Notatki do ćwiczeń

Andrzej Więckowski

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1 Brakety

$$\text{bra: } |\psi\rangle = \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \vdots \end{pmatrix} = \sum_i \psi_i |i\rangle, \quad \text{baza } \{|i\rangle\}\text{: } \textbf{ortonormalna: } \langle i|j\rangle = \delta_{ij}, \textbf{zupełna: } \sum_i |i\rangle\langle i| = \mathbb{1}; \tag{1}$$

$$\text{ket: } \langle\psi| = \begin{pmatrix} \psi_1^* & \psi_2^* & \psi_3^* & \dots \end{pmatrix} = \sum_i \psi_i^* \langle i|; \tag{2}$$

$$\langle\psi|\phi\rangle = \begin{pmatrix} \psi_1^* & \psi_2^* & \psi_3^* & \dots \end{pmatrix} \begin{pmatrix} \phi_1 \\ \phi_2 \\ \phi_3 \\ \vdots \end{pmatrix} = \left(\sum_i \psi_i^* \langle i|\right)\left(\sum_j \phi_j |j\rangle\right) = \sum_{ij} \psi_i^* \phi_i \delta_{ij} = \sum_i \psi_i^* \phi_i \tag{3}$$

$$|\psi\rangle\langle\phi| = \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \vdots \end{pmatrix} \begin{pmatrix} \phi_1^* & \phi_2^* & \phi_3^* & \dots \end{pmatrix} = \begin{pmatrix} \psi_1\phi_1^* & \psi_1\phi_2^* & \psi_1\phi_3^* & \dots \\ \psi_2\phi_1^* & \psi_2\phi_2^* & \psi_2\phi_3^* & \dots \\ \psi_3\phi_1^* & \psi_3\phi_2^* & \psi_3\phi_3^* & \dots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix} = \sum_{nm} \psi_n \phi_m^* |n\rangle\langle m| \tag{4}$$

2 Operatory

Element macierzowy operatora:

$$A_{nm} = \langle n|\hat{A}|m\rangle \tag{5}$$

Operator w bazie $\{|n\rangle\}$:

$$\hat{A} = \sum_{nm} \langle n|A|m\rangle |n\rangle\langle m| = \sum_{nm} A_{nm} |n\rangle\langle m| = \begin{pmatrix} \langle 1|A|1\rangle & \langle 1|A|2\rangle & \langle 1|A|3\rangle & \dots \\ \langle 2|A|1\rangle & \langle 2|A|2\rangle & \langle 2|A|3\rangle & \dots \\ \langle 3|A|1\rangle & \langle 3|A|2\rangle & \langle 3|A|3\rangle & \dots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix} \tag{6}$$

Działanie operatora na ket:

$$\hat{A}|\psi\rangle = \left(\sum_{nm} A_{nm}|n\rangle\langle m|\right)\left(\sum_k \psi_k |k\rangle\right) = \sum_n \underbrace{\sum_m A_{nm}\psi_m}_{(\hat{A}|\psi\rangle)_n} |m\rangle = |\psi'\rangle \tag{7}$$

Wartość oczekiwana w stanie $|\psi\rangle$:

$$\langle A\rangle_\psi = \langle A\rangle = \langle\psi|A|\psi\rangle = \sum_{nm} A_{nm}\langle\psi|n\rangle\langle m|\psi\rangle = \sum_{nm}\sum_{ij} A_{nm}\psi_i^*\delta_{in}\psi_j\delta_{mj} = \sum_{nm}\psi_n^* A_{nm}\psi_m \tag{8}$$

Zagadnienie własne:

$$\hat{A}|a\rangle = a|a\rangle \tag{9}$$

Operator w bazie stanów własnych:

$$\hat{A} = \sum_{aa'}\langle a|\hat{A}|a'\rangle|a\rangle\langle a'| = \sum_{aa'} a\delta_{aa'}|a\rangle\langle a'| = \sum_a a|a\rangle\langle a| \tag{10}$$

3 (Anty-)komutator

Własności komutatora $[A,B] = AB - BA$ and anty-komutatora $\{A,B\} = AB + BA$:

1. $[\alpha A + \beta B, C] = \alpha[A,C] + \beta[B,C]$, gdzie α, β to stałe;
2. $[A,B] = -[B,A]$, $\{A,B\} = \{B,A\}$;
3. $[AB,C] = A[B,C] + [A,C]B$;
4. $[AB,C] = A\{B,C\} - \{A,C\}B$.

4 Kwanotwanie kanoniczne

$$[\hat{x}_i, \hat{p}_j] = i\hbar\delta_{ij}, \quad [\hat{x}_i, \hat{x}_j] = [\hat{p}_i, \hat{p}_j] = 0; \tag{11}$$

$$\text{operator położenia: } \hat{x}_i = x_i; \tag{12}$$

$$\text{operator pędu: } \hat{p}_i = -i\hbar\frac{\partial}{\partial x_i}; \tag{13}$$

5 Zasada nieoznaczoności

Dla hermitowskich operatorów: $A = A^\dagger, B = B^\dagger$ ($\Delta A = \sqrt{(A - \langle A\rangle)^2}$):

$$\Delta A\,\Delta B \geq |\langle \tfrac{1}{2i}[A,B]\rangle|, \qquad \Delta x\,\Delta p \geq \tfrac{\hbar}{2}; \tag{14}$$

6 Zmiana bazy—transformacje

Dane są dwie zupełne, ortonormalne bazy $\{|i\rangle\}|_{i=1,2,3,\ldots}$ oraz $\{|\widetilde{i}\rangle\}$ oraz transformacja unitarna U:

$$U|i\rangle = |\widetilde{i}\rangle, \quad U = \sum_j |\widetilde{j}\rangle\langle j| \tag{15}$$

Elementy macierzowe U:

$$U_{ij} = \langle i|\left(\sum_{j'}|\widetilde{j'}\rangle\langle j'|\right)|j\rangle = \langle i|\widetilde{j}\rangle \tag{16}$$

Postać U w bazie $|i\rangle$

$$U = \sum_{ij} U_{ij} |i\rangle\langle j| = \sum_{ij} \langle i|\widetilde{j}\rangle |i\rangle\langle j| = \begin{pmatrix} \langle 1|\widetilde{1}\rangle & \langle 1|\widetilde{2}\rangle & \langle 1|\widetilde{3}\rangle & \dots \\ \langle 2|\widetilde{1}\rangle & \langle 2|\widetilde{2}\rangle & \langle 2|\widetilde{3}\rangle & \dots \\ \langle 3|\widetilde{1}\rangle & \langle 3|\widetilde{2}\rangle & \langle 3|\widetilde{3}\rangle & \dots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix} \tag{17}$$

Transformacja stanu $|\psi\rangle = \sum_i \psi_i |i\rangle$:

$$|\psi\rangle = \sum_i \underbrace{\left(\sum_j |\widetilde{j}\rangle\langle\widetilde{j}| \right)}_{\mathbb{1}} \psi_i |i\rangle = \sum_j \sum_i \underbrace{\langle\widetilde{j}|i\rangle}_{U^\dagger_{ji}} \psi_i |\widetilde{j}\rangle = \sum_j \left(U^\dagger |\psi\rangle \right)_j |\widetilde{j}\rangle \tag{18}$$

Transformacja U jest unitarna i zachowuję normę $|\psi\rangle$:

$$UU^\dagger = \left(\sum_i |\widetilde{i}\rangle\langle i| \right) \left(\sum_j |j\rangle\langle\widetilde{j}| \right) = \sum_{ij} |\widetilde{i}\rangle \delta_{ij} \langle\widetilde{j}| = \mathbb{1}; \quad \langle\widetilde{\psi}|\widetilde{\psi}\rangle = \langle\psi|U^\dagger U|\psi\rangle = \langle\psi|\psi\rangle \tag{19}$$

Transformacja operatora $A = \sum_{nm} A_{nm} |n\rangle\langle m|$:

$$A = \sum_{nm} A_{nm} \underbrace{\left(\sum_i |\widetilde{i}\rangle\langle\widetilde{i}| \right)}_{\mathbb{1}} |n\rangle\langle m| \underbrace{\left(\sum_j |\widetilde{j}\rangle\langle\widetilde{j}| \right)}_{\mathbb{1}} = \sum_{nmij} A_{nm} |\widetilde{i}\rangle\langle\widetilde{j}| \underbrace{\langle\widetilde{i}|n\rangle}_{U^\dagger_{in}} \underbrace{\langle m|\widetilde{j}\rangle}_{U_{mj}} = \sum_{ij} \underbrace{\left(\sum_{nm} U^\dagger_{in} A_{nm} U_{mj} \right)}_{(U^\dagger A U)_{ij}} |\widetilde{i}\rangle\langle\widetilde{j}| \tag{20}$$

7 Reprezentacja położeniowa

Zagadnienie własne operatora położenia:

$$\hat{x}|x\rangle = x|x\rangle \tag{21}$$

Elementy macierzowe operatora $\hat{x}$:

$$\hat{x}_{xy} = \langle x|\hat{x}|y\rangle = x\delta(x-y), \quad \hat{x}^n_{xy} = x^n \delta(x-y) \tag{22}$$

Stany $|x\rangle$ stanowią ortogonalną zupełną ciągłą bazę:

$$\int \mathrm{d}x\, |x\rangle\langle x| = \mathbb{1}, \quad \langle x|y\rangle = \delta(x-y) \tag{23}$$

Funkcja falowa (definicja):

$$\psi(x) = \langle x|\psi\rangle \tag{24}$$

Iloczyn skalarny:

$$\langle\psi|\phi\rangle = \langle\psi| \underbrace{\left(\int \mathrm{d}x\, |x\rangle\langle x| \right)}_{\mathbb{1}} |\phi\rangle = \int \mathrm{d}x\, \langle\psi|x\rangle\langle x|\phi\rangle = \int \mathrm{d}x\, \psi^*(x)\phi(x) \tag{25}$$

Działanie operatora $\hat{\mathscr{O}}$ na funkcję falową $\psi(x)$—definicja:

$$\hat{\mathscr{O}}\psi(x) = \langle x|\hat{\mathscr{O}}|\psi\rangle = \langle x|\psi'\rangle = \psi'(x) \tag{26}$$

Elementy macierzowe operatora pędu $\hat{p}$ w reprezentacji położeniowej:

$$\hat{p}_{xy} = \langle x|\hat{p}|y\rangle = -i\hbar \frac{\partial}{\partial x} \delta(x-y), \quad \hat{p}^n_{xy} = \langle x|\hat{p}^n|y\rangle = (-i\hbar)^n \frac{\partial^n}{\partial x^n} \delta(x-y) \tag{27}$$

Wartość oczekiwana operatora:

$$\langle A\rangle = \langle\psi|A|\psi\rangle = \langle\psi|\underbrace{\left(\int \mathrm{d}x\,|x\rangle\langle x|\right)}_{\mathbb{1}} A \underbrace{\left(\int \mathrm{d}y\,|y\rangle\langle y|\right)}_{\mathbb{1}}|\psi\rangle = \int\int \mathrm{d}x\,\mathrm{d}y\,\psi^*(x)A_{xy}\psi(y) \tag{28}$$

Wzór (28), kiedy A jest funkcją $\hat{x}$ upraszcza się:

$$\langle A(\hat{x})\rangle = \int\int \mathrm{d}x\,\mathrm{d}y\,\psi^*(x)A(x)\underbrace{\langle x|y\rangle}_{\delta(x-y)}\psi(x) = \int \mathrm{d}x\,\psi^*(x)A(x)\psi(x) \tag{29}$$

Wzór (28), analogicznie kiedy A jest funkcją $\hat{p}$ upraszcza się:

$$\langle A(\hat{p})\rangle = \int\int \mathrm{d}x\,\mathrm{d}y\,\psi^*(x)\left(\sum_{n=0}^{\infty}\frac{1}{n!}\frac{\partial^n A(p)}{\partial p^n}\bigg|_{p=0}\hat{p}^n_{xy}\right)\psi(y) = \int \mathrm{d}x\,\psi^*(x)A(p)\psi(x) \tag{30}$$

W ogólności dla dowolnej obserwabli:

$$\langle A\rangle = \int \mathrm{d}x\,\psi^*(x)A\psi(x) \tag{31}$$