Gaussovy integrály

- jednorozměrné integrály

$$\int_{\mathbb{R}} x^n e^{-ax^2+bx} dx = \sqrt{\frac{\pi}{a}} \frac{\partial^n}{\partial b^n} e^{\frac{b^2}{4a}}, \quad a,b \in \mathbb{C},\ \mathrm{Re}\, a > 0$$

$$\int_{\mathbb{R}} e^{-ax^2+bx} dx = \sqrt{\frac{\pi}{a}} e^{\frac{b^2}{4a}},\ \int_{\mathbb{R}} x e^{-ax^2+bx} dx = \sqrt{\frac{\pi}{a}} e^{\frac{b^2}{4a}} \frac{b}{2a},\ \int_{\mathbb{R}} x^2 e^{-ax^2+bx} dx = \sqrt{\frac{\pi}{a}} e^{\frac{b^2}{4a}} \left(\frac{b^2}{4a^2} + \frac{1}{2a}\right)$$

- vícerozměrné integrály

$$\int_{\mathbb{R}^n} e^{-ax^2+\vec{b}\cdot\vec{x}} d^n x = \left(\frac{\pi}{a}\right)^{\frac{n}{2}} e^{\frac{b^2}{4a}}, \quad a \in \mathbb{C},\ \mathrm{Re}\, a > 0,\ \vec{b} \in \mathbb{C}^n$$

Operátory, komutační relace

- komutační relace $\left[\hat{Q}_j, \hat{P}_k\right] = i\hbar\delta_{jk},\ \left[\hat{L}_j, \hat{Q}_k\right] = i\hbar\varepsilon_{jkl}\hat{Q}_l,\ \left[\hat{L}_j, \hat{P}_k\right] = i\hbar\varepsilon_{jkl}\hat{P}_l$

$$\left[\hat{L}_j, \hat{L}_k\right] = i\hbar\varepsilon_{jkl}\hat{L}_l$$

- sférické souřadnice $\hat{Q}_1 = r\sin\theta\cos\varphi,\ \hat{Q}_2 = r\sin\theta\sin\varphi,\ \hat{Q}_3 = r\cos\theta$

$$\hat{P}_1 = -i\hbar\left(\cos\varphi\sin\theta\frac{\partial}{\partial r} - \frac{\sin\varphi}{r\sin\theta}\frac{\partial}{\partial\varphi} + \frac{\cos\theta\cos\varphi}{r}\frac{\partial}{\partial\theta}\right)$$

$$\hat{P}_2 = -i\hbar\left(\sin\varphi\sin\theta\frac{\partial}{\partial r} + \frac{\cos\varphi}{r\sin\theta}\frac{\partial}{\partial\varphi} + \frac{\cos\theta\sin\varphi}{r}\frac{\partial}{\partial\theta}\right),\ \hat{P}_3 = -i\hbar\left(\cos\theta\frac{\partial}{\partial r} - \frac{\sin\theta}{r}\frac{\partial}{\partial\theta}\right)$$

$$\hat{L}_1 = i\hbar\left(\cos\varphi\cot\theta\frac{\partial}{\partial\varphi} + \sin\varphi\frac{\partial}{\partial\theta}\right),\ \hat{L}_2 = i\hbar\left(\sin\varphi\cot\theta\frac{\partial}{\partial\varphi} - \cos\varphi\frac{\partial}{\partial\theta}\right),\ \hat{L}_3 = -i\hbar\frac{\partial}{\partial\varphi}$$

$$\hat{L}^2 = -\hbar^2\left[\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2} + \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)\right]$$

Lineární harmonický oscilátor

- spektrum $\hat{H}\psi_n = \hbar\omega\left(n + \frac{1}{2}\right)\psi_n, \quad n \in \mathbb{Z}_+$
- vlastní funkce $\psi_n(\xi) = \left(\frac{M\omega}{\pi\hbar}\right)^{\frac{1}{4}} \frac{1}{\sqrt{n!2^n}}\ H_n(\xi)\ e^{-\frac{\xi^2}{2}}, \quad \xi = \sqrt{\frac{M\omega}{\hbar}}x$
- Hermitovy polynomy $H_n(z) = (-1)^n e^{z^2} \frac{d^n}{dz^n} e^{-z^2}$

$$H_0(z) = 1,\ H_1(z) = 2z,\ H_2(z) = 2(2z^2-1),\ H_3(z) = 4z(2z^2-3)$$

- posunovací operátory $\hat{a}_\pm = \sqrt{\frac{M\omega}{2\hbar}}(\hat{Q} \mp \frac{i}{M\omega}\hat{P}),\ [\hat{H}, \hat{a}_\pm] = \pm\hbar\omega\hat{a}_\pm,\ [\hat{a}_-, \hat{a}_+] = \mathbb{1}$

$$\hat{Q} = \sqrt{\frac{\hbar}{2M\omega}}\left(\hat{a}_+ + \hat{a}_-\right),\ \hat{P} = i\sqrt{\frac{M\hbar\omega}{2}}\left(\hat{a}_+ - \hat{a}_-\right),\ \hat{H} = \hbar\omega\left(\hat{a}_+\hat{a}_- + \frac{1}{2}\right)$$

$$\hat{a}_\pm|n\rangle = \alpha_n^\pm|n\pm 1\rangle,\ \alpha_n^- = \sqrt{n},\ \alpha_n^+ = \sqrt{n+1},\ |n\rangle = \frac{1}{\sqrt{n!}}\hat{a}_+^n|0\rangle$$

- koherentní stavy $\hat{a}_-|\alpha\rangle = \alpha|\alpha\rangle, \quad |\alpha\rangle = e^{-\frac{|\alpha|^2}{2}} \sum_{n=0}^{+\infty} \frac{\alpha^n}{\sqrt{n!}}|n\rangle$

$$\hat{a}_-\psi_\alpha = \alpha\psi_\alpha,\ \psi_\alpha(\xi) = e^{\frac{\alpha^2-|\alpha|^2}{2}} \left(\frac{M\omega}{\pi\hbar}\right)^{\frac{1}{4}} e^{-\frac{(\xi-\sqrt{2}\alpha)^2}{2}},\ \alpha \in \mathbb{C}$$

Moment hybnosti

- spektrum $\hat{L}_3 Y_{lm} = m\hbar Y_{lm},\ \hat{L}^2 Y_{lm} = \hbar^2 l(l+1) Y_{lm}, l \in \mathbb{Z}_+,\ m \in \{-l, \ldots, l\}$
- kulové funkce $Y_{lm}(\theta,\varphi) = C_{lm}\ P_l^m(\cos\theta)\ e^{im\varphi}, \quad |C_{lm}|^2 = \frac{(2l+1)(l-m)!}{4\pi(l+m)!}$
- Legenderovy polynomy $P_l^m(t) = \frac{(1-t^2)^{\frac{m}{2}}}{2^l l!} \frac{d^{l+m}}{dt^{l+m}}(t^2-1)^l$

$$Y_{00}(\theta,\varphi) = \frac{1}{\sqrt{4\pi}},\ Y_{11}(\theta,\varphi) = -\sqrt{\frac{3}{8\pi}}\sin\theta e^{i\varphi},\ Y_{10}(\theta,\varphi) = \sqrt{\frac{3}{4\pi}}\cos\theta,\ Y_{1-1}(\theta,\varphi) = \sqrt{\frac{3}{8\pi}}\sin\theta e^{-i\varphi}$$

- posunovací operátory $\hat{L}_\pm = \hat{L}_1 \pm i\hat{L}_2,\ [\hat{L}_3, \hat{L}_\pm] = \pm\hbar\hat{L}_\pm,\ [\hat{L}^2, \hat{L}_\pm] = 0$

$$\hat{L}_\pm|l,m\rangle = \alpha_{lm}^\pm|l, m\pm 1\rangle,\ \alpha_{lm}^\pm = \hbar\sqrt{l(l+1) - m(m\pm 1)}$$

Izotropní oscilátor

- spektrum hamiltoniánu $\hat{H}\psi_{n,l,m} = \hbar\omega(2n+l+\frac{3}{2})\ \psi_{n,l,m},\ n, l \in \mathbb{Z}_+,\ m \in \{-l, \ldots, l\}$
- společné vlastní funkce $\hat{H},\ \hat{L}_3,\ \hat{L}^2$ $\psi_{n,l,m}(\xi,\theta,\varphi) = K_{nl}\ \xi^l\ e^{-\frac{\xi^2}{2}}\ L_n^{l+\frac{1}{2}}(\xi^2)\ Y_{lm}(\theta,\varphi)$

$$\xi = r\sqrt{\frac{M\omega}{\hbar}}, \quad |K_{nl}| = \frac{2}{\pi^{\frac{1}{4}}}\left(\frac{M\omega}{\hbar}\right)^{\frac{3}{4}}\left(\frac{2^{n+l}n!}{(2n+2l+1)!!}\right)^{\frac{1}{2}}$$

- Lagguerovy polynomy $L_n^\beta(z) = \frac{1}{n!}\ e^z z^{-\beta}\ \frac{d^n}{dz^n}\ (e^{-z}z^{n+\beta})$

$$L_0^\beta(z) = 1,\ L_1^\beta(z) = 1 + \beta - z$$

Vodíkový atom

- bodové spektrum hamiltoniánu $\hat{H}\psi_{N,l,m} = -\frac{R}{N^2}\ \psi_{N,l,m},\ N = n + l + 1,\ R = \frac{MQ^2}{2\hbar^2}$
- společné vlastní funkce $\hat{H},\ \hat{L}_3,\ \hat{L}^2$ $\psi_{N,l,m}(\xi,\theta,\varphi) = K_{Nl}\ \left(\frac{2r}{Na}\right)^l e^{-\frac{r}{Na}} L_{N-l-1}^{2l+1}(\frac{2r}{Na}) Y_{lm}(\theta,\varphi)$

$$a = \frac{\hbar^2}{|Q|M}, \quad |K_{Nl}| = \frac{2}{N^2}\left(\frac{(N-l-1)!}{a^3(N+l)!}\right)^{\frac{1}{2}}$$

Částice v nekonečné potenciálové jámě

- spektrum hamiltoniánu $\hat{H}\psi_n = E_n\psi_n, \quad E_n = \frac{1}{2M}\left(\frac{n\pi\hbar}{2a}\right)^2,\ n \in \mathbb{N}$
- vlastní funkce $\psi_n(x) = \frac{1}{\sqrt{a}}\sin\left(\frac{n\pi}{2a}(x-a)\right)$

Kvantové tuhé těleso

- spektrum hamiltoniánu $\hat{H}\psi_m(\varphi) = -\frac{\hbar^2}{2I}\frac{d^2\psi_m}{d\varphi^2} = E_m\psi_m(\varphi),\ E_m = \frac{m^2\hbar^2}{2I},\ m \in \mathbb{Z}$
- vlastní funkce $\psi_m(\varphi) = \frac{1}{\sqrt{2\pi}}e^{im\varphi}$

Zobecněné vlastní funkce

- operátor hybnosti $(\phi_{\vec{p}}, \hat{P}_j\psi) = p_j(\phi_{\vec{p}}, \psi), \quad \phi_{\vec{p}}(\vec{x}) = \frac{1}{(2\pi\hbar)^{\frac{3}{2}}}e^{\frac{i}{\hbar}\vec{p}\cdot\vec{x}}$

$$(\phi_{\vec{p}}, \psi) = \frac{1}{(2\pi\hbar)^{\frac{3}{2}}}\int\limits_{\mathbb{R}^3} e^{-\frac{i}{\hbar}\vec{p}\cdot\vec{x}}\psi(\vec{x})d^3x = \widetilde{\psi}(\vec{p}), \quad (\phi_{\vec{p}}, \phi_{\vec{p}'}) = \delta(\vec{p} - \vec{p'})$$

- operátor polohy $(\delta_{\vec{a}}, \hat{Q}_j\psi) = a_j(\delta_{\vec{a}}, \psi), \quad \delta_{\vec{a}}(\vec{x}) = \delta(\vec{x} - \vec{a})$

$$(\delta_{\vec{a}}, \psi) = \int\limits_{\mathbb{R}^3} \delta(\vec{x} - \vec{a})\psi(\vec{x})d^3x = \psi(\vec{a}), \quad (\delta_{\vec{a}}, \delta_{\vec{a}'}) = \delta(\vec{a} - \vec{a'})$$

Integrály pohybu

- $\hat{A}$ je integrál pohybu $\iff$ $\frac{i}{\hbar}[\hat{H}, \hat{A}] + \frac{\partial\hat{A}}{\partial t} = 0$

Spin

- složky spinu $[\hat{S}_j, \hat{S}_k] = i\hbar\epsilon_{jkl}\hat{S}_l, \quad \hat{S}_j = \frac{\hbar}{2}\sigma_j$
- Pauliho matice $[\sigma_j, \sigma_k] = 2i\epsilon_{jkl}\sigma_l, \quad \{\sigma_j, \sigma_k\} = 2\delta_{jk}\mathbb{1}, \quad \sigma_j\sigma_k = \delta_{jk}\mathbb{1} + i\epsilon_{jkl}\sigma_l$

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},\ \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix},\ \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

- spinor s kladnou projekcí do směru $\vec{n} = (\sin\theta\cos\varphi, \sin\theta\sin\varphi, \cos\theta)$

$$(\vec{n}\cdot\vec{\sigma})\ \psi_{\vec{n}} = \psi_{\vec{n}} \implies \psi_{\vec{n}} = \begin{pmatrix} e^{-i\frac{\varphi}{2}}\cos\frac{\theta}{2} \\ e^{i\frac{\varphi}{2}}\sin\frac{\theta}{2} \end{pmatrix}$$

- řešení Pauliho rovnice pro spin v homogenním magnetickém poli $\vec{B}(\vec{x}, t) = \vec{B}$

$$\begin{pmatrix} \psi_1(t) \\ \psi_2(t) \end{pmatrix} = \exp\left\{-\frac{i}{\hbar}\hat{\vec{\mu}}\cdot\vec{B}t\right\}\begin{pmatrix} \psi_1(0) \\ \psi_2(0) \end{pmatrix} = \left\{\cos\left(\frac{\mu_0}{\hbar}|\vec{B}|t\right)\mathbb{1} - i\frac{\sin\left(\frac{\mu_0}{\hbar}|\vec{B}|t\right)}{|\vec{B}|}\vec{B}\cdot\vec{\sigma}\right\}\begin{pmatrix} \psi_1(0) \\ \psi_2(0) \end{pmatrix}$$

Poruchová teorie

$\hat{H} = \hat{H}_0 + \varepsilon\hat{H}',\ \hat{H}_0|\psi_k\rangle = E_k^{(0)}|\psi_k\rangle,\ \hat{H}|\psi_k(\varepsilon)\rangle = E_k(\varepsilon)|\psi_k(\varepsilon)\rangle,\ E_k(\varepsilon) = E_k^{(0)} + \varepsilon E_k^{(1)} + \varepsilon^2E_k^{(2)} + \dots$

- oprava prvního řádu $E_k^{(1)} = \langle\psi_k|\hat{H}'|\psi_k\rangle$
- oprava druhého řádu $E_k^{(2)} = \sum\limits_{j\neq k}\frac{\left|\langle\psi_j|\hat{H}'|\psi_k\rangle\right|^2}{E_k - E_j}$