end{pmatrix} \overset{!}{=} 0$$

$$x^3 + 0 + 0 - x - x - 0 \overset{!}{=} 0$$

$$x^3 - 2x = 0$$

$$x(x^2-2) = 0$$

$$x = 0, \pm\sqrt{2}$$

$x = -\sqrt{2}$: $\quad \frac{\alpha - E}{\beta} = x = -\sqrt{2}$

$$\underline{E = \alpha + \sqrt{2}\beta}$$

(III) pst. pro zákl. stav:

$$-\sqrt{2}\cdot a + 1\cdot b + 0\cdot c = 0$$
$$1\cdot a + (-\sqrt{2})\cdot b + 1\cdot c = 0$$
$$0\cdot a + 1\cdot b + (-\sqrt{2})\cdot c = 0$$

+ normalizace $|a|^2 + |b|^2 + |c|^2 = 1$

$$|a|^2 + |b|^2 + |c|^2 = 1$$

$-\sqrt{2}a + b = 0$

$|a|^2 = \frac{|b|^2}{2}$

$\sqrt{2}c = b$

$|c|^2 = \frac{|b|^2}{2}$

$$\frac{|b|^2}{2} + |b|^2 + \frac{|b|^2}{2} = 1$$

$|b|^2 = \frac{1}{2} \Rightarrow |b| = \frac{1}{\sqrt{2}}$

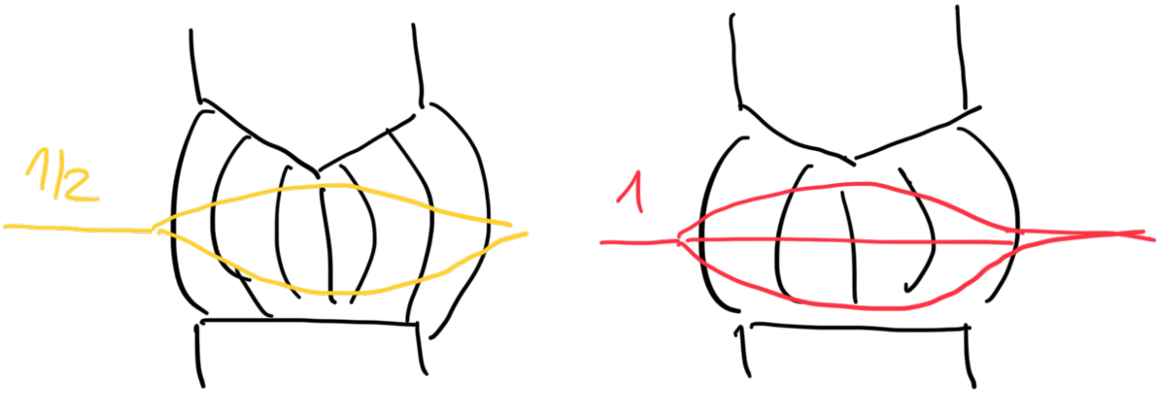
$|a| = \frac{1}{2}$

$|c| = \frac{1}{2}$

$\Rightarrow$ psti: 25 % na C_1 nebo C_3

50 % na C_2

③ STERN-GERLACH



(I) spin 1 $\rightarrow$ projekce $-1, 0, +1$

(II) báze $\{ |+z\rangle, |0z\rangle, |-z\rangle \}$

$$S_z |+z\rangle = +1\, |+z\rangle$$
$$S_z |0z\rangle = 0\, |0z\rangle$$
$$S_z |-z\rangle = -1\, |-z\rangle$$

$$\Rightarrow \quad S_z = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

$$|+z\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \quad |0z\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \quad |-z\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

(III) $S_\pm = S_1 \pm i S_2$

(IV)

$$J_\pm |j, m\rangle = \sqrt{j(j+1) - m(m\pm1)}\, |j, m\pm1\rangle$$

$$S_+ |-z\rangle = \sqrt{1\cdot(1+1) - (-1)\cdot((-1)+1)}\, |0z\rangle = \sqrt{2}\, |0z\rangle$$
$$S_+ |0z\rangle = \sqrt{2}\, |+z\rangle$$
$$S_+ |+z\rangle = 0$$

$$S_- |-z\rangle = 0$$
$$S_- |0z\rangle = \sqrt{2}\, |-z\rangle$$
$$S_- |+z\rangle = \sqrt{2}\, |0z\rangle$$

$$\Rightarrow \quad S_+ = \sqrt{2} \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix} \qquad S_- = \sqrt{2} \begin{pmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$$

(V) $S_x = \frac{1}{2}(S_+ + S_-) = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$

$S_y = \frac{i}{2}(S_- - S_+) = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix}$

(VI) $S_x|\lambda x\rangle = \lambda|\lambda x\rangle \quad \lambda = -1, 0, +1$

$$\lambda=1: \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}\begin{pmatrix} a \\ b \\ c \end{pmatrix} = 1\begin{pmatrix} a \\ b \\ c \end{pmatrix} \Rightarrow \begin{matrix} b = \sqrt{2}a \\ a+c = \sqrt{2}b \\ b = \sqrt{2}c \end{matrix}$$

$$\underbrace{|a|^2}_{\frac{|b|^2}{2}} + |b|^2 + \underbrace{|c|^2}_{\frac{|b|^2}{2}} = 1 \Rightarrow |b|^2 = \frac{1}{2}$$

$$|b| = \frac{1}{\sqrt{2}} \Rightarrow \begin{matrix} a = 1/2 \\ c = 1/2 \end{matrix}$$

$$\Rightarrow |+x\rangle = \frac{1}{2}\begin{pmatrix} 1 \\ \sqrt{2} \\ 1 \end{pmatrix}$$

$$|0x\rangle = \frac{1}{2}\begin{pmatrix} \sqrt{2} \\ 0 \\ -\sqrt{2} \end{pmatrix}$$

$$|-x\rangle = \frac{1}{2}\begin{pmatrix} 1 \\ -\sqrt{2} \\ 1 \end{pmatrix}$$

analogicky jako pro $|+x\rangle$

$S_y|\lambda y\rangle = \lambda|\lambda y\rangle \quad \lambda = -1, 0, +1$

$$|-y\rangle = \begin{pmatrix} -1 \\ i\sqrt{2} \\ 1 \end{pmatrix} \quad |0y\rangle = \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix} \quad |+y\rangle = \begin{pmatrix} -1 \\ -i\sqrt{2} \\ 1 \end{pmatrix}$$

pro kontrolu DÚ