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É 2.88

2 zh + jav. zh

HF - 1 -> pótverseny

pcs10.elte.hu/index.html

CM: $x(t) \longrightarrow m\frac{d^2x}{dt^2} = -\frac{dV}{dx}$

QM: $\Psi(x,t) \longrightarrow i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + V\cdot\Psi$

$|\Psi(x,t)|^2 dx$ ↘ valószínűség $\in [x, x+dx]$

időbeli változás

- Schrödinger - egyenlet
- hullámfv. összeomlás

$\Psi$ m. $\Rightarrow \alpha\cdot\Psi$ is m. $\forall \alpha \in \mathbb{C}$

$\int |\Psi|^2 dx = 1$ normálás

$\Psi$ négyzetesen integrálható

$t = 0 \quad \int |\Psi(x,0)|^2 dx = 1 \Rightarrow \int |\Psi(x,t)|^2 dx = 1$

$$\frac{\partial\Psi}{\partial t} = \frac{i\hbar}{2m}\frac{\partial^2\Psi}{\partial x^2} - \frac{i}{\hbar}V\cdot\Psi$$

$$\frac{\partial\Psi^*}{\partial t} = -\frac{i\hbar}{2m}\frac{\partial^2\Psi^*}{\partial x^2} + \frac{i}{\hbar}V\cdot\Psi^*$$

$$\frac{\partial}{\partial t}\int |\Psi(x,t)|^2 dx = \int \frac{\partial}{\partial t}(\Psi^*\Psi)\, dx =$$

$$= \int \left(-\frac{i\hbar}{2m}\frac{\partial^2\Psi^*}{\partial x^2}\Psi + \cancel{\frac{i}{\hbar}V\Psi^*\Psi} + \frac{i\hbar}{2m}\Psi^*\frac{\partial^2\Psi}{\partial x^2} - \cancel{\frac{i}{\hbar}V\Psi^*\Psi}\right) dx$$

$$= \frac{i\hbar}{2m} \int \left( \psi^* \frac{\partial^2 \psi}{\partial x^2} - \frac{\partial^2 \psi^*}{\partial x^2} \psi \right) dx =$$

$$= \frac{i\hbar}{2m} \int \frac{\partial}{\partial x} \left( \psi^* \frac{\partial \psi}{\partial x} - \frac{\partial \psi^*}{\partial x} \psi \right) dx =$$

$$= \frac{i\hbar}{2m} \left[ \psi^* \frac{\partial \psi}{\partial x} - \frac{\partial \psi^*}{\partial x} \psi \right]_{-\infty}^{+\infty} = 0$$

várható érték $\quad \langle x \rangle = \int_{-\infty}^{+\infty} x \cdot |\psi|^2 \, dx$

$$\frac{d}{dt} \langle x \rangle = \int x \frac{\partial}{\partial t} |\psi|^2 \, dx = \frac{i\hbar}{2m} \int x \cdot \frac{\partial}{\partial x} \left( \psi^* \psi' - \psi^{*\prime} \cdot \psi \right) dx$$

$$= -\frac{i\hbar}{2m} \int 1 \cdot \left( \psi^* \frac{\partial \psi}{\partial x} - \frac{\partial \psi^*}{\partial x} \psi \right) dx =$$

$$= -\frac{i\hbar}{2m} \int \psi^* \frac{\partial \psi}{\partial x} \cdot 2 = -\frac{i\hbar}{m} \int \psi^* \frac{\partial \psi}{\partial x} = \langle v \rangle$$

$$\langle p \rangle = m \langle v \rangle = -i\hbar \int \psi^* \frac{\partial}{\partial x} \psi$$

$$x \longrightarrow \langle x \rangle = \int \psi^* \cdot x \cdot \psi \, dx$$

$$p \longrightarrow \langle p \rangle = \int \psi^* \cdot \left( -i\hbar \frac{\partial}{\partial x} \right) \psi \, dx$$

$$Q(x, p) \longrightarrow \langle Q \rangle = \int \psi^* \, Q\left(x, -i\hbar \frac{\partial}{\partial x}\right) \psi \, dx$$

vektor fogalom: $<$ valós komponens
komponens $\in \mathbb{C}$

$V \ni u, v$

$u + v = w \in V$

$\exists 0: \; 0 + v = v$

$a \cdot v = w \in V$

$\exists 1: \; 1 \cdot v = v$

disztributív

lin. kombináció $a \cdot v + b \cdot u$

$v_1, v_2, \ldots$ -től $u$ lin. független

$u \neq a_1 \cdot v_1 + a_2 \cdot v_2 + \ldots$

bázis, dimenzió

skalárszorzat $\langle u, v \rangle = \langle v, u \rangle^*$

$\langle u, u \rangle \geq 0$ és $\langle u, u \rangle = 0 \iff u = 0$

$$\langle u, a_1 \cdot v_1 + a_2 \cdot v_2 \rangle = a_1 \cdot \langle u, v_1 \rangle + a_2 \cdot \langle u, v_2 \rangle$$

$$\langle a_1 \cdot u_1 + a_2 \cdot u_2, v \rangle = a_1^* \langle u_1, v \rangle + a_2^* \cdot \langle u_2, v \rangle$$

CS $\left|\langle u, v \rangle\right|^2 \leq \left|\langle u, u \rangle\right| \cdot \langle v, v \rangle$

$$\hat{T}(a \cdot u + b \cdot v) = a \cdot \hat{T} u + b \cdot \hat{T} v$$

$\hat{T} \leftrightarrow \underline{\underline{T}}$ $\quad (\tilde{\underline{\underline{T}}})_{ik} = \underline{\underline{T}}_{ki}$ $\quad (\underline{\underline{T}}^*)_{ik} = \underline{\underline{T}}^*_{ik}$

$\underline{\underline{T}}^+ = \tilde{\underline{\underline{T}}}^*$

$[\underline{\underline{S}}, \underline{\underline{T}}] = \underline{\underline{S}}\,\underline{\underline{T}} - \underline{\underline{T}}\,\underline{\underline{S}}$

$\underline{\underline{T}}^{-1} \cdot \underline{\underline{T}} = \mathbb{1}$ $\quad$ $\det \underline{\underline{T}} \neq 0$

hermitikus $\quad \underline{\underline{T}}^{+} = \underline{\underline{T}}$

unitér $\quad \underline{\underline{T}}^{+} = \underline{\underline{T}}^{-1}$

<u>sajátérték</u> $\quad \hat{T} v = \lambda v \qquad (\underline{\underline{T}} - \lambda \mathbb{1}) v = 0$

$$\det(\underline{\underline{T}} - \lambda \mathbb{1}) = 0$$

<u>lin. tr. adjungáltja</u>

$$\langle \hat{T}^{+} u, v \rangle = \langle u, \hat{T} v \rangle$$

önadjungált op. $\quad \hat{T}^{+} = \hat{T}$

1. sé $\in \mathbb{R}$
2. kül. sé.-hez tartozó sv.-ok ortogonálisak
3. sv.-ok kifeszítik a teret

$$\hat{T} e_i = \lambda e_i \qquad u = \sum_{i=1}^{n} c_i \cdot e_i$$

$$c_j = \langle e_j, u \rangle$$

<u>függvénytérel</u>

- vektorok $\to$ fvek
- skalárszorzat $\to$ integrálás
- lin. tr. $\to$ operátor $\qquad \hat{O}: f \to g$

$$\langle f | g \rangle = \int_{D} f^{*} g \, dx \qquad \langle f | g \rangle^{*} = \langle g | f \rangle$$

$$\int |f|^2 \, dx < \infty$$

$P(N)$ polinomok

$$f(x) = a_0 + a_1 \cdot x + \dots + a_{N-1} \cdot x^{N-1}$$

$e_1 = 1 \quad e_2 = x \quad e_3 = x^2 \quad \dots$ bázis

de nem teljes ortonormált rendszer

$\hat{T}$ operátor lineáris

$$\hat{D} = \frac{d}{dx} \quad \checkmark \qquad \hat{x} = x \quad \lightning$$

$$\frac{df}{dx} = \lambda \cdot f \qquad f = A \cdot e^{\lambda x}$$

$P(N)$-en csak $\lambda = 0 \quad f = \text{const}$

$L^2(\mathbb{R})$-en nincs

$$\langle \hat{T}^+ f | g \rangle = \langle f | \hat{T} g \rangle$$

$$\langle f | \hat{x} \cdot g \rangle = \int f^* \cdot x \cdot g \cdot dx = \int (x \cdot f)^* g \cdot dx = \langle \hat{x} f | g \rangle$$

$$\Rightarrow \hat{x}^+ = \hat{x} \qquad x \in \mathbb{R}$$

$$\langle f | \hat{D} g \rangle = \int f^* \frac{dg}{dx} dx = - \int \frac{df^*}{dx} g \, dx = \langle -\hat{D} f | g \rangle$$

$$\Rightarrow \hat{D}^+ = -\hat{D} \quad \text{antiherm.}$$

$$(i \cdot \hat{D})^+ = i \cdot \hat{D} \qquad (\hat{D}^2)^+ = \hat{D}^2$$

<u>Hilbert tér</u>

teljes: $\forall$ Cauchy sorozat konvergens

$$\mathbb{Q} \qquad 1 - \frac{1}{2} + \frac{1}{3} - \frac{1}{4} + \dots = \ln 2 \qquad \mathbb{Q} \to \mathbb{R}$$

$P(\mathbb{N})$ nem teljes $\longrightarrow$ $L^2(\mathbb{R})$

$$f = \sum_{j=1}^{\infty} a_j \cdot e_j$$

1. részecske állapota $L^2 \ni \Psi$ $\qquad \int |\Psi|^2 \, dx = 1$

mennyiség $\rightarrow$ operátor

$$x \longrightarrow \hat{x} = x$$

$$p \longrightarrow \hat{p} = -i\hbar \frac{\partial}{\partial x}$$

$$Q(x,p) \longrightarrow Q\left(x, -i\hbar \frac{\partial}{\partial x}\right)$$

$$T = \frac{p^2}{2m} \longrightarrow \hat{T} = \frac{1}{2m}\left(-i\hbar \frac{\partial}{\partial x}\right)^2 = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2}$$

2. $\langle Q \rangle = \langle \Psi | \hat{Q} \Psi \rangle \in \mathbb{R}$ $\Leftarrow$

$$\hat{Q}^{+} = \hat{Q} \qquad \langle \hat{Q}\Psi | \Psi \rangle = \langle \Psi | \hat{Q} \Psi \rangle$$

3. $|\Psi\rangle$ állapot; megmérjük $Q$-t

$$\hat{Q}|e_n\rangle = \lambda_n |e_n\rangle \qquad |\Psi\rangle = \sum_{n=1}^{\infty} c_n |e_n\rangle$$

$$c_n = \langle e_n | \Psi \rangle$$

$\lambda_n$ lesz az eredmény $|c_n|^2$ valószínűséggel

QM → állapot: teljes rendszer

(egyszerre mérhetők, de másik nem)

$f$: $f_n$ lehetséges értékek, $\Psi_n(x)$ sajátfüggvények

$f \to \hat{f}$ operátor: $\hat{f}\,\Psi_n = f_n \cdot \Psi_n$

$$\Psi(x) = \sum_n c_n \cdot \Psi_n(x) \qquad \int \Psi^*(x)\,\Psi(x)\,dx = 1$$

ortogonalitás

$$\int \Psi_n^*(x)\,\Psi_m(x)\,dx = \delta_{nm} \qquad \sum_n |c_n|^2 = 1 \;\to\; p_n = |c_n|^2 = \left|\int \Psi_n^*(x)\,\Psi(x)\,dx\right|^2$$

Folytonos spektrum

$f$ mennyiség $\hat{f}$, sajátértékek $f \in \mathbb{R}$ $\quad \Psi_f(x)$

$$\Psi(x) = \int df \cdot c(f) \cdot \Psi_f(x)$$

$$p(f, f+df) = |c(f)|^2 \cdot df$$

$$1 = \int dx\, \Psi^*(x)\,\Psi(x) = \int dx \int df' \int df\; c^*(f')\,c(f)\,\Psi_{f'}^*(x)\,\Psi_f(x) =$$

$$= \int df' \int df\, \{c^*(f')\,c(f)\} \underbrace{\int dx\; \Psi_{f'}^*(x)\,\Psi_f(x)}_{\delta(f-f')} =$$

$$= \int df\, |c(f)|^2 = 1$$

miért? ortogonalitás

$$c(f) = \int \Psi_f^*(x)\,\Psi(x)\,dx = \int df' \cdot c(f') \cdot \underbrace{\int dx \cdot \Psi_f^*(x)\,\Psi_{f'}(x)}_{\delta(f-f')}$$

$\Psi(x) = \int df' \cdot c(f') \cdot \Psi_{f'}(x)$

$\delta(f-f') \to f = f'$-re $\infty$

(~~[illegible]~~)

$$i\hbar \frac{\partial \Psi}{\partial t} = \hat{H}\Psi$$

Hamilton-op.

$$\Psi(x,t) = T(t)\cdot \Psi(x)$$

$$i\hbar\, \dot{T}(t)\cdot \Psi(x) = T(t)\cdot \hat{H}\,\Psi(x)$$

$$i\hbar \frac{\dot{T}(t)}{T(t)} = \frac{\hat{H}\,\Psi(x)}{\Psi(x)} = E$$

$$T(t) = e^{-\frac{i}{\hbar}E\cdot t} \qquad \hat{H}\,\Psi = E\cdot\Psi$$

$$\hat{H}\,\Psi_n(x) = E_n\cdot \Psi_n(x) \qquad \Psi(x,t) = \Psi_n(x)\cdot e^{-\frac{i}{\hbar}E_n t}$$

Stac. állapotok / Energia-s. á.

$$|\Psi(x,t)|^2 = |\Psi_n(x)|^2 - \text{áll}$$

$$\hat{f}: \quad \bar{f} = \int \Psi^*(x)\,\hat{f}\,\Psi(x)\,dx$$

Kl. mech. $\rightarrow \quad H = \frac{p^2}{2m} + V(x)$

$$\hat{H} = \frac{1}{2m}\hat{p}^2 + V(x)$$

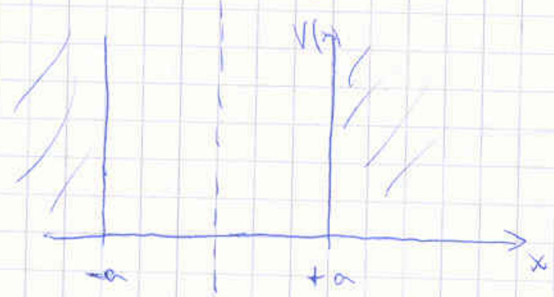
$$\hat{p} = -i\hbar\frac{\partial}{\partial x} \qquad \hat{\underline{p}} = -i\hbar\,\underline{\nabla}$$

$$-\frac{\hbar^2}{2m}\Delta\Psi_n(x) + V(x)\,\Psi_n(x) = E_n\Psi_n(x)$$

$$\Psi(x,t=0) = \sum_n c_n\,\Psi_n(x) \longrightarrow c_n = \int \Psi_n^*(x)\,\Psi(x,t=0)\,dx$$

$$\Psi(x,t) = \sum_n c_n\, e^{-\frac{i}{\hbar}E_n t}\cdot \Psi_n(x)$$

1. példa: potenciálgödör, 1d




Belül: $-\frac{\hbar^2}{2m}\psi''(x) = E\cdot\psi(x)$ ⟶ határfeltétel: $\psi(x)$ folytonos

Kívül: $\psi(x) \equiv 0$

$$\psi''(x) = -\underbrace{\frac{2mE}{\hbar^2}}_{k^2}\cdot\psi(x) \qquad E = \frac{\hbar^2 k^2}{2m}$$

$$\psi(x) = A\cdot\sin(kx) + B\cdot\cos(kx)$$

$$\psi(-a) = -A\sin(ka) + B\cos(ka) = 0$$
$$\psi(+a) = +A\sin(ka) + B\cos(ka) = 0$$

$$A\cdot\sin(ka) = 0 \qquad B\cdot\cos(ka) = 0$$

I. $\sin(ka) = 0 \qquad B = 0$

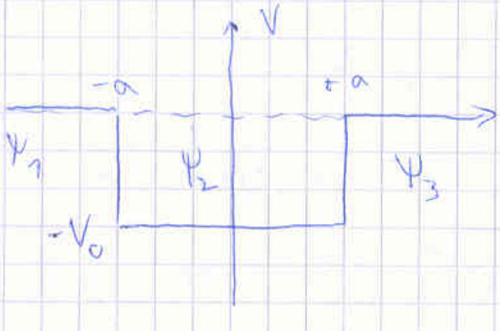
$$k\cdot a = n\pi \qquad E_n = \Big(\underbrace{\frac{n\cdot\pi}{a}}_{\frac{2n\cdot\pi}{2a}}\Big)^2\cdot\frac{\hbar^2}{2m}$$

II. $\cos(ka) = 0 \qquad A = 0$

$$ka = \frac{\pi}{2} + n\cdot\pi \qquad E'_n = \left(\frac{(2n+1)\pi}{2a}\right)^2\cdot\frac{\hbar^2}{2m}$$

Összevonva: $E_n = \left(\frac{n\cdot\pi}{2a}\right)^2\cdot\frac{\hbar^2}{2m}$

2. példa: potenciálvölgy, 1d




$$-\frac{\hbar^2}{2m}\psi''(x)+V(x)\psi(x)=E\cdot\psi(x) \qquad \Big/ \int_{x_0-\varepsilon}^{x_0+\varepsilon}$$

$$-\frac{\hbar^2}{2m}\int_{x_0-\varepsilon}^{x_0+\varepsilon}\psi''(x)\,dx+\int_{x_0-\varepsilon}^{x_0+\varepsilon}V(x)\psi(x)\,dx=E\cdot\int_{x_0-\varepsilon}^{x_0+\varepsilon}\psi(x)\,dx$$

V sima fv. (nincs benne Dirac-δ)

$$-\frac{\hbar^2}{2m}\left(\psi'(x_0+\varepsilon)-\psi'_0(x_0-\varepsilon)\right)+\cancel{V(x_0)\psi(x_0)\cdot 2\varepsilon}=\cancel{E\,\psi(x_0)\cdot 2\varepsilon}$$

$\varepsilon\to 0 \Rightarrow \psi'$ folytonos $x_0$-ban

$$-\frac{\hbar^2}{2m}\psi_1''=E\cdot\psi_1 \qquad \kappa^2=-\frac{2mE}{\hbar^2} \qquad E<0$$

$$-\frac{\hbar^2}{2m}\psi_2''-V_0\cdot\psi_2=E\cdot\psi_2 \qquad k^2=+\frac{2m(E+V_0)}{\hbar^2}$$

$$-\frac{\hbar^2}{2m}\psi_3''=E\cdot\psi_3$$

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$$\psi_1''-\kappa^2\cdot\psi_1=0$$
$$\psi_3''-\kappa^2\cdot\psi_3=0$$
$$\psi_2''+k^2\cdot\psi_2=0$$

$\Psi_1 = A\cdot e^{\kappa x} + B\cdot e^{-\kappa x}$

normálhatóság

$\Psi_3 = C\cdot e^{\kappa x} + D\cdot e^{-\kappa x}$ $\quad B=0 \quad C=0$

$\Psi_2 = K\cdot e^{ikx} + L\cdot e^{-ikx}$

$\Psi$ folytonos: $A\cdot e^{-\kappa\cdot a} = K\cdot e^{-ika} + L\cdot e^{ika}$

$D\cdot e^{-\kappa a} = K\cdot e^{+ika} + L\cdot e^{-ika}$

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$\Psi'$ folytonos: $\kappa\cdot A\, e^{-\kappa\cdot a} = ik\cdot K\cdot e^{-ika} - ikL\cdot e^{+ika}$

$-\kappa\cdot D\cdot e^{-\kappa a} = ik\cdot K\cdot e^{ika} - ikL\cdot e^{-ika}$

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$[\hat{p},\hat{x}] = ?$

$[\hat{p},\hat{x}]\,\Psi = \hat{p}\hat{x}\Psi - \hat{x}\hat{p}\Psi = -i\hbar\frac{\partial}{\partial x}(x\Psi) + x\cdot i\hbar\frac{\partial\Psi}{\partial x} =$

$= -i\hbar\cdot\Psi \Rightarrow [\hat{p},\hat{x}] = -i\hbar$

$[\hat{p},\hat{A}(x)] = -i\hbar\frac{\partial\hat{A}}{\partial x}$

operátor négyzete $\left(\frac{d}{dx}+x\right)^2 = ?$

$\left(\frac{d}{dx}+x\right)\left(\frac{d}{dx}+x\right)\Psi = \frac{d^2}{dx^2}\Psi + \frac{d}{dx}(x\Psi) + x\frac{d\Psi}{dx} + x^2\Psi =$

$= \frac{d^2}{dx^2}\Psi + 2x\frac{d\Psi}{dx} + (x^2+1)\Psi$

$\Rightarrow \left(\frac{d}{dx}+x\right)^2 = \frac{d^2}{dx^2} + 2x\frac{d}{dx} + (x^2+1)$

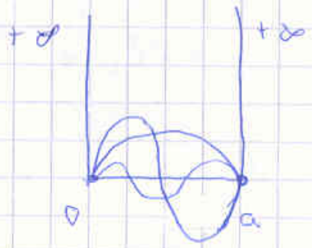
eltolás $\hat{T}(a)\,\Psi(x) = \Psi(x-a)$

$$\hat{T}(a)\,\Psi(x) = \sum_{n=0}^{\infty} \frac{(-a)^n}{n!} \frac{d^n}{dx^n}\Psi(x) = \underbrace{\sum_{n=0}^{\infty} \frac{\left(-a\frac{d}{dx}\right)^n}{n!}}_{e^{-a\cdot\frac{d}{dx}}} \Psi(x)$$

$$\boxed{\hat{T}(a) = e^{-a\frac{d}{dx}} = e^{\frac{i a \hat{p}}{\hbar}}}$$

$$\hat{p} = -i\hbar\frac{d}{dx}$$

végtelen potenciálgödör




$$k_n = \frac{n\cdot\pi}{a}$$

$$E_n = \frac{\hbar^2 k_n^2}{2m} = \frac{n^2\pi^2\hbar^2}{2m\cdot a^2}$$

$$\Psi_n(x) = \sqrt{\frac{2}{a}}\sin(k_n x) = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{a}\right)$$

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\underline{\Psi} + V\cdot\underline{\Psi} = i\hbar\frac{d\underline{\Psi}}{dt}$$

$$\underline{\Psi}(x,t) = \Psi(x)\cdot\Phi(t)$$

$$\swarrow \qquad \searrow$$

$$-\frac{\hbar^2}{2m}\frac{d^2\Psi}{dx^2} + V\cdot\Psi = E\cdot\Psi \qquad \Phi(t) = e^{-\frac{i}{\hbar}Et}$$

1) $\langle x\rangle = \text{konst}$, $\langle Q(x,p)\rangle = \text{konst}$ (stacionárius állapot)

2) $E$ = állandó

3) $\underline{\Psi}(x,t) = \sum_{n=0}^{\infty} c_n \Psi_n e^{-\frac{i}{\hbar}E_n t}$

$E > V_{min} \rightarrow$ hfv. normálhatósághoz

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \underset{\substack{\uparrow \\ \text{valós}}}{V(x)}$$

$$\Psi_n(x,t) = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{a}\right) e^{-i\frac{n^2\pi^2\hbar}{2ma^2}t}$$

$$\Psi(x,t) = \sum_{n=1}^{\infty} c_n \cdot \Psi_n(x,t)$$

$$\Psi(x,0) = \sum_{n=1}^{\infty} c_n \cdot \underbrace{\Psi_n(x,0)}_{\sqrt{\frac{2}{a}}\cdot\sin\left(\frac{n\pi x}{a}\right)}$$

$$c_n = \int_0^a \Psi_n^*(x,0)\,\Psi(x,0)\,dx = \int_0^a \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{a}\right)\Psi(x,0)\,dx$$

Végtelen gödörben $\sigma_x \cdot \sigma_p \geq \frac{\hbar}{2}$

$$\sigma_x^2 = \langle x^2\rangle - \langle x\rangle^2$$

$$\langle x\rangle_1 = \int_0^a \sqrt{\frac{2}{a}}\sin\left(\frac{\pi x}{a}\right)\cdot x\,\sqrt{\frac{2}{a}}\sin\left(\frac{\pi x}{a}\right) = \frac{2}{a}\int_0^a x\cdot\sin^2\left(\underbrace{\frac{\pi x}{a}}_{y}\right)dx$$

$$= \frac{2}{a}\cdot\left(\frac{a}{\pi}\right)^2 \underbrace{\int_0^\pi y\cdot\sin^2 y\,dy}$$

$$\int_0^\pi \frac{1-\cos(2y)}{2}\,y\,dy = \underbrace{\left[\frac{y^2}{4}\right]_0^\pi}_{\frac{\pi^2}{4}} - \frac{1}{2}\left\{\underbrace{\left[y\cdot\frac{\sin(2y)}{2}\right]_0^\pi}_{0} - \underbrace{\int_0^\pi \frac{\sin(2y)}{2}\,dy}_{0}\right\}$$

$$= \frac{2a}{\pi^2}\cdot\frac{\pi^2}{4} = \frac{a}{2}$$

$$\langle x^2\rangle_1 = \frac{2}{a}\cdot\left(\frac{a}{\pi}\right)^3\cdot\underbrace{\int_0^\pi y^2\cdot \sin^2 y\; dy}$$

$$\int_0^\pi \frac{1-\cos 2y}{2}\, y^2\, dy = \int_0^\pi \frac{y^2}{2}\, dy - \frac{1}{2}\left\{\underbrace{\left[y^2\cdot\frac{\sin(2y)}{2}\right]_0^\pi}_{0} - \int_0^\pi 2y\cdot\frac{\sin 2y}{2}\, dy\right\}$$

$$= \frac{\pi^3}{6} + \frac{1}{2}\int_0^\pi y \sin(2y)\, dy =$$

$$= \frac{\pi^3}{6} + \frac{1}{2}\left\{\underbrace{\left[y\,\frac{-\cos(2y)}{2}\right]_0^\pi}_{-\frac{1}{2}\pi} - \underbrace{\int_0^\pi \frac{-\cos(2y)}{2}\, dy}_{0}\right\} = \frac{\pi^3}{6} - \frac{\pi}{4}$$

$$\langle x^2\rangle_1 = \frac{2a^2}{\pi^3}\left(\frac{\pi^3}{6} - \frac{\pi}{4}\right) = \frac{a^2}{3} - \frac{a^2}{2\pi^2}$$

$$\sigma_x^2 = a^2\left(\frac{1}{3} - \frac{1}{2\pi^2}\right) - \frac{a^2}{4} \qquad \sigma_x = \sqrt{\frac{1}{12} - \frac{1}{2\pi^2}}\cdot a$$

$$\langle p\rangle_1 = \langle \psi_1 | -i\hbar\, \psi_1'\rangle = \ldots \int_0^a \sin\left(\frac{\pi x}{a}\right)\cos\left(\frac{\pi x}{a}\right) dx = 0$$

$$\langle p^2\rangle_1 = \langle \psi_1 | -\hbar^2\, \psi_1''\rangle = -\hbar^2\cdot\frac{2}{a}\cdot\int_0^a -\sin^2\left(\underbrace{\frac{\pi x}{a}}_{y}\right)\cdot\left(\frac{\pi}{a}\right)^2 dx =$$

$$= \frac{2\pi^2\hbar^2}{a^3}\cdot\frac{a}{\pi}\cdot\underbrace{\int_0^\pi \sin^2 y\; dy}_{\frac{\pi}{2}} = \frac{\hbar^2\pi^2}{a^2}$$

$$\sigma_p^2 = \frac{\hbar^2\pi^2}{a^2} \qquad \sigma_p = \frac{\hbar\pi}{a}$$

$$\sigma_x\cdot\sigma_p = \sqrt{\frac{\pi^2}{12} - \frac{1}{2}}\cdot\hbar \simeq 0{,}57\,\hbar$$

## Dirac-delta potenciál

$$V(x) = -V_0 \cdot \delta(x)$$

$$\delta(k \cdot x) = \frac{1}{|k|} \cdot \delta(x) \qquad \frac{d\Theta(x)}{dx} = \delta(x)$$

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} - V_0 \cdot \delta(x)$$

$$\hat{H}\Psi = E \cdot \Psi$$

$$-\frac{\hbar^2}{2m}\Psi''(x) - V_0 \cdot \delta(x)\,\Psi(x) = E \cdot \Psi(x)$$

$$\Psi''(x) = -\frac{2mE}{\hbar^2}\Psi(x) - \frac{2mV_0}{\hbar^2}\delta(x)\,\Psi(x)$$

$$\Psi''(x) = -\frac{2mE}{\hbar^2}\Psi(x) \quad \text{ha } x \neq 0$$

$x=0$ -ban derivált ugrik

$$\Psi'(+0) - \Psi'(-0) = -\frac{2mV_0}{\hbar^2}\Psi(0) \leftarrow \Psi(+0) = \Psi(-0) = \Psi(0)$$

folytonos


$$\Psi_1(0) = \Psi_2(0)$$

$$\Psi_2'(0) - \Psi_1'(0) = -\frac{2mV_0}{\hbar^2}\Psi(0)$$

$E<0$ kötött állapotok $\quad -\frac{2mE}{\hbar^2} = \kappa^2 \rightarrow E = -\frac{\hbar^2\kappa^2}{2m}$

$$\Psi_1'' = \kappa^2 \cdot \Psi_1 \rightarrow \Psi_1(x) = A \cdot e^{\kappa x} + \cancel{B \cdot e^{-\kappa \cdot x}}$$

$$\Psi_2'' = \kappa^2 \cdot \Psi_2 \rightarrow \Psi_2(x) = \cancel{C \cdot e^{\kappa \cdot x}} + D \cdot e^{-\kappa x}$$

$B=0 \quad C=0$ hogy négyzetesen integrálható legyen

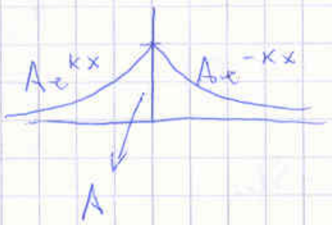
$$\Psi_1(0) = \Psi_2(0) \Rightarrow A = D$$

$$\Psi_2'(0) - \Psi_1'(0) = -\kappa \cdot D - \kappa \cdot A = -2\kappa \cdot A = -\frac{2mV_0}{\hbar^2} \cdot A$$

$$\Downarrow$$

$$\kappa = \frac{mV_0}{\hbar^2}$$

$$E = -\frac{\hbar^2}{2m}\left(\frac{mV_0}{\hbar^2}\right)^2 = -\frac{mV_0^2}{2\hbar^2}$$




$$\int |\Psi|^2 \, dx = 1$$

$$2 \cdot \int_0^\infty \left| A \cdot e^{-\kappa \cdot x} \right|^2 dx =$$

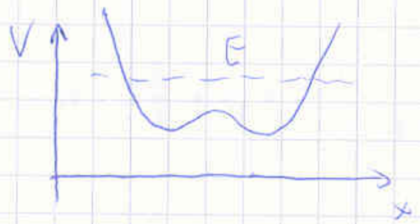
$$= 2 \cdot |A|^2 \cdot \int_0^\infty e^{-2\kappa \cdot x} \, dx = 2 \cdot |A|^2 \cdot \underbrace{\left[\frac{e^{-2\kappa \cdot x}}{-2\kappa}\right]_0^\infty}_{\frac{1}{2\kappa}} =$$

$$= \frac{|A|^2}{\kappa} = 1$$

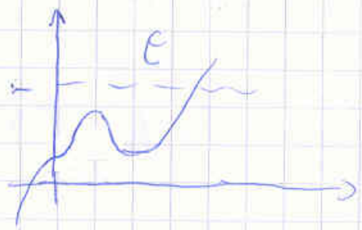
$$\rightarrow |A|^2 = \kappa \rightarrow \text{pl. } A = \sqrt{\kappa} = \sqrt{\frac{mV_0}{\hbar^2}}$$

$$\left.\begin{aligned} \langle x \rangle = 0 \quad & \langle x^2 \rangle = \ldots \\ \langle p \rangle = 0 \quad & \langle p^2 \rangle = \ldots \end{aligned}\right\} \Rightarrow \sigma_p \cdot \sigma_x = \frac{\hbar}{2}$$

$\int |\Psi|^2 \, dx = 1 \rightarrow$ ha ezt nem követeljük meg, akkor az előbb lehetett volna $E > 0$ is kötött állapotok




szórási állapotok

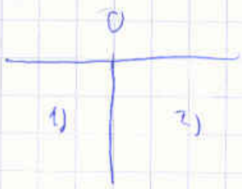



- normálható
- megszámlálható sok
- $E < V(-\infty)$ $E < V(+\infty)$

- nem normálható
- nem megszámlálható
- egyébként

---

$E > 0$ megoldások:




$$k^2 = \frac{2mE}{\hbar^2}$$

$$\psi'' = -k^2 \cdot \psi \qquad E = \frac{\hbar^2 k^2}{2m}$$

1) $\psi_1 = A \cdot e^{ikx} + B \cdot e^{-ikx}$

2) $\psi_2 = F \cdot e^{ikx} + G \cdot e^{-ikx}$

$$\psi_1(0) = \psi_2(0) \rightarrow A + B = F + G$$

$$\psi_2'(0) - \psi_1'(0) = ikF - ikG - ikA + ikB = -\frac{2mV_0}{\hbar^2}(A+B)$$

$$F - G = A - B + 2i \cdot \underbrace{\frac{mV_0}{k \cdot \hbar^2}}_{\beta}(A+B) = (1+2i\beta)A - (1-2i\beta)B$$

$$\Psi_1(x,t) = A\cdot e^{i\left(kx-\frac{E}{\hbar}t\right)} + B\cdot e^{-i\left(kx+\frac{E}{\hbar}t\right)} =$$

$$= A\cdot e^{ik\left(x-\frac{\hbar k}{2m}t\right)} + B\cdot e^{-ik\left(x+\frac{\hbar k}{2m}t\right)}$$

↓ jobbra terjedő ↓ balra terjedő

síkhullám

A : balról bejövő

B : balra ki

F : jobbra ki

G : jobbról be

balról érkező részecske → $G=0$

$$\frac{|B|^2}{|A|^2} ; \frac{|F|^2}{|A|^2} = ?$$

$\frac{|B|^2}{|A|^2} = R$ → reflexió

$\frac{|F|^2}{|A|^2} = T$ → transzmisszió

$R+T=1$

$$F = A(1+2i\beta) - B(1-2i\beta) = A+B$$

$$2i\beta(A+B) = 2B$$

$$A = \left(\frac{1}{i\beta}-1\right)B = \frac{1-i\beta}{i\beta}\cdot B$$

$$R = \frac{|B|^2}{|A|^2} = \left|\frac{i\beta}{1-i\beta}\right|^2 = \frac{\beta^2}{1+\beta^2}$$

$$T = \frac{|F|^2}{|A|^2} = 1-R = \frac{1}{1+\beta^2}$$

$\beta = \frac{m \cdot V_0}{\hbar^2} \cdot \frac{\hbar}{\sqrt{2mE}}$   $\beta^2 = \frac{m^2 V_0^2}{\hbar^2} \cdot \frac{1}{2mE}$

R, T csak $V_0^2$-től függ

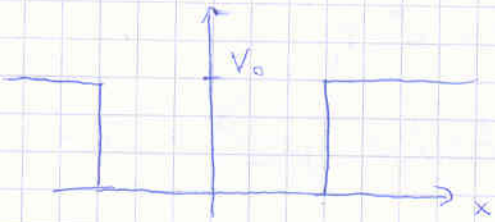
ekvivalensek

$E < V(+\infty)$
$E < V(-\infty)$   vagy

$\Downarrow$   $\Downarrow$

kötött álla.   szórás
normálható   $\emptyset$ norm.

lin. kombinációk mindkét esetben normálhatók, ha $E > V_{min}$





V páros → $\Psi_n$ ps v. ptl. fv.
$V(x) = V(-x)$

$\Psi(x)$ mo. → $\Psi(-x)$ is mo.

$\left.\begin{array}{l}\Psi(x) + \Psi(-x) \\ \Psi(x) - \Psi(-x)\end{array}\right\}$ is mo.

1d) kötött állapotok nem degeneráltak

$\hat{H}\Psi_1 = E \cdot \Psi_1$

$\hat{H}\Psi_2 = E \cdot \Psi_2$

$$-\frac{\hbar^2}{2m}\psi_1'' + V\cdot\psi_1 = E\cdot\psi_1 \qquad /\cdot\psi_2$$

$$-\quad -\frac{\hbar^2}{2m}\psi_2'' + V\cdot\psi_2 = E\cdot\psi_2 \qquad /\cdot\psi_1$$

$$-\frac{\hbar^2}{2m}\left(\psi_1''\psi_2 - \psi_1\psi_2''\right) = 0$$

$$\underbrace{\psi_1''\psi_2 - \psi_1\psi_2''}_{\left(\psi_1'\psi_2 - \psi_1\cdot\psi_2'\right)'} = 0$$

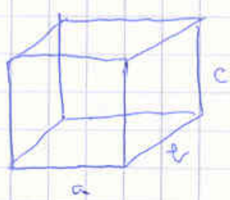
$\psi_1'\psi_2 - \psi_1\cdot\psi_2' = C = 0$ (négyzetes integrálhatóság miatt)

$$\psi_1'\psi_2 = \psi_1\cdot\psi_2'$$

$$\frac{\psi_1'}{\psi_1} = \frac{\psi_2'}{\psi_2} \qquad \ln\psi_1 = \ln\psi_2 + C'$$

$$\psi_1 = \underset{\underset{1}{\parallel}}{C''}\cdot\psi_2$$

## QM több dimenzióban




V belül 0, kívül $\infty$

$$-\frac{\hbar^2}{2m}\Delta\psi = E\cdot\psi$$

$$\Delta\psi = -\frac{2mE}{\hbar^2}\psi = -k^2\psi \qquad E = \frac{\hbar^2k^2}{2m}$$

$$\psi = X(x)\,Y(y)\,Z(z)$$

$$X'' \cdot Y \cdot Z + X \cdot Y'' \cdot Z + X \cdot Y \cdot Z'' = -k^2 X \cdot Y \cdot Z$$

$$\underset{-k_1^2}{\underset{\parallel}{\frac{X''}{X}}} + \underset{-k_2^2}{\underset{\parallel}{\frac{Y''}{Y}}} + \underset{-k_3^2}{\underset{\parallel}{\frac{Z''}{Z}}} = -k^2$$

$$X'' = -k_1^2 X \qquad X = A \sin(k_1 x) + B \cos(k_1 x)$$

határfelt: $X(0) = X(a) = 0$

$$X(x) = \sqrt{\frac{2}{a}} \sin(k_1 x) \qquad \sin(k_1 a) = 0 \Rightarrow k_1 = \frac{n_1 \pi}{a}$$

$$X(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n_1 \pi x}{a}\right)$$

$$E = \frac{\hbar^2}{2m}\left(k_1^2 + k_2^2 + k_3^2\right) = \frac{\hbar^2 \pi^2}{2m}\left(\frac{n_1^2}{a^2} + \frac{n_2^2}{b^2} + \frac{n_3^2}{c^2}\right)$$

$a \geq b \geq c \qquad n_1, n_2, n_3 = 1, 2, 3, \ldots$

$$E_1 = E_{111} = \frac{\hbar^2 \pi^2}{2m}\left(\frac{1}{a^2} + \frac{1}{b^2} + \frac{1}{c^2}\right)$$

$$E_2 = E_{211} = \frac{\hbar^2 \pi^2}{2m}\left(\frac{2}{a^2} + \frac{1}{b^2} + \frac{1}{c^2}\right)$$

spec.: $a = b = c$ kocka

$$E = \frac{\hbar^2 \pi^2}{2ma^2}\left(n_1^2 + n_2^2 + n_3^2\right)$$

$$E_1 = E_{111}$$

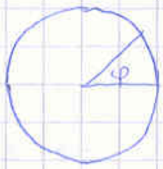
$$E_2 = E_{211} = E_{121} = E_{112}$$

$$E_3 = E_{221} = E_{212} = E_{122}$$

$$E_4 = E_{311} = E_{131} = E_{113}$$

$$\Psi(x,y,z) = \left(\frac{2}{a}\right)^{\frac{3}{2}} \cdot \sin\left(\frac{n_1 \pi x}{a}\right) \sin\left(\frac{n_2 \pi x}{a}\right) \sin\left(\frac{n_3 \pi x}{a}\right)$$

Síkrotátor




$$\hat{H} = \frac{\hat{p}_\varphi^2}{2\Theta} \qquad \hat{p}_\varphi = -i\hbar \frac{\partial}{\partial \varphi}$$

$$-\frac{\hbar^2}{2\Theta} \frac{\partial^2 \Psi}{\partial \varphi^2} = E \cdot \Psi$$

$$\frac{\partial^2 \Psi}{\partial \varphi^2} = -\underbrace{\frac{2\Theta E}{\hbar^2}}_{m^2} \Psi \qquad E > 0 \qquad E = \frac{m^2 \cdot \hbar^2}{2 \cdot \Theta}$$

$$\Psi = A \cdot e^{im\varphi} \qquad \int_0^{2\pi} |\Psi|^2 \, d\varphi = 1$$

$$|A|^2 \cdot 2\pi = 1 \rightarrow A = \frac{1}{\sqrt{2\pi}}$$

$$\varphi \rightarrow \varphi + 2\pi$$

$$e^{im\varphi} = e^{im(\varphi + 2\pi)}$$

$$1 = e^{im \cdot 2\pi} \qquad m \in \mathbb{Z}$$

$$E = \frac{\hbar^2 m^2}{2\Theta}$$

$m = 0 \rightarrow$ alapállapot

$m = \pm 1 \rightarrow$ kétszeresen degenerált

$m = \pm 2$

⋮

$\hat{p} = -i\hbar\nabla \qquad \hat{H} = -\frac{\hbar^2}{2m}\Delta$

$\hat{r} = r \qquad [\hat{r}_i, \hat{p}_j] = i\hbar\cdot\delta_{ij}$

$\hat{H}\Psi = E\cdot\Psi$

$\Psi(r,\vartheta,\varphi) = R(r)\,\Theta(\vartheta)\,\Phi(\varphi)$

$\varphi$: $\Phi(\varphi) = e^{im\varphi} \qquad m\in\mathbb{Z}$

$\vartheta$: $\Theta(\vartheta) = A\cdot P_\ell^m(\cos\vartheta)$ asszociált Legendre

$\ell = 0,1,2,\ldots$

$m = -\ell,\ldots,0,\ldots,+\ell$

$\Theta\cdot\Phi \to Y_\ell^m$ gömbfüggvények

$\underline{L} = \underline{r}\times\underline{p} \qquad L_x = y p_z - z p_y = -i\hbar(y\partial_z - z\partial_y)$

$L_\ell = -i\hbar\cdot\varepsilon_{\ell ij}\cdot x_i\cdot\partial_j$

$$[L_i, L_j]\Psi = (-i\hbar)^2\Big((\varepsilon_{ik\ell}\,x_k\,\partial_\ell)(\varepsilon_{jmn}\,x_m\,\partial_n) -$$

$$-(\varepsilon_{jmn}\,x_m\,\partial_n)(\varepsilon_{ik\ell}\,x_k\,\partial_\ell)\Big)\Psi =$$

$$= -\hbar^2\cdot\varepsilon_{ik\ell}\,\varepsilon_{jmn}\Big(x_k\,\partial_\ell(x_m\,\partial_n\Psi) - x_m\,\partial_n(x_k\,\partial_\ell\Psi)\Big) =$$

$$= -\hbar^2\cdot\varepsilon_{ik\ell}\,\varepsilon_{jmn}\Big(\cancel{x_k x_m\,\partial_\ell\partial_n\Psi} - \cancel{x_m x_k\,\partial_n\partial_\ell\Psi}$$

$$+ x_k\cdot\delta_{\ell m}\,\partial_n\Psi - x_m\cdot\delta_{nk}\cdot\partial_\ell\Psi\Big) =$$

$$= \ldots = i\hbar\cdot\varepsilon_{ijk}\cdot L_k\,\Psi$$

$$[L_i, L_j] = i\hbar\, \varepsilon_{ijk}\, L_k$$

$$\underline{L}^2 = L_x^2 + L_y^2 + L_z^2$$

$$[L^2, L_i] = 0$$

$$L^2 \psi_e^m = \hbar^2 e(e+1)\, \psi_e^m$$

$$L_z \psi_e^m = m \cdot \hbar \cdot \psi_e^m$$

$e = 0, 1, 2, \ldots$

$$L_\pm = L_x \pm i L_y$$

$m = -e, \ldots, e$

$$L_\pm \psi_e^m = \hbar \sqrt{e(e+1) - m(m\pm 1)}\; \psi_e^{m\pm 1}$$

$$\langle \psi_e^m , \psi_{e'}^{m'} \rangle = \delta_{mm'} \cdot \delta_{ee'}$$

$$\langle L_x \rangle = \langle \psi_e^m \,|\, L_x \psi_e^m \rangle = \langle \psi_e^m \,|\, -\tfrac{i}{\hbar}[L_y, L_z]\, \psi_e^m \rangle =$$

$$= -\frac{i}{\hbar} \langle \psi_e^m \,|\, (L_y L_z - L_z L_y)\, \psi_e^m \rangle =$$

$$= -\frac{i}{\hbar} \Big( \langle \psi_e^m \,|\, L_y \underbrace{L_z \psi_e^m}_{m\hbar \cdot \psi_e^m} \rangle - \langle \underbrace{L_z \psi_e^m}_{m\hbar \cdot \psi_e^m} \,|\, L_y \psi_e^m \rangle \Big)$$

$\hat{L}_z^+ = \hat{L}_z$

$$= -\frac{i}{\hbar} \cdot m\hbar \Big( \langle \psi_e^m \,|\, L_y \psi_e^m \rangle - \langle \psi_e^m \,|\, L_y \psi_e^m \rangle \Big) = 0$$

$\langle L_x^2 \rangle = ?$ $\qquad L_x = \dfrac{L_+ + L_-}{2}$

$$L_x^2 = \frac{1}{4}\left( L_+ L_+ + L_- L_- + L_+ L_- + L_- L_+ \right)$$

$$\langle L_x^2\rangle = \frac{1}{4}\langle\psi_\ell^m|(\underbrace{L_+L_+}_{\Downarrow\atop 0} + \underbrace{L_-L_-}_{\Downarrow\atop 0} + L_+L_- + L_-L_+)\,\psi_\ell^m\rangle =$$

$$= \frac{\hbar^2}{4}\langle\psi_\ell^m|\psi_\ell^m\rangle\Big(\sqrt{\ell(\ell+1) - m(m-1)}\,\sqrt{\ell(\ell+1) - (m-1)m} +$$

$$+ \sqrt{\ell(\ell+1) - m(m+1)}\cdot\sqrt{\ell(\ell+1) - (m+1)m}\Big)$$

$$= \frac{\hbar^2}{4}\Big(\ell(\ell+1) - m(m-1) + \ell(\ell+1) - m(m+1)\Big) =$$

$$= \frac{\hbar^2}{4}\left(2\ell(\ell+1) - 2m^2\right) = \frac{\hbar^2}{2}\left(\ell(\ell+1) - m^2\right) = \sigma_{L_x}^2$$

<u>Spin</u>

$S_i \qquad S^2 = \sum_i S_i^2$

$[S_i, S_j] = i\hbar\cdot\varepsilon_{ijk}\,S_k$

$[S^2, S_i] = 0 \qquad S_\pm$

ofv. $|s\ m\rangle$

$S^2\,|s\ m\rangle = \hbar\,s(s+1)\,|s\ m\rangle$

$S_z\,|s\ m\rangle = \hbar\cdot m\,|s\ m\rangle$

$S_\pm\,|s\ m\rangle = \hbar\sqrt{s(s+1) - m(m\pm1)}\,|s\ m\pm1\rangle$

$s = 0, \frac{1}{2}, 1, \ldots$

$m = -s, -s+1, \ldots, s$

$\mathcal{H}_1$ 1. részecske állapotai

$\mathcal{H}_2$ 2. részecske állapotai

$$\left.\begin{matrix}\mathcal{H}_1 \\ \mathcal{H}_2\end{matrix}\right\} \to \mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2$$

összetett rendszer

$\varphi_a, \varphi_b \in \mathcal{H}_1$

$\varphi_c, \varphi_d \in \mathcal{H}_2$

$$\langle \varphi_a \otimes \varphi_c \mid \varphi_b \otimes \varphi_d \rangle_{\mathcal{H}} = \langle \varphi_a \mid \varphi_b \rangle_{\mathcal{H}_1} \cdot \langle \varphi_c \mid \varphi_d \rangle_{\mathcal{H}_2}$$

$A_1 : \mathcal{H}_1 \to \mathcal{H}_1$

$A_2 : \mathcal{H}_2 \to \mathcal{H}_2$

$A : \mathcal{H} \to \mathcal{H} \qquad A = \mathbb{1} \otimes A_2 + A_1 \otimes \mathbb{1}$

$s = \frac{1}{2} \qquad \left|\frac{1}{2}\ \frac{1}{2}\right\rangle \qquad \left|\frac{1}{2}\ -\frac{1}{2}\right\rangle \qquad \chi_+ = \begin{pmatrix}1\\0\end{pmatrix} \qquad \chi_- = \begin{pmatrix}0\\1\end{pmatrix}$

$$\chi = a \cdot \chi_+ + b \cdot \chi_- = \begin{pmatrix}a\\b\end{pmatrix}$$

$$S_z \cdot \chi_+ = \hbar \cdot \frac{1}{2} \cdot \chi_+ \qquad S_z \cdot \chi_- = \hbar \cdot \left(-\frac{1}{2}\right) \cdot \chi_-$$

$S_z \to |a|^2$ valószínűséggel $+\frac{1}{2}\hbar$

$|b|^2$ valószínűséggel $-\frac{1}{2}\hbar$

$1/2$ spin $\quad \left|\frac{1}{2}\ \frac{1}{2}\right\rangle \quad \left|\frac{1}{2}\ -\frac{1}{2}\right\rangle$

$$\chi_+ = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \qquad \chi_- = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \qquad \chi = a\chi_+ + b\chi_- = \begin{pmatrix} a \\ b \end{pmatrix}$$

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

$$S_z \chi_+ = \frac{1}{2}\hbar\chi_+ \qquad S_z\chi_- = -\frac{1}{2}\hbar\chi_-$$

$S_z$ mérése: $\quad \frac{\hbar}{2} \quad |a|^2$

$\qquad\qquad -\frac{\hbar}{2} \quad |b|^2$

$S_x$-et mérjük?

$$S_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \longrightarrow \lambda_{1/2} = \pm\frac{\hbar}{2}$$

$$\begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix} = \chi_+^{(x)} \qquad \begin{pmatrix} \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} \end{pmatrix} = \chi_-^{(x)}$$

$$\chi = c\chi_+^{(x)} + d\chi_-^{(x)} = \begin{pmatrix} \frac{c+d}{\sqrt{2}} \\ \frac{c-d}{\sqrt{2}} \end{pmatrix} = \begin{pmatrix} a \\ b \end{pmatrix}$$

$$c = \frac{a+b}{\sqrt{2}} \qquad d = \frac{a-b}{\sqrt{2}}$$

$S_x$ mérése: $\quad \frac{\hbar}{2} \quad \frac{(a+b)^2}{2}$

$\qquad\qquad -\frac{\hbar}{2} \quad \frac{(a-b)^2}{2}$

$\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2 \qquad A_1 : \mathcal{H}_1 \to \mathcal{H}_1$

$\qquad\qquad\qquad\qquad\quad A_2 : \mathcal{H}_2 \to \mathcal{H}_2$

$A : \mathcal{H} \to \mathcal{H} \qquad \mathbb{1} \otimes A_2 + A_1 \otimes \mathbb{1}$

2 részecske

$\chi_1, \chi_2$

$$S_z (\chi_1 \otimes \chi_2) = (\mathbb{1} \otimes S_z^{(2)} + S_z^{(1)} \otimes \mathbb{1}) (\chi_1 \otimes \chi_2) =$$

$$= \chi_1 \otimes S_z^{(2)} \chi_2 + S_z^{(1)} \chi_1 \otimes \chi_2 =$$

$$= \chi_1 \otimes \hbar m_2 \chi_2 + \hbar m_1 \chi_1 \otimes \chi_2 =$$

$$= \hbar \underbrace{(m_1 + m_2)}_{m} (\chi_1 \otimes \chi_2)$$

$$|s_1 \; m_1\rangle \otimes |s_2 \; m_2\rangle \Rightarrow |s \; m\rangle \qquad m = m_1 + m_2$$

$\frac{1}{2} \otimes \frac{1}{2}$ $\qquad\qquad s = s_1 + s_2, \ldots, |s_1 - s_2|$

1. lépés legnagyobb $s$, legnagyobb $m$

$$\begin{pmatrix} s = 1 & s = 0 \\ m = 1, 0, -1 & m = 0 \end{pmatrix}$$

$S_-$: $|1 \; 1\rangle \to |1 \; 0\rangle \to |1 \; -1\rangle$; $|1 \; 0\rangle \xrightarrow{\text{ort.}} |0 \; 0\rangle$

$$|1 \; 1\rangle = |\tfrac{1}{2} \; \tfrac{1}{2}\rangle \otimes |\tfrac{1}{2} \; \tfrac{1}{2}\rangle$$

2. lépés $\qquad S_- |s \; m\rangle = \hbar \sqrt{s(s+1) - m(m-1)} \, |s \; m-1\rangle$

$$S_- |1 \; 1\rangle = \hbar \sqrt{2 - 0} \, |1 \; 0\rangle$$

$$S_-\left(\left|\tfrac12\ \tfrac12\right\rangle \otimes \left|\tfrac12\ \tfrac12\right\rangle\right) = \hbar \underbrace{\sqrt{\left(\tfrac12\right)\left(\tfrac32\right) - \left(\tfrac12\right)\left(-\tfrac12\right)}}_{1} \left|\tfrac12\ -\tfrac12\right\rangle \otimes \left|\tfrac12\ \tfrac12\right\rangle$$

$$+ \left|\tfrac12\ \tfrac12\right\rangle \otimes 1 \cdot \left|\tfrac12\ -\tfrac12\right\rangle$$

$$\Rightarrow \left|1\ 0\right\rangle = \frac{1}{\sqrt{2}} \left|\tfrac12\ -\tfrac12\right\rangle \otimes \left|\tfrac12\ \tfrac12\right\rangle +$$

$$+ \frac{1}{\sqrt{2}} \left|\tfrac12\ \tfrac12\right\rangle \otimes \left|\tfrac12\ -\tfrac12\right\rangle$$

<u>2. lépés újra</u>

$$S_- \left|1\ 0\right\rangle = \ldots$$

$$S_-\left(\frac{1}{\sqrt{2}} \left(\left|\tfrac12\ -\tfrac12\right\rangle \otimes \left|\tfrac12\ \tfrac12\right\rangle + \left|\tfrac12\ \tfrac12\right\rangle \otimes \left|\tfrac12\ -\tfrac12\right\rangle\right)\right) =$$

$$= \ldots \cdot \left|\tfrac12\ -\tfrac12\right\rangle \otimes \left|\tfrac12\ -\tfrac12\right\rangle$$

$$\Rightarrow \left|1\ -1\right\rangle = \left|\tfrac12\ -\tfrac12\right\rangle \otimes \left|\tfrac12\ -\tfrac12\right\rangle$$

---

$$\left|1\ 0\right\rangle \cdot \left|0\ 0\right\rangle = 0 \qquad |a|^2 + |b|^2 = 1$$

$$\left|0\ 0\right\rangle = a \left|\tfrac12\ -\tfrac12\right\rangle \otimes \left|\tfrac12\ \tfrac12\right\rangle + b \left|\tfrac12\ \tfrac12\right\rangle \otimes \left|\tfrac12\ -\tfrac12\right\rangle$$

$$0 = \left(\frac{1}{\sqrt{2}} \left|\tfrac12\ -\tfrac12\right\rangle \otimes \left|\tfrac12\ \tfrac12\right\rangle + \frac{1}{\sqrt{2}} \left|\tfrac12\ \tfrac12\right\rangle \otimes \left|\tfrac12\ -\tfrac12\right\rangle\right) \cdot$$

$$\cdot \left(a \left|\tfrac12\ -\tfrac12\right\rangle \otimes \left|\tfrac12\ \tfrac12\right\rangle + b \left|\tfrac12\ \tfrac12\right\rangle \otimes \left|\tfrac12\ -\tfrac12\right\rangle\right)$$

$$0 = a\cdot\frac{1}{\sqrt{2}} + 0 + 0 + b\cdot\frac{1}{\sqrt{2}} \to a = -b$$

$$|0\ \ 0\rangle = \frac{1}{\sqrt{2}}\left|\tfrac{1}{2}\ \ -\tfrac{1}{2}\right\rangle \otimes \left|\tfrac{1}{2}\ \ \tfrac{1}{2}\right\rangle - \frac{1}{\sqrt{2}}\left|\tfrac{1}{2}\ \ \tfrac{1}{2}\right\rangle \otimes \left|\tfrac{1}{2}\ \ -\tfrac{1}{2}\right\rangle$$

<u>$j_1 \otimes j_2$</u>

$$j_1 + j_2 = j \qquad m = j$$

$$|j_1 + j_2\ \ j_1 + j_2\rangle = |j_1\ \ j_1\rangle \otimes |j_2\ \ j_2\rangle$$

$$|j\ \ m\rangle = \sum_{m = m_1 + m_2} C^{j_1 j_2 j}_{m_1 m_2 m}\ |j_1\ \ m_1\rangle \otimes |j_2\ \ m_2\rangle$$

$$\uparrow$$

Clebsch - Gordon eh.

előbb pl.: $C^{-\frac{1}{2}\ \frac{1}{2}\ 0}_{-\frac{1}{2}\ \frac{1}{2}\ 0} = \frac{1}{\sqrt{2}}$

$$C^{\frac{1}{2}\ \frac{1}{2}\ 0}_{\frac{1}{2}\ -\frac{1}{2}\ 0} = -\frac{1}{\sqrt{2}}$$

<u>1. lépés</u>

$$\begin{tikzcd}
|j\ \ j\rangle \arrow[d] & & \\
|j\ \ j-1\rangle \arrow[r] \arrow[d] & |j-1\ \ j-1\rangle \arrow[d] & \\
|j\ \ j-2\rangle & |j-1,\ j-2\rangle \arrow[r] & |j-2\ \ j-2\rangle \\
\vdots & & \\
|j\ \ -j\rangle & &
\end{tikzcd}$$

$s_1 = 1 \quad m_1 = 1, 0, -1$

$s_2 = \frac{1}{2} \quad m_2 = \frac{1}{2}, -\frac{1}{2}$

$s = \frac{3}{2}, \frac{1}{2}$

1) $\left|\frac{3}{2}\ \frac{3}{2}\right\rangle = |1\ 1\rangle \otimes \left|\frac{1}{2}\ \frac{1}{2}\right\rangle$

2)
$$S_- \left|\frac{3}{2}\ \frac{3}{2}\right\rangle = \hbar \underbrace{\sqrt{\frac{3}{2}\left(\frac{3}{2}+1\right) - \frac{3}{2}\left(\frac{3}{2}-1\right)}}_{\sqrt{3}} \left|\frac{3}{2}\ \frac{1}{2}\right\rangle$$

$$S_-\left(|1\ 1\rangle \otimes \left|\frac{1}{2}\ \frac{1}{2}\right\rangle\right) = \hbar\sqrt{1(1+1) - 0}\ |1\ 0\rangle \left|\frac{1}{2}\ \frac{1}{2}\right\rangle +$$

$$+ |1\ 1\rangle\ \hbar\sqrt{\frac{1}{2}\,\frac{3}{2} - \frac{1}{2}\left(-\frac{1}{2}\right)}\ \left|\frac{1}{2}\ -\frac{1}{2}\right\rangle =$$

$$= \hbar\sqrt{2}\ |1\ 0\rangle \left|\frac{1}{2}\ \frac{1}{2}\right\rangle + \hbar\ |1\ 1\rangle \left|\frac{1}{2}\ -\frac{1}{2}\right\rangle$$

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

$$C^{1\ \frac{1}{2}\ \frac{3}{2}}_{0\ \frac{1}{2}\ \frac{1}{2}} \qquad\qquad C^{1\ \frac{1}{2}\ \frac{3}{2}}_{1\ -\frac{1}{2}\ \frac{1}{2}}$$

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

2) $\left|\frac{3}{2}\ -\frac{1}{2}\right\rangle = ?$

$$S_- \left|\frac{3}{2}\ \frac{1}{2}\right\rangle = \hbar \underbrace{\sqrt{\frac{3}{2}\left(\frac{3}{2}+1\right) - \frac{1}{2}\left(\frac{1}{2}-1\right)}}_{2} \left|\frac{3}{2}\ -\frac{1}{2}\right\rangle$$

$$S_-(\dots) = \sqrt{\tfrac{2}{3}}\,\hbar\sqrt{2}\,|1\ -1\rangle\left|\tfrac{1}{2}\ \tfrac{1}{2}\right\rangle + \sqrt{\tfrac{2}{3}}\,|1\ 0\rangle\,\hbar\,1\cdot\left|\tfrac{1}{2}\ -\tfrac{1}{2}\right\rangle$$

$$+\tfrac{1}{\sqrt{3}}\hbar\sqrt{2}\,|1\ 0\rangle\left|\tfrac{1}{2}\ -\tfrac{1}{2}\right\rangle$$

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

$$\Rightarrow \left|\tfrac{3}{2}\ -\tfrac{1}{2}\right\rangle = \tfrac{1}{\sqrt{3}}|1\ -1\rangle\left|\tfrac{1}{2}\ \tfrac{1}{2}\right\rangle + \sqrt{\tfrac{2}{3}}\,|1\ 0\rangle\left|\tfrac{1}{2}\ -\tfrac{1}{2}\right\rangle$$

3) $$\left|\tfrac{1}{2}\ -\tfrac{1}{2}\right\rangle = -\sqrt{\tfrac{2}{3}}\,|1\ -1\rangle\left|\tfrac{1}{2}\ \tfrac{1}{2}\right\rangle + \tfrac{1}{\sqrt{3}}|1\ 0\rangle\left|\tfrac{1}{2}\ -\tfrac{1}{2}\right\rangle$$

$$\left|\tfrac{3}{2}\ -\tfrac{3}{2}\right\rangle = |1\ -1\rangle\left|\tfrac{1}{2}\ -\tfrac{1}{2}\right\rangle$$

$j_1 = 1 \quad j_2 = \frac{1}{2}$ rendszer

$j = \frac{3}{2} \quad m = \frac{1}{2}$ tudom, egyértelműen

mekkora a valószínűsége, hogy $m_1 = 0 \quad m_2 = \frac{1}{2}$ ?

$$\left|C^{j_1 j_2 j}_{m_1 m_2 m}\right|^2 = \frac{2}{3}$$

$$|j\ m\rangle = \sum_{\substack{m_1, m_2 \\ m_1+m_2=m}} C^{j_1 j_2 j}_{m_1 m_2 m}\,|j_1\ m_1\rangle \otimes |j_2\ m_2\rangle$$

$$|j_1\ m_1\rangle \otimes |j_2\ m_2\rangle = \sum_j C^{j_1 j_2 j}_{m_1 m_2 m}\,|j\ m\rangle \qquad m = m_1 + m_2$$

$$\left|\tfrac{1}{2}\ \tfrac{1}{2}\right\rangle \otimes \left|\tfrac{1}{2}\ -\tfrac{1}{2}\right\rangle = \frac{1}{\sqrt{2}}|1\ 0\rangle + \frac{1}{\sqrt{2}}|0\ 0\rangle$$

$$C^{\frac{1}{2}\,\frac{1}{2}\,1}_{\frac{1}{2}\,-\frac{1}{2}\,0} \qquad C^{\frac{1}{2}\,\frac{1}{2}\,0}_{\frac{1}{2}\,-\frac{1}{2}\,0}$$

$s_1 = s_2 = \frac{1}{2}$

$m_1 = \frac{1}{2} \qquad m_2 = -\frac{1}{2}$

mekkora a valószínűsége, hogy $s=1$ $m=0$?

$|C|^2 = \frac{1}{2}$

$$|1\ 1\rangle \left|\tfrac{1}{2}\ -\tfrac{1}{2}\right\rangle = \frac{1}{\sqrt{3}}\left|\tfrac{3}{2}\ \tfrac{1}{2}\right\rangle - \sqrt{\frac{2}{3}}\left|\tfrac{1}{2}\ \tfrac{1}{2}\right\rangle$$

<u>Variációs módszer</u>

1d

$E_0 = ?$ felső becslés

$E_0 \le \langle\Psi|\hat{H}\Psi\rangle = E_{a_1, a_2, \dots}$

$\Psi(a_1, a_2, \dots, a_N)$

$E_{a_1, a_2, \dots}$ minimuma $\qquad \dfrac{\partial E_{a_1, a_2, \dots}}{\partial a_i} = 0$

ha $\Psi$ nem normált: $\dfrac{\langle\Psi|\hat{H}\Psi\rangle}{\langle\Psi|\Psi\rangle}$

pl.: $V(x) = V_0|x|$

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V_0|x|$$

$$\psi = \frac{1}{a^2 + x^2} \cdot \cancel{A} \qquad (A \dots)$$

$$\langle \psi | \psi \rangle \neq 1 \qquad \int_{-\infty}^{+\infty} \frac{1}{(a^2+x^2)^2}\, dx = \frac{1}{a^3} \int_{-\infty}^{+\infty} \frac{1}{(1+y^2)^2}\, dy =$$

$$y = \frac{x}{a}$$

$$= \frac{1}{a^3} \int_{-\infty}^{+\infty} \left( \frac{1+y^2}{(1+y^2)^2} - \frac{y^2}{(1+y^2)^2} \right) dy =$$

$$= \underbrace{\frac{1}{a^3} \int_{-\infty}^{+\infty} \frac{1}{1+y^2}\, dy}_{\left[\operatorname{arctg} y\right]_{-\infty}^{+\infty} = \pi} - \frac{1}{a^3} \int_{-\infty}^{+\infty} \frac{y^2}{(1+y^2)^2}\, dy$$

$$\left( \frac{1}{1+y^2} \right)' = -\frac{1}{(1+y^2)^2} \cdot 2y$$

$$\frac{1}{2} \int_{-\infty}^{+\infty} \frac{-2y}{(1+y^2)^2}\, y\, dy = \frac{1}{2} \underbrace{\left[ \frac{1}{1+y^2}\, y \right]_{-\infty}^{+\infty}}_{0} - \frac{1}{2} \underbrace{\int_{-\infty}^{+\infty} \frac{1}{1+y^2}\, dy}_{\pi}$$

$$= \frac{1}{a^3} \left( \pi - \frac{\pi}{2} \right) = \frac{1}{a^3} \cdot \frac{\pi}{2}$$

$$\langle \psi | V_0 |x| \psi \rangle = V_0 \int_{+\infty}^{+\infty} \frac{1}{(a^2+x^2)^2} |x|\, dx = \frac{V_0}{a^2} \int_{-\infty}^{+\infty} \frac{|y|}{(1+y^2)^2}\, dy =$$

$$= 2 V_0 \frac{1}{a^2} \int_0^{\infty} \frac{y}{(1+y^2)^2}\, dy = \frac{V_0}{a^2} \left[ -\frac{1}{1+y^2} \right]_0^{\infty} = \frac{V_0}{a^2}$$

$$\langle\psi| -\frac{\hbar^2}{2m}\psi''\rangle =$$

$$\psi' = -\frac{1}{(a^2+x^2)^2}\cdot 2x$$

$$\psi'' = \frac{-2(a^2+x^2)^2 + 2x\cdot 2(a^2+x^2)\,2x}{(a^2+x^2)^2} = \frac{-2a^4-4a^2x^2-2x^4+8x^2a^2+8x^4}{(a^2+x^2)^4} =$$

$$= \frac{-2a^4+4a^2x^2+6x^4}{(a^2+x^2)^4}$$

$$= \frac{\hbar^2}{m}\int_{-\infty}^{+\infty}\frac{a^4-2a^2x^2-3x^4}{(a^2+x^2)^5}\,dx = \frac{\hbar^2}{m}\cdot\frac{1}{a^5}\cdot B \qquad B=\frac{\pi}{4}$$

$$E_a = \frac{\langle\psi|\hat{H}\psi\rangle}{\langle\psi|\psi\rangle} = \frac{\frac{\hbar^2}{m}\cdot\frac{1}{a^5}\cdot\frac{\pi}{4}+\frac{V_0}{a^2}}{\frac{1}{a^3}\cdot\frac{\pi}{2}} = \frac{\hbar^2}{2m}\cdot\frac{1}{a^2}+\frac{2V_0}{\pi}\cdot a$$

$$\frac{\partial E_a}{\partial a} = -\frac{\hbar^2}{m}\cdot\frac{1}{a^3}+\frac{2V_0}{\pi} = 0$$

$$a_{min} = \sqrt{\frac{\hbar^2\pi}{2V_0 m}}$$

$$E_{min} = E_a\Big|_{a_{min}} \geq E_0$$

Spin $|s\ m\rangle$

$S^2,\ S_z$

$$S^2|s\ m\rangle = \hbar^2 s(s+1)\,|s\ m\rangle$$

$$S_z\,|s\ m\rangle = \hbar m\,|s\ m\rangle$$

$$S_\pm\,|s\ m\rangle = \hbar\sqrt{s(s+1)-m(m\pm 1)}\ |s\ m\pm 1\rangle$$

$$|s_1\ m_1\rangle \otimes |s_2\ m_2\rangle \to |s\ m\rangle$$

$$|s\ m\rangle = \sum_{\substack{m_1, m_2 \\ m_1+m_2=m}} C^{s_1\,s_2\,s}_{m_1\,m_2\,m}\,|s_1\ m_1\rangle \otimes |s_2\ m_2\rangle$$

$$|s_1\ m_1\rangle \otimes |s_2\ m_2\rangle = \sum_{s} C^{s_1\,s_2\,s}_{m_1\,m_2\,m}\,|s\ m\rangle$$

Variációs módszer

$V(x)$ bonyolult

$$E_0 \le \frac{\langle\psi|\hat{H}\psi\rangle}{\langle\psi|\psi\rangle} \qquad \psi(a_1, a_2, \ldots)$$

$$V(x) = -\alpha\cdot\delta(x) \qquad E_0 = -\frac{m\alpha^2}{2\hbar^2}$$

$$\psi = A\cdot e^{-bx^2}$$

$$\int|\psi|^2 = 1 \qquad \int|\psi|^2\,dx = |A|^2\cdot\int_{-\infty}^{+\infty} e^{-2bx^2}\,dx = |A|^2\cdot\sqrt{\frac{\pi}{2b}} = 1$$

$$A = \left(\frac{2b}{\pi}\right)^{1/4}$$

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} - \alpha\cdot\delta(x)$$

$$\int \psi^* \left(-\alpha\,\delta(x)\right)\psi\, dx = |A|^2(-\alpha)\int_{-\infty}^{+\infty} e^{-2bx^2}\,\delta(x)\,dx =$$

$$= |A|^2\cdot(-\alpha) = -\alpha\sqrt{\frac{2b}{\pi}}$$

$$\psi' = A(-2bx)\,e^{-bx^2}$$

$$\psi'' = A\left(-2b + (-2bx)^2\right)e^{-bx^2} = A\cdot 2b\cdot\left(2bx^2-1\right)e^{-bx^2}$$

$$-\frac{\hbar^2}{2m}\int \psi^*\psi''\,dx = -\frac{\hbar^2}{2m}|A|^2\int_{-\infty}^{+\infty} 2b\left(2bx^2-1\right)e^{-2bx^2}\,dx =$$

$$= -\frac{\hbar^2\cdot b}{m}\sqrt{\frac{2b}{\pi}}\int_{-\infty}^{+\infty}\left(\underbrace{2b\cdot x^2\cdot e^{-2bx^2}}_{2b\cdot\frac{2\sqrt{\pi}}{4(2b)^{3/2}}} - \underbrace{e^{-2bx^2}}_{\sqrt{\frac{\pi}{2b}}}\right)$$

$$= -\frac{\hbar^2 b}{m}\left(-1+\frac{1}{2}\right) = +\frac{\hbar^2 b}{2m}$$

$$\langle\psi|\hat{H}\psi\rangle = \frac{\hbar^2 b}{2m} - \alpha\sqrt{\frac{2b}{\pi}} = f(b)$$

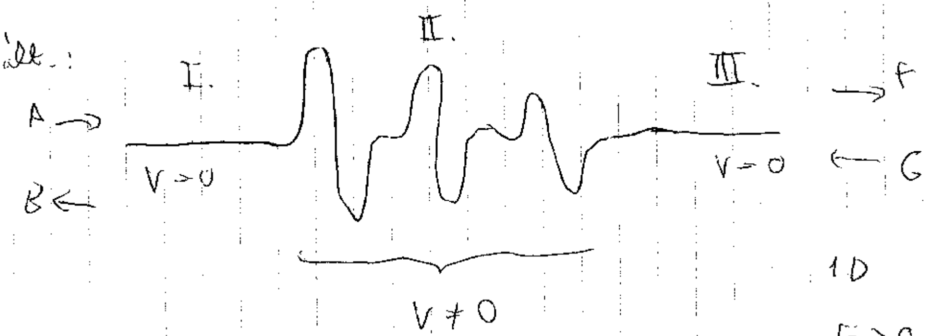
$$f'(b) = \frac{\hbar^2}{2m} - \sqrt{\frac{2}{\pi}}\,\alpha\cdot\frac{1}{2\sqrt{b}} = 0$$

$$\frac{\hbar^2}{m} = \sqrt{\frac{2}{\pi b}}\cdot\alpha \qquad b_{min} = \frac{2\alpha^2 m^2}{\hbar^4\pi}$$

$$f(b_{min}) = -\frac{m\alpha^2}{\pi\cdot\hbar^2} > E_0$$

# Szórásmátrix, transzfer mátrix

Ált.:




1D

$E > 0$

$k = \sqrt{\frac{2mE}{\hbar^2}}$

$$\Psi_{I}(x) = A e^{ikx} + B e^{-ikx}$$

$$\Psi_{III}(x) = F \cdot e^{ikx} + G \cdot e^{-ikx}$$

$$\Psi_{II}(x) = C \cdot f(x) + D \cdot g(x)$$

4 határfeltétel $\quad 2 + 2$

$A, B, \cancel{C, D}, F, G$

$$B = S_{11} A + S_{12} G$$

$$F = S_{21} A + S_{22} G$$

$$S = \begin{pmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{pmatrix}$$

$$\begin{pmatrix} B \\ F \end{pmatrix} = S \begin{pmatrix} A \\ G \end{pmatrix}$$

balról: $G = 0$

$$R_L = \left|\frac{B}{A}\right|^2 = |S_{11}|^2 \qquad T_L = \left|\frac{F}{A}\right|^2 = |S_{21}|^2$$

jobbról: $A = 0$

$$R_R = \left|\frac{F}{G}\right|^2 = |S_{22}|^2 \qquad T_R = \left|\frac{B}{G}\right|^2 = |S_{12}|^2$$

$E < 0$

$$\Psi_I(x) = A \cdot e^{-\kappa x} + B \cdot e^{+\kappa x} \qquad \kappa = \sqrt{\frac{-2mE}{\hbar^2}}$$

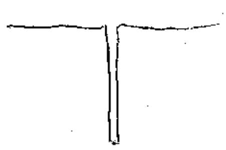
$$\Psi_{II}(x) = C \cdot f(x) + D \cdot g(x)$$

$$\Psi_{III}(x) = F \cdot e^{-\kappa x} + G \cdot e^{+\kappa x}$$

$$k \to +i\kappa$$

$$A, G = 0 \qquad B \neq 0 \qquad F \neq 0$$

$$\begin{pmatrix} B \\ F \end{pmatrix} = S \begin{pmatrix} A \\ G \end{pmatrix}$$ $S$ tartalmaz '$\infty$' elemet

pl.: 

$$T = \left|\frac{F}{A}\right|^2 = \frac{1}{1+\beta^2} \qquad \beta^2 = \left(\frac{mV_0}{\hbar^2 k}\right)^2$$

$$T = \frac{1}{1 + \frac{m^2 V_0^2}{\hbar^4 k^2}} \xrightarrow[k \to i\kappa]{} \frac{1}{1 - \frac{m^2 V_0^2}{\hbar^2 \kappa^2}} \to \infty$$

$$\kappa^2 = \frac{m^2 V_0^2}{\hbar^4}$$

$\kappa = \frac{mV_0}{\hbar^2}$ a kötött állapot energiája

Transzfer mátrix

$$F = M_{11} \cdot A + M_{12} \cdot B \qquad B = S_{11} A + S_{12} G$$

$$G = M_{21} \cdot A + M_{22} \cdot B \qquad F = S_{21} A + S_{22} G$$

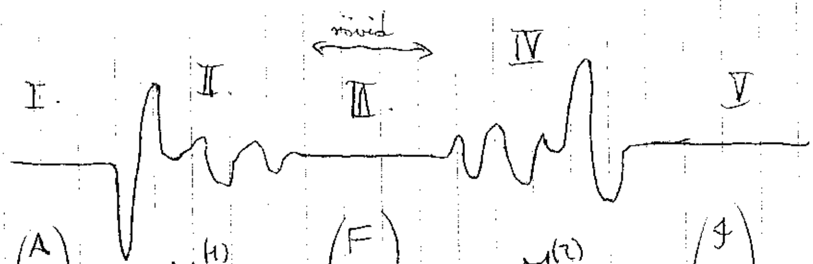
$$B = \underbrace{\frac{1}{M_{22}}}_{S_{12}} \cdot G - \underbrace{\frac{M_{21}}{M_{22}}}_{S_{11}} \cdot A \qquad B = \frac{1}{M_{12}} \cdot F - \frac{M_{11}}{M_{12}} A$$

$$F = M_{11} A + M_{12} \left( \frac{1}{M_{22}} G - \frac{M_{21}}{M_{22}} A \right) =$$

$$= \underbrace{A \left( M_{11} - \frac{M_{12} M_{21}}{M_{22}} \right)}_{S_{21}} + G \cdot \underbrace{\frac{M_{12}}{M_{22}}}_{S_{22}}$$

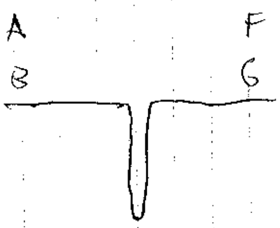
$$R_L = |S_{11}|^2 = \left| -\frac{M_{21}}{M_{22}} \right|^2$$

$$T_L = |S_{21}|^2 = \left| M_{11} - \frac{M_{12} M_{21}}{M_{22}} \right|^2$$




$$\begin{pmatrix} A \\ B \end{pmatrix} \quad M^{(1)} \quad \begin{pmatrix} F \\ G \end{pmatrix} \quad M^{(2)} \quad \begin{pmatrix} J \\ K \end{pmatrix}$$

$$M = M^{(2)} M^{(1)} \qquad \begin{pmatrix} J \\ K \end{pmatrix} = M \begin{pmatrix} A \\ B \end{pmatrix}$$

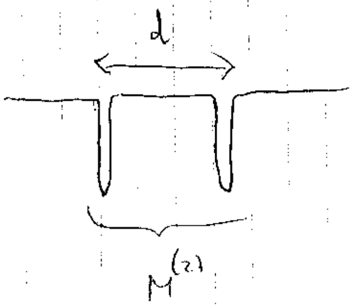



$$A + B = F + G$$

$$F - G = A(1 + 2i\beta) - B(1 - 2i\beta)$$

$$F = \_\_\_ \cdot A + \_\_\_ \cdot B$$

$$G = \_\_\_ \cdot A + \_\_\_ \cdot B$$




$$M^{(2)} = M^{(1)} M^{(0)} M^{(1)}$$

$$M^{(1)} = \begin{pmatrix} 1+i\beta & +i\beta \\ -i\beta & 1-i\beta \end{pmatrix} \qquad M^{(d)} = \begin{pmatrix} e^{ikd} & 0 \\ 0 & e^{-ikd} \end{pmatrix}$$

$$M^{(2)} = \begin{pmatrix} 1+i\beta & +i\beta \\ -i\beta & 1-i\beta \end{pmatrix} \begin{pmatrix} e^{ikd} & 0 \\ 0 & e^{-ikd} \end{pmatrix} \begin{pmatrix} 1+i\beta & +i\beta \\ -i\beta & 1-i\beta \end{pmatrix} - \dots$$

$$T_L = \left| M_{11} - \frac{M_{12} \cdot M_{21}}{M_{22}} \right|^2 = T_L(d, \beta, k)$$

<u>Perturbációszámítás</u>

$$\hat{H} = \hat{H}_0 + \hat{K} \qquad E_n^{(0)} \psi_n^{(0)} = \hat{H}_0 \psi_n^{(0)} \qquad \hat{H} \to E, \psi \,?$$

$$E_n = E_n^{(0)} + E_n^{(1)} + E_n^{(2)} + \dots \qquad \hat{H} \psi_n = E_n \psi_n \; ↯$$

$$\psi_n = \psi_n^{(0)} + \psi_n^{(1)} + \psi_n^{(2)} + \dots$$

<u>Feltétel:</u> · $K$ "kicsi" $\quad \| K \psi_n \| \ll |E_n - E_k| \quad \forall n \neq k$

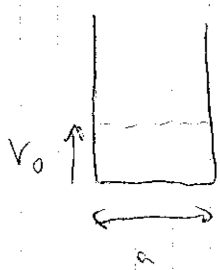
· egyszeres sajátérték

$$E_n^{(1)} = \langle \psi_n^{(0)} | \hat{K} \psi_n^{(0)} \rangle$$

$$\psi_n^{(1)} = \sum_{m \neq n} \frac{\langle \psi_m^{(0)} | \hat{K} \psi_n^{(0)} \rangle}{E_n^{(0)} - E_m^{(0)}} \psi_m^{(0)}$$

$$E_n^{(2)} = \sum_{m \neq n} \frac{\left| \langle \psi_m^{(0)} | K \psi_n^{(0)} \rangle \right|^2}{E_n^{(0)} - E_m^{(0)}}$$

① 1D




$$\psi_n^{(0)} = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right)$$

$$K(x) = V_0$$

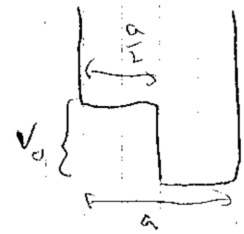
$$\hat{H} = \hat{H}_0 + \hat{K}$$

$$E_n^{(1)} = \langle \psi_n^{(0)} | V_0 \, \psi_n^{(0)} \rangle = V_0 \cdot 1$$

$$E_n^{(2)} = \sum_{n \neq m} \delta_{nm} = 0 \qquad \langle \psi_m^{(0)} | K \, \psi_n^{(0)} \rangle = V_0 \cdot \delta_{mn}$$

② 

$$K(x) = \begin{cases} V_0 & x < \frac{a}{2} \\ 0 & x \geq \frac{a}{2} \end{cases}$$



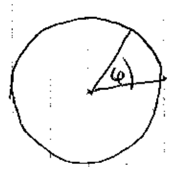

$$E_n^{(1)} = \langle \psi_n^{(0)} | K \, \psi_n^{(0)} \rangle = \int_0^{\frac{a}{2}} V_0 \sin^2\left(\frac{n\pi x}{a}\right) \cdot \frac{2}{a} =$$

$$= \frac{2V_0}{a} \cdot \frac{a}{2} \cdot \frac{1}{2} = \frac{V_0}{2}$$

$$E_n^{(2)} = ? \qquad K_{nm} = \langle \psi_n^{(0)} | K \, \psi_m^{(0)} \rangle = \frac{2}{a} V_0 \int_0^{a/2} \underbrace{\sin\left(\frac{n\pi x}{a}\right) \sin\left(\frac{m\pi x}{a}\right)}_{\frac{1}{2}\left[\cos\left(\frac{(n-m)\pi x}{a}\right) - \cos\left(\frac{(n+m)\pi x}{a}\right)\right]} dx$$

③ 2D rotator

$$\hat{H}_0 = -\frac{\hbar^2}{2G} \frac{d^2}{d\varphi^2}$$




$$\psi_m^{(0)} = \frac{1}{\sqrt{2\pi}} e^{im\varphi} \qquad m \in \mathbb{Z}$$

$$E_n^{(0)} = \frac{n^2 \hbar^2}{2\Theta} \qquad \hat{K} = \varepsilon \cdot \cos\varphi \qquad \hat{K}(x,y) = \varepsilon \cdot \cancel{(\cos)} \, \frac{x}{R}$$

$$K_{kn} = \int_0^{2\pi} \frac{1}{2\pi} \left(e^{ik\varphi}\right)^* \varepsilon \cos\varphi \cdot e^{in\varphi} \, d\varphi =$$

$$= \frac{\varepsilon}{2\pi} \int_0^{2\pi} e^{i(n-k)\varphi} \cdot \frac{e^{i\varphi} + e^{-i\varphi}}{2} \, d\varphi =$$

$$= \frac{\varepsilon}{4\pi} \int_0^{2\pi} \Big( \underbrace{e^{i(n-k+1)\varphi}}_{2\pi \delta_{n,k-1}} + \underbrace{e^{i(n-k-1)\varphi}}_{2\pi \delta_{n,k+1}} \Big) \, d\varphi$$

$$K_{kn} = \frac{\varepsilon}{2} \left( \delta_{n,k-1} + \delta_{n,k+1} \right)$$

$$K_{nn} = 0 \qquad E_n^{(1)} = 0$$

1 db alapálla $n=0$

2 db gerjesztett álla $n>0$

$$E_0^{(2)} = \sum_{k \neq 0} \frac{|K_{kn}|^2}{E_0^{(0)} - E_k^{(0)}}$$

$$E_0^{(2)} = \sum_{k \neq 0} \frac{\frac{\varepsilon^2}{4} \left( \delta_{0,k-1} + \delta_{0,k+1} \right)}{0 - \frac{k^2 \hbar^2}{2\Theta}} =$$

$$= \frac{\varepsilon^2}{4} \left( \frac{1}{-\frac{\hbar^2}{2\Theta}} + \frac{1}{-\frac{\hbar^2}{2\Theta}} \right) = -\frac{\varepsilon^2}{4} \cdot \frac{4\Theta}{\hbar^2} = -\frac{\varepsilon^2 \cdot \Theta}{\hbar^2}$$

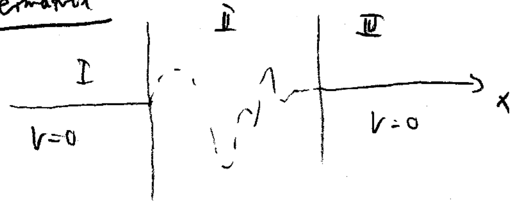
$$E_0 = \underset{\Downarrow \atop 0}{E_0^{(0)}} + \underset{\Downarrow \atop 0}{E_0^{(1)}} + E_0^{(2)} = -\frac{\varepsilon^2 \cdot \Theta}{\hbar^2}$$

$$f(b_{min}) = \frac{\hbar^2 \frac{2\alpha^2 m^2}{\hbar^4 \pi}}{2m} - \alpha \sqrt{\frac{2}{\pi}}\sqrt{\frac{2}{\pi}} \frac{\alpha m}{\hbar^2} = \frac{\alpha^2 m}{\hbar^2 \pi} - \frac{\alpha^2 m \, 2}{\hbar^2 \pi} = - \frac{\alpha^2 m}{\hbar^2 \pi} \geq E_0$$

$\frac{x \cdot 20}{2}$

## Szórásmátrix, transzfermátrix

1D probléma ált.




$E > 0$

$$\psi_{I}(x) = A e^{ikx} + B e^{-ikx}$$

$$\psi_{III}(x) = F e^{ikx} + G e^{-ikx}$$

$$\psi_{II}(x) = C f(x) + D g(x)$$

4 határfeltétel: $\psi$ folytonos

$\psi'$ is, ha $V$ sima

6 ismeretlen, $A B \cancel{C} \cancel{D} F G$

$$B = S_{11} A + S_{12} G$$

$$F = S_{21} A + S_{22} G$$

$$\begin{pmatrix} B \\ F \end{pmatrix} = \underline{\underline{S}} \begin{pmatrix} A \\ G \end{pmatrix}$$

$R_L$ reflexió: $\left|\frac{B}{A}\right|^2 = |S_{11}|^2$ balról

$T_L$ áthaladás $\left|\frac{F}{A}\right|^2 = |S_{21}|^2$

$$R_R = \left|\frac{F}{G}\right|^2 = |S_{22}|^2$$

$$T_R = \left|\frac{B}{G}\right|^2 = |S_{12}|^2$$

---

ha $E < 0$

$$\psi_{I}(x) = B e^{\kappa x} + \cancel{A e^{-\kappa x}} \qquad \kappa = \sqrt{\frac{-2mE}{\hbar^2}}$$

$$\psi_{II} = C f(x) + D g(x)$$

kötött

$$\psi_{III} = \cancel{G e^{\kappa x}} + F e^{-\kappa x}$$

$$\begin{pmatrix} B \\ F \end{pmatrix} = S \begin{pmatrix} A \\ G \end{pmatrix}$$ viszont $A, G = 0$

X.20 / 3

Pl:  $T=\left|\frac{F}{A}\right|^2 = \frac{1}{1+\beta^2}$ $\beta^2 = \left(\frac{m v_0}{\hbar^2 k}\right)^2$

$$T = \frac{1}{1+\frac{m v_0}{\hbar^2 k}} \xrightarrow[k\to ik]{} \frac{1}{1-\frac{m^2 v_0^2}{\hbar^4 k^2}} \to \infty$$

$k^2 = \frac{m^2 v_0^2}{\hbar^4}$ $k = \frac{m v_0}{\hbar^2}$

a kötött állapot energiája

Transfer mátrix

$F = M_{11} A + M_{12} B$ $B = S_{11} A + S_{12} G$

$G = M_{21} A + M_{22} B$ $F = S_{21} A + S_{22} G$

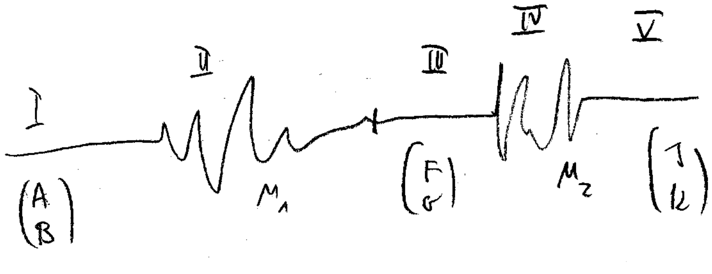
$$B = \frac{1}{M_{12}} F - \frac{M_{11}}{M_{12}} A$$

$$B = \underbrace{\frac{1}{M_{22}}}_{S_{12}} G - \underbrace{\frac{M_{21}}{M_{22}}}_{S_{11}} A$$

$$F = M_{11} A + M_{12}\left(\frac{1}{M_{22}} G - \frac{M_{21}}{M_{22}} A\right) = A\underbrace{\left(M_{11} - \frac{M_{21}}{M_{22}} M_{12}\right)}_{S_{21}} + G \underbrace{\frac{M_{12}}{M_{22}}}_{S_{22}}$$

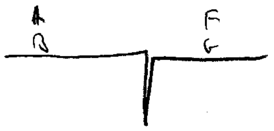
$$R_L = |S_{11}|^2 = \left|\frac{-M_{21}}{M_{22}}\right|^2$$

$$T_L = |S_{21}|^2 = \left|M_{12} - \frac{M_{21}}{M_{22}}\right|^2$$




$\binom{F}{G} = M_1 \binom{A}{B}$ ez így nem OK, szabad terjedési hiányzik

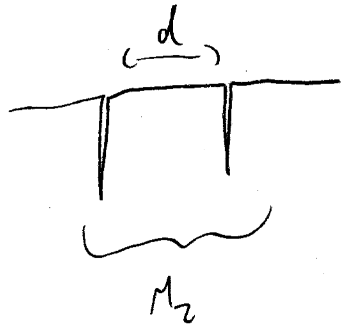
$\binom{J}{K} = M_2 \binom{F}{G} = M_2 M_1 \binom{A}{B}$




$$A+B = F+G$$

$$F-G = A(1+2i\beta) - B(1-2i\beta)$$

$$M = \begin{pmatrix} 1+i\beta & -i\beta \\ -i\beta & 1-i\beta \end{pmatrix}$$




$$M_2 = M \cdot \underset{\substack{\uparrow \\ \text{szabad} \\ \text{terjedés}}}{M_0} \cdot M = \begin{pmatrix} 1+i\beta & -i\beta \\ -i\beta & 1-i\beta \end{pmatrix} \begin{pmatrix} e^{ikd} & 0 \\ 0 & e^{-ikd} \end{pmatrix} \begin{pmatrix} 1+i\beta & -i\beta \\ -i\beta & 1-i\beta \end{pmatrix}$$

$$T_L = \left| M_{11} - \frac{M_{12} M_{21}}{M_{22}} \right|^2 = T_L(d, \beta, k)$$

## Perturbációszámítás

ismert

$$\hat{H} = \hat{H}_0 + \hat{K} \qquad E_n^{(0)} \psi_n^{(0)} = \hat{H}_0 \psi_n^{(0)} \qquad \hat{H} \to E, \psi\,?$$

0-adrendű

$$\hat{H} \psi_n = E_n \psi_n$$ de ezt nem tudjuk megoldani

egzakt ↓    ↓ közelítés, rend

$$E_n = E_n^{(0)} + E_n^{(1)} + E_n^{(2)} + \dots$$

**Feltétel:**
- $K$ „kicsi" $\|K \psi_n\| \ll |E_n - E_k| \quad \forall n \neq k$
- egyszeres sajátértékek

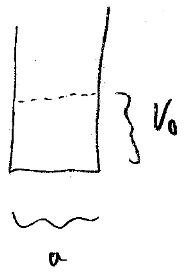
$$E_n^{(1)} = \langle \psi_n^{(0)} | \hat{K} \psi_n^{(0)} \rangle$$

$$E_n^{(2)} = \sum_{m \neq n} \frac{|\langle \psi_m^{(0)} | K \psi_n^{(0)} \rangle|^2}{E_n^{(0)} - E_m^{(0)}}$$

$$\psi_n^{(1)} = \sum_{m \neq n} \frac{\langle \psi_m^{(0)} | K \psi_n^{(0)} \rangle}{E_n^{(0)} - E_m^{(0)}} \psi_m^{(0)}$$

$\frac{x \cdot 20}{5.}$

1D ①




$$\psi_n^{(0)} = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right)$$

$$K(x) = V_0$$

$$\hat{H} = \hat{H}_0 + V_0$$

$$E_n^{(1)} = \langle \psi_n^{(0)} \cdot V_0 \cdot \psi_n^{(0)} \rangle = V_0 \cdot 1$$

$$E_n^{(2)} = \sum_{m \neq n} \delta_{nm} = 0 \qquad \langle \psi_n^{(0)} | K \psi_m^{(0)} \rangle = V_0 \delta_{nm}$$

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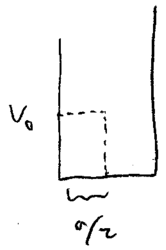
②




$$K(x) = \begin{cases} V_0 & x < a/2 \\ 0 & x \geq a/2 \end{cases}$$

$$E_n^{(1)} = \langle \psi_n^{(0)} K \psi_n^{(0)} \rangle = \int_0^{a/2} V_0 \sin^2\left(\frac{n\pi x}{a}\right) \frac{2}{a} = \frac{2V_0}{a} \frac{a/2}{2} = \frac{V_0}{2}$$

$$E_n^{(2)} =$$

$$K_{nm} = \langle \psi_n^{(0)} | K \psi_m^{(0)} \rangle = \frac{2}{a} V_0 \int_0^{a/2} \sin\left(\frac{n\pi x}{a}\right) \sin\left(\frac{m\pi x}{a}\right) dx = \ldots$$

---

③ 2D rotátor

$$\hat{H}_0 = \frac{-\hbar^2}{2\Theta} \frac{d^2}{d\varphi^2} \qquad \hat{K} = \varepsilon \cos\varphi \qquad \hat{K}(x,y) = \varepsilon x$$

$$\psi_n^{(0)} = \frac{1}{\sqrt{2\pi}} e^{in\varphi} \quad n \in \mathbb{Z}$$

$$E_n^{(0)} = \frac{n^2\hbar^2}{2\Theta}$$

$$K_{kn} = \int_0^{2\pi} \frac{1}{2\pi} \left(e^{ik\varphi}\right)^* \varepsilon \cos\varphi \, e^{in\varphi} d\varphi = \frac{\varepsilon}{2\pi} \int_0^{2\pi} e^{i(n-k)\varphi} \frac{e^{i\varphi} + e^{-i\varphi}}{2} d\varphi =$$

$$= \frac{\varepsilon}{4\pi} \int_0^{2\pi} \left( \underbrace{e^{i(n-k+1)\varphi}}_{2\pi \delta_{n,k-1}} + \underbrace{e^{i(n-k-1)\varphi}}_{2\pi \delta_{n,k+1}} \right) d\varphi = \frac{\varepsilon}{2} \left(\delta_{n,k-1} + \delta_{n,k+1}\right) \qquad K_{nn} = 0 \qquad E_n^{(1)} = 0, \forall n$$

$E_0^{(2)}$ nem alkalmazható, mert csak az alapállapot nem degenerált X. 20. 6.

$$E_0^{(2)} = \sum_{l\neq 0} \frac{\frac{\varepsilon^2}{4}\left(\delta_{n,l-1}+\delta_{n,l+1}\right)}{0-\frac{l^2\hbar^2}{2\Theta}} = \frac{\varepsilon^2}{4}\left[\frac{1}{-\frac{\hbar^2}{2\Theta}}+\frac{1}{-\frac{\hbar^2}{2\Theta}}\right] = \frac{-\varepsilon^2}{4}\frac{4\Theta}{\hbar^2} = -\frac{\varepsilon^2\Theta}{\hbar^2}$$

$$E_0 = E_0^{(0)}+E_0^{(1)}+E_0^{(2)} = \frac{-\varepsilon^2\Theta}{\hbar^2}$$

XI. 10.

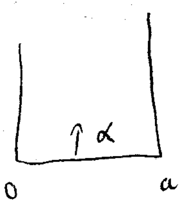
Perturbációszámítás

$$H_0\psi_n^{(0)} = E_n^{(0)}\psi_n^{(0)} \qquad H_0+K=H$$

$$E_n^{(1)} = \langle\psi_n^{(0)}|K\psi_n^{(0)}\rangle \qquad \psi_n^{(1)} = \sum_{l\neq n}\frac{\langle\psi_l^{(0)}|K\psi_n^{(0)}\rangle}{E_n^{(0)}-E_l^{(0)}}\psi_l^{(0)}$$

$$E_n^{(2)} = \sum_{l\neq n}\frac{|\langle\psi_l^{(0)}|K\psi_n^{(0)}\rangle|^2}{E_n^{(0)}-E_l^{(0)}}$$

pl:




$$K=\alpha\cdot\delta(x-a/2) \qquad E_n^{(1)}=? \qquad E_n^{(2)}=?$$

$$\psi_n^{(0)} = \sqrt{\frac{2}{a}}\sin\frac{n\pi x}{a}$$

$$E_n^{(0)} = \frac{n^2\pi^2\hbar^2}{2ma^2}$$

$$K_{ln}=? \qquad K_{nn} = \int_0^a\left(\sqrt{\frac{2}{a}}\sin\frac{n\pi x}{a}\right)^2\cdot\alpha\cdot\delta(x-a/2)\,dx = \frac{2\alpha}{a}\sin^2\left(\frac{n\pi}{2}\right) \begin{cases}\frac{2\alpha}{a} & \text{ha } n \text{ ptl}\\ 0 & \text{ha } n \text{ ps}\end{cases}$$

$$K_{ln} = \frac{2\alpha}{a}\sin\frac{n\pi}{2}\sin\frac{l\pi}{2} = \frac{2\alpha}{a}\cdot\begin{cases}0 & l \text{ vagy } n \text{ ps}\\ \pm 1 & l \text{ és } n \text{ ptl}\end{cases}$$

ha n ptl: $$E_n^{(2)} = \sum_{\substack{l\neq n\\ l\text{ ptl}}}\frac{4\alpha^2}{a^2}\frac{1}{\frac{n^2\pi^2\hbar^2}{2ma^2}-\frac{l^2\pi^2\hbar^2}{2ma^2}} = \frac{4\alpha^2}{a^2}\frac{2ma^2}{\pi^2\hbar^2}\overbrace{\sum_{\substack{l\neq n\\ l\text{ ptl}}}\frac{1}{n^2-l^2}}^{=\frac{1}{4n^2}} = \frac{\alpha^2 2ma^2}{a^2n^2\pi^2\hbar^2}$$

# Harmonikus oszcillátor

$$-\frac{\hbar^2}{2m}\psi'' + \frac{1}{2}m\omega^2x^2\psi = E\psi$$

$V = \frac{1}{2} m\omega^2 x^2$

$$\hbar\omega\left(\frac{-\hbar}{2m\omega}\frac{d^2}{dx^2} + \frac{1}{2}\frac{m\omega}{\hbar}x^2\right)\psi = E\psi$$ ↖ szeretnénk felírni $c\cdot(p^2+u^2)$ alakban

$$a_- := \sqrt{\frac{\hbar}{2m\omega}}\frac{d}{dx} + \sqrt{\frac{m\omega}{2\hbar}}x = \sqrt{\frac{1}{2m\omega\hbar}}\,ip + \sqrt{\frac{m\omega}{2\hbar}}x = \frac{1}{\sqrt{2m\omega\hbar}}(ip + m\omega x)$$

$$a_+ := \frac{1}{\sqrt{2m\omega\hbar}}(-ip + m\omega x)$$

$$\hbar\omega\left(a_+a_- + \frac{1}{2}\right) = H \qquad [a_-, a_+] = 1$$

Áll: ha $\psi$ sf-e $H$-nak $E$ sé-vel, vagyis $H\psi = E\psi \Rightarrow \begin{cases} H(a_+\psi) = (\hbar\omega + E)(a_+\psi) \\ H(a_-\psi) = (-\hbar\omega + E)(a_-\psi)\end{cases}$

$E \geq 0$ mindig és $\exists\, \psi_0 : a_-\psi_0 = 0$

$$(ip + m\omega x)\psi_0 = 0$$

$$\hbar\frac{d}{dx}\psi_0 = -m\omega x\psi_0$$

$$\psi_0 = C' e^{-\frac{m\omega x^2}{2\hbar}} \Rightarrow E_0 = \frac{1}{2}\hbar\omega$$

$$E_n = \hbar\omega\left(\frac{1}{2} + n\right) \qquad \psi_n = A_n (a_+)^n e^{-\frac{m\omega x^2}{2\hbar}}$$

↑ Hermite polinomok

Új bázis

$|n\rangle$ legyen az az állapot melyre $H|n\rangle = \hbar\omega\left(\frac{1}{2}+n\right)|n\rangle$

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

$a_-|n\rangle = \sqrt{n}\,|n-1\rangle$

$$x = \sqrt{\frac{\hbar}{2m\omega}}(a_+ + a_-) \qquad p = \sqrt{\frac{m\omega\hbar}{2}}\, i(a_+ - a_-)$$

$\Delta x \cdot \Delta p \overset{?}{\geq} \frac{\hbar}{2}$

$\langle n|x|n\rangle = \langle n|a_+ + a|n\rangle \cdot \sqrt{\frac{\hbar}{2m\omega}} \sim \langle n|n+1\rangle + \langle n|n-1\rangle = 0$

hasonlóan $\langle n|p|n\rangle = 0$

$\langle x^2\rangle = \frac{\hbar}{2m\omega} \langle n|\, a_+a_+ + a_+a + aa_+ + aa\,|n\rangle = \frac{\hbar}{2m\omega} \langle n|\, a_-a_+ + a_+a_-|n\rangle = \frac{\hbar}{2m\omega}(2n+1)$

$\langle p^2\rangle = \frac{-m\hbar\omega}{2} \langle n|\, a_+a_+ - a_+a_- - a_-a_+ + a_-a_-|n\rangle = -\frac{m\omega\hbar}{2}(-2n-1) = \frac{m\omega\hbar}{2}(2n+1)$

$$\left.\begin{aligned} \Delta x &= \sqrt{\langle x^2\rangle} \\ \Delta p &= \sqrt{\langle p^2\rangle} \end{aligned}\right\} \quad \Delta x\Delta p = \hbar\sqrt{n+\tfrac{1}{2}}^{\,2} \qquad n=0 \rightarrow \quad \Delta x\Delta p = \hbar\cdot\frac{1}{2}$$

Perturbáció: $K = \varepsilon \cdot x^3$, azaz $H = H_0 + K = \frac{-\hbar^2}{2m} + \frac{1}{2}m\omega^2x^2 + \varepsilon x^3$

$E_n^{(1)} =$

$K = \varepsilon \cdot \left(\frac{\hbar}{2m\omega}\right)^{3/2}(a_+ + a_-)(a_+ + a_-)(a_+ + a_-)$

$[a, a_+] = 1$

$K = \varepsilon\left(\frac{\hbar}{2m\omega}\right)^{3/2}\left(aaa + 3a_+a_+a + 3a_+aa + a_+a_+a_+ + 3a_- + 3a_+\right)$

# Kvantum gyak

## Perturbációszámítás

Ha nem degenerált állapot és $\| K | \psi_n \rangle \| << | E_{n_1} - E_{n_2} |$ $(n_1 \neq n_2)$

## Harmonikus oszcillátor

$\frac{1}{2} m\omega^2 x^2 = V(x)$ $\qquad H = \hbar\omega(a_+ a + 1/2)$ $\qquad \psi$ megoldáshoz $E$

$$\left\{ \begin{array}{l} a = \frac{1}{\sqrt{2m\omega\hbar}}(ip + m\omega x) \\ a_+ = (a)^+ \end{array} \right.$$

$(a_+ + a)\sqrt{\frac{\hbar}{2m\omega}} = x$

$(a_+ - a) i \sqrt{\frac{m\hbar\omega}{2}} = p$

$[a, a_+] = 1$

$\Downarrow$

$a a_+ = a_+ a + 1$

$a_+ \psi$ megoldáshoz $E + \hbar\omega$

$a \psi$ megoldáshoz $E - \hbar\omega$

ha $K = \varepsilon x^3$

$$\left. \begin{array}{l} E_n^{(1)} = ? \\ E_n^{(2)} = ? \end{array} \right\} K_{ln} = \langle \psi_l^{(0)} | K \psi_n^{(0)} \rangle$$

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

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

$a_+$ balra

$a$ jobbra csoportosítandó

$$\hat{K} = \varepsilon \left(\frac{\hbar}{2m\omega}\right)^{3/2} (a_+ a_+ a_+ + a_+ a_+ a + a_+ a a_+ + a a_+ a_+ + a_+ a a + a a_+ a + a a a_+ + a a a)$$

$a_+ a a_+ \to a_+ a_+ a + a_+$

$a a_+ a_+ \to a_+ a a_+ + a_+ \to a_+ a_+ a + 2a_+$

$a a_+ a \to a_+ a a + a$

$a a a_+ \to a a_+ a + a \to a_+ a a + 2a$

$$K_1 = \varepsilon \left(\frac{\hbar}{2m\omega}\right)^{3/2} (a_+ a_+ a_+ + 3 a_+ a_+ a + 3a_+ + 3a + 3 a_+ a a + a a a)$$

$a_+ a_+ a_+ |n\rangle = \sqrt{(n+1)(n+2)(n+3)}\, |n+3\rangle$

$a_+ a_+ a |n\rangle = \sqrt{n \cdot n(n+1)}\, |n+1\rangle$

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

$a a a |n\rangle = \sqrt{n(n-1)(n-2)}\, |n-3\rangle$

$\langle l | n \rangle = \delta_{ln}$

$$K_{ln} = \varepsilon \left(\frac{\hbar}{2m\omega}\right)^{3/2} \Big[ \sqrt{(n+1)(n+2)(n+3)}\, \delta_{l,n+3} +$$
$$+ 3\sqrt{n^2(n+1)}\, \delta_{l,n+1} + 3\sqrt{n+1}\, \delta_{l,n+1} + 3\sqrt{n}\, \delta_{l,n-1} +$$
$$+ 3\sqrt{(n-1)^2 n}\, \delta_{l,n-1} +$$
$$+ \sqrt{n(n-1)(n-2)}\, \delta_{l,n-3} \Big]$$

$E_n^{(1)} = K_{nn} = 0$

$$E_n^{(2)} = \sum_{k \neq n} \frac{|K_{kn}|^2}{\left(E_n^{(0)} - E_k^{(0)}\right)} = \varepsilon^2 \left(\frac{\hbar}{2m\omega}\right)^3 \sum_{k\neq n} \frac{1}{\hbar\omega(n-k)} \Big( (n+1)(n+2)(n+3)\, \delta_{k,n+3} + \left(3(n+1)\sqrt{n+1}\right)^2 \delta_{k,n+1}$$

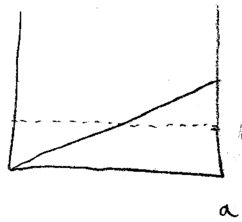
$$+ \left(3n\sqrt{n}\right)^2 \delta_{k,n-1} + n(n-1)(n-2)\, \delta_{k,n-3} \Big) =$$

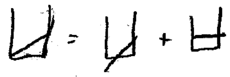
$$= \varepsilon^2 \left(\frac{\hbar}{2m\omega}\right)^3 \frac{1}{\hbar\omega} \left( \frac{(n+1)(n+2)(n+3)}{-3} + \frac{3(n+1)^3}{-1} + \frac{3n^3}{1} + \frac{n(n-1)(n-2)}{3} \right) =$$

$$= \frac{\varepsilon^2 \hbar^2}{(2m)^3 \omega^4} \left( 20n^3 + 30n^2 + 40n + 15 \right)$$

$\| K |n\rangle \| \ll \hbar\omega$ mikor teljesül? $\quad n^{3/2} \ll \frac{1}{\varepsilon\hbar} \omega^2 (2m)^{3/2}$

~~ha~~ $V(x) = \varepsilon \cdot x$





$$E_n^{(1)} = \int \left( \sqrt{\frac{2}{a}} \sin\frac{n\pi x}{a} \right)^2 \varepsilon x \, dx = \varepsilon \, a/2$$

$\varepsilon a/2$

$$K_{kn} = \varepsilon \frac{2}{a} \int_0^a \sin\frac{n\pi x}{a} \, x \cdot \sin\frac{k\pi x}{a} \, dx = \varepsilon \frac{2}{a} \int_0^\pi y \sin(ny) \sin(ky) \, dy =$$

$\frac{\pi x}{a} = y$

$$= \varepsilon \frac{2a}{\pi^2} \int_0^\pi y \frac{1}{2} \left[ \cos((n-k)y) - \cos((n+k)y) \right] dy = \frac{\varepsilon a}{\pi^2} \left( \left[ y \frac{\sin((n-k)y)}{n-k} \right]_0^\pi - \int_0^\pi \frac{\sin((n-k)y)}{n-k} dy - \right.$$

$$\left. - \left[ y \frac{\sin((n+k)y)}{n+k} \right]_0^\pi + \int_0^\pi \frac{\sin((n+k)y)}{n+k} dy \right) =$$

$$= \frac{ka}{\pi^2} \left( \frac{\cos((n-k)\pi) - 1}{(n-k)^2} - \frac{\cos((n+k)\pi) - 1}{(n+k)^2} \right)$$

ha $\left.\begin{matrix} n-\ell \\ n+\ell \end{matrix}\right\}$ páros, akkor $= \frac{\varepsilon a}{\pi^2}(0-0)=0$

ha $\left.\begin{matrix} n-\ell \\ n+\ell \end{matrix}\right\}$ páratlan, akkor $= \frac{\varepsilon a}{\pi^2}\left(\frac{-2}{(n-\ell)^2} - \frac{2}{(n+\ell)^2}\right) = -\frac{2\varepsilon a}{\pi^2}\frac{4n\ell}{(n-\ell)^2(n+\ell)^2} = -\frac{8\varepsilon a n}{\pi^2}\frac{\ell}{(n^2-\ell^2)^2}$

$$E_n^{(2)} = \sum_{\ell\neq n}\frac{64\varepsilon^2 a^2 n^2}{\pi^4}\frac{\ell^2}{(n^2-\ell^2)^4}\frac{1}{\underbrace{\frac{\hbar^2\pi^2}{2ma^2}(n^2-\ell^2)}_{E_n^{(0)}-E_\ell^{(0)}}} = \underbrace{\frac{128\,\varepsilon^2 m a^4 n^2}{\hbar^2\pi^6}}_{:=A}\sum_{\ell\neq n}\frac{\ell^2}{(n^2-\ell^2)^5}$$

ha $n$ páros (akkor $\ell$ páratlan) $= A\cdot\sum_{\ell\ \text{ptl}}\frac{\ell^2}{(n^2-\ell^2)^5} = A\,\frac{1}{3072}\,\frac{\pi^2(n^2\pi^2-15)}{n^6}$

állítólag

ha $n$ páratlan $= A\cdot\sum_{\ell\ \text{ps}}\frac{\ell^2}{(n^2-\ell^2)^5} = A\,\frac{1}{3072}\,\frac{\pi^2(n^2\pi^2-15)}{n^6}$

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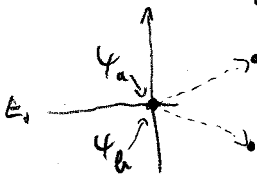
Degenerált perturbációszámítás

ha egy energiához több állapot tartozik

$E_a$ a perturbált rendszerben

$\alpha\psi_a+\beta\psi_b$




$\gamma\psi_a+\delta\psi_b$

$E_b$ a perturbált rendszerben

$(\alpha,\beta)$ és $(\gamma,\delta)$-t a $\underline{\underline{W}}$ határozza meg

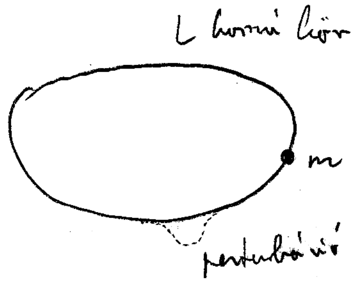
$H_0\psi_a^{(0)} = E_0\,\psi_a^{(0)}$

$H_0\psi_b^{(0)} = E_0\,\psi_b^{(0)}$

$W_{ij} := \langle\psi_i^{(0)}|K\psi_j^{(0)}\rangle \qquad \begin{pmatrix} W_{aa} & W_{ab} \\ W_{ba} & W_{bb}\end{pmatrix}$

$H_0 + K = H$

perturbáljuk




$$\psi'' = \frac{-2mE}{\hbar^2}\psi$$

$$\psi(x)\,,\quad x\in[0,L]\,,\quad E\geq 0$$

$$\psi = A e^{\pm ikx}$$

$$\psi(x) = \psi(x+L) \Rightarrow e^{ikL} = 1 \Rightarrow kL = 2n\pi$$

$$\psi_n(x) = \frac{1}{\sqrt{L}} e^{i\frac{2n\pi}{L}x} \qquad n\in\mathbb{Z}$$

$\uparrow$

$$\int_0^L \left|A e^{ikx}\right|^2 \overset{!}{=} 1 \text{ normálásból}$$

$$E_n^{(0)} = \frac{\hbar^2}{2m}k^2 = \frac{\hbar^2}{2m}\frac{4n^2\pi^2}{L^2}$$ $n=0$-t kivéve 2 állapotnak van ennyi energiája

$$K := -V_0 e^{-x^2/a^2} \qquad a \ll L$$

$$E_0^{(1)} = \langle \psi_0^{(0)} | K | \psi_0^{(0)} \rangle = \int_{-L/2}^{L/2} \frac{1}{L}\underbrace{e^{i\frac{2\cdot 0\cdot\pi}{L}}}_{1}\left(-V_0 e^{-x^2/a^2}\right)dx \approx \int_{-\infty}^{\infty}\frac{-V_0 e^{-x^2/a^2}}{L} = \frac{-V_0}{L}\sqrt{\frac{\pi}{1/a^2}} = \frac{-V_0}{L}\sqrt{\pi}\,a$$

$$E_1^{(1)} = \int_{-\infty}^{\infty}\frac{1}{L}\underbrace{\left|e^{i\frac{2\pi x}{L}}\right|^2}_{1}\left(-V_0 e^{-x^2/a^2}\right)dx = \frac{-V_0}{L}\sqrt{\pi}\,a$$

$$\psi_n := \psi_a \qquad \psi_{-n} := \psi_b$$

$$W_{aa} = \langle \psi_a | K\psi_a \rangle = \frac{-V_0}{L}a\sqrt{\pi} = W_{bb} \qquad W_{ab} = \int_{-\infty}^{\infty}\frac{1}{L}\left(e^{i\frac{n2\pi x}{L}}\right)^*\left(-V_0 e^{-x^2/a^2}\right)\left(e^{-i\frac{n\pi 2x}{L}}\right)dx$$

de itt is integrálhatok

itt integrálok

$$\frac{-x^2}{a^2} - i\frac{4n\pi x}{L} = \frac{-1}{a^2}\left(x^2 + \frac{i4n\pi + a^2}{L}\right) = \frac{-1}{a^2}\Big(\underbrace{x + \frac{i2n\pi \cdot a^2}{L}}_{y}\Big) - \frac{4n^2\pi^2a^2}{L^2}$$

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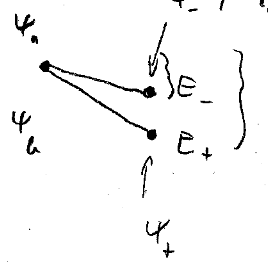
$$W_{ab} = \frac{-V_0}{L}\int_c e^{-x^2/a}\underbrace{e^{-\frac{4n^2\pi^2a^2}{L^2}}}_{:=B}dy = \frac{-V_0}{L}\sqrt{\pi}\,a\cdot B$$

$$W_{ba} = (W_{ab})^* = \frac{-V_0}{L}\sqrt{\pi}\,aB \qquad W = \frac{-V_0}{L}\sqrt{\pi}\,a\begin{pmatrix}1 & B\\ B & 1\end{pmatrix}$$

$$(1-\lambda)^2 - B^2 = 0 \qquad \lambda_\pm = 1 \pm B$$

$$E_\pm = \frac{-V_0}{L}\sqrt{\pi}\,a(1\pm B) \qquad E^{(0)} = \frac{\hbar^2}{2m}\frac{4n^2\pi^2}{L^2}$$

$\psi_- \neq \psi_a, \psi_b$ hanem lin. komb.




$$\begin{pmatrix}1 & B\\ B & 1\end{pmatrix}\begin{pmatrix}\alpha\\ \beta\end{pmatrix} = (1\pm B)\begin{pmatrix}\alpha\\ \beta\end{pmatrix}$$

$\alpha + B\beta = (1+B)\alpha$

$B\beta = B\alpha$

$\beta = \alpha$

$$\psi_\pm = \frac{1}{\sqrt{2}}\left(\psi_n(x) \pm \psi_{-n}(x)\right)$$

$$\langle\psi_+|K\psi_+\rangle = E_+ = \frac{1}{2}\left(\langle\psi_n|K\psi_{-n}\rangle + \langle\psi_{-n}|K\psi_n\rangle + \langle\psi_n|K\psi_n\rangle + \langle\psi_{-n}|K\psi_{-n}\rangle\right)$$

$$\langle\psi_-|K\psi_-\rangle = E_-$$

Áll: $A$ hermitikus $[A,K]=0$ $[A,H]$ operátorra $A\psi_a^{(0)} = \mu\psi_a^{(0)}$ $\quad A\psi_b^{(0)} = \nu\psi_b^{(0)}$

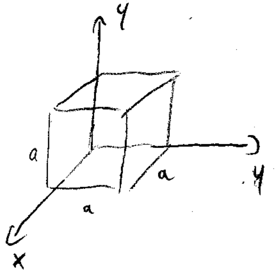
Ebben a bázisban $W_{ab} = 0$, azaz pont a jó lin. kombinációkat vannak

$$[A, e^{-x^2/a^2}] = 0 \quad \text{pl. } A = P, \text{ amire } P\psi(x) = \psi(-x)$$

$P\psi_n = \psi_{-n}$ $\qquad P = \begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}$, sajátvektorai $\sqrt{\frac{1}{2}}(\psi_n + \psi_{-n})$, s.é.: 1

$P\psi_{-n} = \psi_n$ $\qquad \sqrt{\frac{1}{2}}(\psi_n - \psi_{-n})$, s.é.: $-1$

X1.23




$$\psi^{(0)}_{n_1,n_2,n_3} = \sqrt{\frac{2}{a}}\sin\frac{n_1\pi x}{a}\sqrt{\frac{2}{a}}\sin\frac{n_2\pi y}{a}\sqrt{\frac{2}{a}}\sin\frac{n_3\pi z}{a}$$

$$E_{n_1n_2n_3} = \frac{\hbar^2\pi^2}{2ma^2}\left(n_1^2+n_2^2+n_3^2\right) \qquad n_i\in\mathbb{Z}^+,\ i\in\{1,2,3\}$$

$E_{alap} = E_{111}$

$E_1 = E_{112} = E_{121} = E_{211} = \frac{\hbar^2\pi^2}{2ma^2}\,6$

$\psi_{112} = \psi_a$

$\psi_{121} = \psi_b$

$\psi_{211} = \psi_c$

$$K = \begin{cases} V_0 & 0<x<a/2 \quad 0<y<a/2 \\ 0 & \text{amúgy} \end{cases}$$

$$E_{al}^{(1)} = \underbrace{\int_0^{a/2}\left|\sqrt{\frac{2}{a}}\sin\left(\frac{\pi x}{a}\right)\right|^2}_{1/2}\underbrace{\int_0^{a/2}\left|\sqrt{\frac{2}{a}}\sin\frac{\pi y}{a}\right|^2}_{1/2}\underbrace{\int_0^{a}\left|\sqrt{\frac{2}{a}}\sin\frac{\pi z}{a}\right|^2}_{1} V_0 = \frac{V_0}{4} = \langle\psi_{1,1,1}|K|\psi_{1,1,1}\rangle$$

$$W_{aa} = V_0\int_0^{a/2}\left|\sqrt{\frac{2}{a}}\sin\frac{\pi x}{a}\right|^2\int_0^{a/2}\left|\sqrt{\frac{2}{a}}\sin\frac{\pi y}{a}\right|^2\int_0^{a}\left|\sqrt{\frac{2}{a}}\sin\frac{n z}{a}\right|^2 = \frac{V_0}{4}$$

$$W_{bb} = \frac{V_0}{4}$$

$$W_{cc} = \frac{V_0}{4}$$

$$W_{ab} = \langle\psi_a|K|\psi_b\rangle = c\cdot\underbrace{\sin\ldots}_{x}\ \underbrace{\sin\ldots}_{y}\ \underbrace{\int_0^a \sin\frac{2\pi z}{a}\sin\frac{\pi z}{a}\,dz}_{0} = 0$$

$$W_{ac} = c\cdot\underbrace{\sin\ldots}_{x\text{-os rész}}\ \underbrace{\sin\ldots}_{y\text{-os rész}}\int_0^a \sin\frac{2\pi z}{a}\sin\frac{\pi z}{a}\,dz = 0$$

$$W_{bc} = V_0\left(\frac{2}{a}\right)^3\int_0^{a/2}\sin\frac{\pi x}{a}\sin\frac{2\pi x}{a}\,dx\int_0^{a/2}\sin\frac{\pi y}{a}\sin\frac{2\pi y}{a}\,dy\ \overbrace{\int_0^a\left|\sin\frac{\pi z}{a}\right|^2 dz}^{\frac{a}{2}}$$

$$= \left(\frac{2}{a}\right)^2\left(\int_0^{a/2}\sin\left(\frac{2\pi x}{a}\right)\sin\left(\frac{\pi x}{a}\right)\right)^2 V_0 = \left(\frac{2}{a}\right)^2\left(\frac{2a}{3\pi}\right)^2 V_0 = \frac{16}{9}\frac{V_0}{\pi^2} = \frac{V_0}{4}\underbrace{\frac{64}{9\pi^2}}_{=k}$$

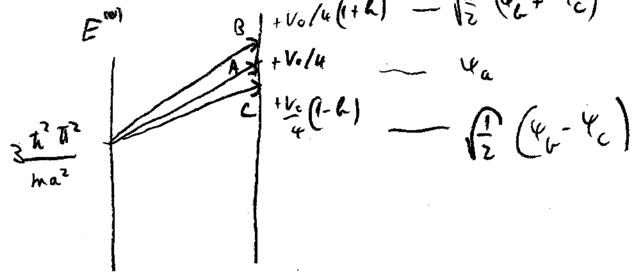
$\frac{x(.2)}{2}$

$$W = \frac{V_0}{4}\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & h \\ 0 & h & 1 \end{pmatrix} \qquad (1-\lambda)^3 - h^2(1-\lambda) = 0$$

$$\lambda_1 = 1 \qquad \lambda^2 - 2\lambda + 1 - h^2 = 0$$

$$\lambda_{2,3} = \frac{2 \pm \sqrt{4 - 4(1-h^2)}}{2} = \frac{2 \pm 2h}{2} = 1 \pm h$$

$$E_{1A} = \frac{V_0}{4}$$




$$E_{1B} = \frac{V_0}{4}(1+h)$$

$$E_{1C} = \frac{V_0}{4}(1-h)$$

Belátható:

$$\left\langle \sqrt{\tfrac{1}{2}}(\psi_b + \psi_c) \middle| K \middle| \sqrt{\tfrac{1}{2}}(\psi_b + \psi_c) \right\rangle = \frac{V_0}{4}(1+h)$$

$W$ sajátvektorai:

$$\lambda_1 = 1 \Rightarrow \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$$

$$\lambda_2 = 1+h \Rightarrow \begin{pmatrix} 0 \\ 1/\sqrt{2} \\ 1/\sqrt{2} \end{pmatrix}$$

$$\lambda_3 = 1-h \Rightarrow \begin{pmatrix} 0 \\ 1/\sqrt{2} \\ -1/\sqrt{2} \end{pmatrix}$$

---

$$H\Psi = i\hbar\frac{\partial\Psi}{\partial t} \Rightarrow \Psi(x,t) = \psi(x)\cdot e^{-i\frac{E}{\hbar}t}$$

A megoldás ilyen alakúak lin. kombinációja

$\langle E \rangle$ állandó, de így kombinálni pl nem tárgyalhatunk

$$H(t) = H_0 + K(t)$$

$$H_0 \varphi_k^{(0)} = E_k^{(0)} \varphi_k^{(0)} \qquad \varphi_k^{(0)} \text{ T.ON.R.} \qquad t=0\text{-ban } \psi(0) = \varphi_i^{(0)}$$

$$\psi(t) = \sum_k c_k(t)\,\varphi_k^{(0)} \qquad W_{i\to k}(t) = |c_k(t)|^2$$

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3

$$c_k(t) = \delta_{ki} - \frac{i}{\hbar}\int_{\tau=0}^{t} e^{i\omega_{ki}\tau} K_{ki}(\tau)\,d\tau - \frac{1}{\hbar^2}\int_{\tau_2=0}^{t}\int_{\tau_1=0}^{\tau_2}\sum_j e^{i\omega_{kj}\tau_2} e^{i\omega_{ji}\tau_1}\cdot K_{kj}(\tau_2) K_{ji}(\tau_1)\,d\tau_1 d\tau_2$$

$$\omega_{ki} = \frac{E_k^{(0)} - E_i^{(0)}}{\hbar}$$

① Harmonikus oszcillátor

$$H_0 = \frac{p^2}{2m} + \frac{1}{2} m\omega^2 x^2 \qquad K(t) = \varepsilon x^3 \chi_{[0,T]}(t)$$

$t=0$ alapállapot

$t \geq T$ 1. gerj. áll. valószínűsége

$$\omega_{ki} = \omega(k-i)$$

$$K_{kn} = \varepsilon\left(\frac{\hbar}{2m\omega}\right)^{3/2}\left( \quad \delta_{k,n+3} + \frac{\sqrt{n+1}}{(n+1)\cdot 3}\,\delta_{k,n+1} + \quad \delta_{k,n-1} \quad \delta_{k,n-3}\right.$$

0. rend $\delta_{10} = 0$

1. rend: $K_{10} \neq 0$ $\qquad K_{10} = \varepsilon\left(\frac{\hbar}{2m\omega}\right)^{3/2} \underbrace{\sqrt{0+1}\,(0+1)\cdot 3}_{3}$ $\qquad \omega_{10} = \omega(1-0) = \omega$

2. rend $K_{1j} K_{j0} = 0$

$$\chi_{[0,T]} \to T$$

$$c_k(t) = -\frac{i}{\hbar}\int_{\tau=0}^{T} e^{i\omega\tau}\,\varepsilon\cdot\left(\frac{\hbar}{2m\omega}\right)^{3/2} 3\,d\tau = \frac{-i\varepsilon}{\hbar}\left(\frac{\hbar}{2m\omega}\right)^{3/2}\left[\frac{e^{i\omega\tau}}{i\omega}\right]_0^T\cdot 3 =$$

$$= \frac{-i\varepsilon}{\hbar}\sqrt{\frac{\hbar}{2m\omega}}^{\,3}\frac{1}{i\omega}\left(e^{i\omega T} - 1\right)\cdot 3$$

$$W_{0\to 1}(t) = \left|c_k(t)\right|^2 = 9\cdot\frac{\varepsilon^2\hbar^3}{\hbar^2(2m\omega)^3}\frac{1}{\omega^2}\left(e^{i\omega T} - 1\right)\left(e^{-i\omega T} - 1\right) =$$

$$= 9\frac{\varepsilon^2\hbar}{8m^3\omega^5}\left(1 + 1 - e^{i\omega T} - e^{-i\omega T}\right) = \frac{9\varepsilon^2\hbar}{4m^3\omega^5}\left[1 - \cos(\omega T)\right]$$

Harmonikus oszcillátorra
$i$ - ik állapotban $t=0$. ban

$$W_{i\to k}(t) = |c_k(t)|^2 \qquad \psi = \sum_k c_k(t)\, \varphi_k^{(0)}$$

$k$-ba megyünk a $T$-re

$$c_k(t) = \delta_{ki} - \frac{i}{\hbar}\int_{\tau=0}^{t} e^{i\omega_{ki}\tau} K_{ki}(\tau)\,d\tau \underbrace{- \frac{1}{\hbar^2}\int_{\tau_2=0}^{t}\int_{\tau_1=0}^{\tau_2}\sum_j e^{i\omega_{kj}\tau_2} e^{i\omega_{ji}\tau_1} \cdot K_{kj}(\tau_2) K_{ji}(\tau_1)\,d\tau_1\,d\tau_2}_{:= C_k^{(2)}}$$

$$K = \varepsilon \cdot x^3 \chi_{[0,T]}(t)$$

$$K_{kn} = \varepsilon\left(\frac{\hbar}{2m\omega}\right)^{3/2}\left(\dots \delta_{k,n-3} + \dots \delta_{k,n-1} + 3\sqrt{n+1}\,(n+1)\,\delta_{k,n+1} + \sqrt{n+1}\sqrt{n+2}\sqrt{n+3}\,\delta_{k,n+3}\right)\chi_{[0,T]}(t)$$

0. rend $= \delta_{00} = 1$

1. rend $= 0$

2. rend : $\underbrace{K_{01}K_{10}}_{|K_{01}|^2} + \underbrace{K_{03}K_{30}}_{|K_{03}|^2}$ $\quad 0\to1,\ 1\to0 \quad 0\to3,\ 3\to0$

$$\omega_{kn} = \hbar\omega(k-n)$$

$$c_k^{(2)} = \frac{-1}{\hbar^2}\left[\int_{\tau_2=0}^{T} e^{i\omega(0-1)\tau_2}\,\underset{j=1}{|K_{01}|^2}\int_{\tau_1=0}^{\tau_2} e^{i\omega(1-0)\tau_1}\,d\tau_1 + \int_{\tau_2=0}^{T} e^{i\omega(0-3)\tau_2}\,|K_{03}|^2\int_{\tau_1=0}^{\tau_2} e^{i\omega(3-0)\tau_1}\,d\tau_1\right] =$$

$$= \frac{-\varepsilon^2\hbar}{8m^3\omega^3}\left[9(0+1)^3\int_{\tau_2=0}^{T} e^{-i\omega\tau_2}\left[\frac{e^{i\omega\tau_1}}{i\omega}\right]_0^{\tau_2} d\tau_2 + (0+1)(0+2)(0+3)\int_{\tau_2=0}^{T} e^{-i3\omega\tau_2}\left[\frac{e^{i3\omega\tau_1}}{i3\omega}\right]_0^{\tau_2} d\tau_2\right] =$$

$$= \frac{-\varepsilon^2\hbar}{8m^3\omega^3}\left[\frac{9}{i\omega}\int_0^T\left(1-e^{i\omega\tau_2}\right)d\tau_2 + \frac{6}{3i\omega}\int_0^T\left(1-e^{3i\omega\tau_2}\right)d\tau_2\right] =$$

$$= \frac{\varepsilon^2\hbar i}{8m^3\omega^4}\left[9\left(T-\frac{1}{i\omega}\left(e^{i\omega T}-1\right)\right) + 2\left(T-\frac{1}{3i\omega}\left(e^{i3\omega T}-1\right)\right)\right]$$

$$W_{0\to0}(t) = \left|1 + (\dots)\right|^2$$

$$\varphi_n^{(0)} = e^{in\varphi}\frac{1}{\sqrt{2\pi}} \qquad E_n^{(0)} = \frac{\hbar n^2}{2\Theta}$$

$$K = \varepsilon \sin(\varphi/2)\, \chi_{[0,T]}(t)$$

$$K_{kn} = \varepsilon \int_0^{2\pi} \frac{1}{2\pi}\left(e^{ik\varphi}\right)^* \sin\varphi/2\, e^{in\varphi}\, d\varphi = \frac{\varepsilon}{2\pi}\frac{1}{2i}\int_0^{2\pi} e^{-ik\varphi}\left(e^{i\frac{\varphi}{2}} - e^{-i\frac{\varphi}{2}}\right)e^{in\varphi}\, d\varphi =$$

$$= \frac{\varepsilon}{4\pi i}\int_0^{2\pi}\left[e^{i(n-k+1/2)\varphi} - e^{i(n-k-1/2)\varphi}\right]d\varphi = \frac{\varepsilon}{4\pi i}\left[\left[\frac{e^{i(n-k+1/2)\varphi}}{i(n-k+1/2)}\right]_0^{2\pi} - \left[\frac{e^{i(n-k-1/2)\varphi}}{i(n-k-1/2)}\right]_0^{2\pi}\right] =$$

$$= \frac{\varepsilon(-i)}{4\pi i}\left(\frac{-1-1}{n-k+1/2} - \frac{-1-1}{n-k-1/2}\right) = \frac{-\varepsilon}{4\pi}(-2)\frac{n-k-1/2-(n-k+1/2)}{\left[(n-k)+1/2\right]\left[(n-k)-1/2\right]} =$$

$$= \frac{\varepsilon}{2\pi}\frac{-1}{(n-k)^2-1/4}$$

$$E_0^{(1)} = K_{00} = \frac{2\varepsilon}{\pi}$$

$$E_n^{(2)} = \sum_{k\neq 0}\frac{|K_{k0}|^2}{E_0^{(0)}-E_k^{(0)}} = \frac{\varepsilon^2}{4\pi^2}\frac{1}{\frac{\hbar^2}{2\Theta}}\sum_{k\neq 0}\frac{\left(\frac{1}{(0-k)^2-1/4}\right)^2}{0-k^2} = \frac{\varepsilon^2\Theta}{2\pi^2\hbar^2}\sum\frac{-1}{k^2(k^2-1/4)^2} = \frac{-\varepsilon^2\Theta}{2\pi^2\hbar^2}\overbrace{\sum_{k>0}\frac{1}{k^2(k^2-1/4)}}^{\approx 1{,}99}\cdot 2 =$$

$$W_{nn} = \frac{\varepsilon}{2\pi}\frac{1}{1/4} = \frac{2\varepsilon}{\pi}$$

$$W_{(-n)(-n)} = \frac{2\varepsilon}{\pi}$$

$$W_{n(-n)} = \frac{\varepsilon}{2\pi}\frac{-1}{4n^2-1/4} = W_{(-n)n}$$

$$W = \frac{2\varepsilon}{\pi}\begin{pmatrix}1 & k\\ k & 1\end{pmatrix} \quad \text{ha} \quad k = \frac{1}{4}\frac{-1}{4n^2-1/4}$$

$$\lambda_1 = 1+k \quad \begin{pmatrix}\sqrt{1/2}\\ \sqrt{1/2}\end{pmatrix}$$

$$\lambda_2 = 1-k \quad \begin{pmatrix}\sqrt{1/2}\\ -\sqrt{1/2}\end{pmatrix}$$

$$\left.\begin{aligned} E_{n+} &= \frac{2\varepsilon}{\pi}(1+k)\\ E_{n-} &= \frac{2\varepsilon}{\pi}(1-k)\end{aligned}\right\}\ \text{ha } n\neq 0$$

$$E_0^{(1)} = \frac{2\varepsilon}{\pi} \qquad \text{ha } n=0$$

$W_{0\to 1}(t) = ?$  $t > T$

$K = \varepsilon \cos\frac{\varphi}{2}\, \chi_{[0,T]}(t)$

$$K_{kn} = \frac{-\varepsilon}{(n-k)^2 - 1/4}\,\frac{1}{2\pi} \qquad \omega_{kn} = \frac{E_k^{(0)} - E_n^{(0)}}{\hbar} = \frac{\hbar}{2\Theta}\left(k^2-n^2\right)$$

0. rend $= \delta_{ki} = 0$

1. rend $$\frac{-i}{\hbar}\int_{\tau=0}^{t} e^{i\omega_{10}\tau}K_{10}\,d\tau = \frac{i\varepsilon}{2\pi\hbar}\int_{\tau=0}^{t} e^{i\frac{\hbar}{2\Theta}\tau}\frac{1}{1-1/4}\,d\tau = \frac{i\varepsilon}{2\pi\hbar}\,\frac{4}{3}\left(\frac{e^{i\frac{\hbar}{2\Theta}T}-1}{i\frac{\hbar}{2\Theta}}\right) =$$

$$= \frac{2\varepsilon}{3\pi\hbar^2}\,2\Theta\left(e^{i\frac{\hbar}{2\Theta}T}-1\right)$$

Melyik T-re $e^{i\frac{\hbar}{2\Theta}T}=1$ (ekkor $W^{(1)}_{0\to 1}=0$)

$T = \frac{4\Theta\pi}{\hbar}N$  $N\in\mathbb{Z}^+$ hogy $T>0$ legyen

$A = \frac{\hbar}{2\Theta}$

2. rend $$\frac{-1}{\hbar^2}\int_{\tau_2=0}^{T}\int_{\tau_1=0}^{\tau_2}\sum_j e^{i\omega_{1j}\tau_2}\,e^{i\omega_{j0}\tau_1}\underbrace{K_{1j}K_{j0}}_{\frac{\varepsilon^2}{4\pi^2}\frac{-1}{(1-j)^2-1/4}\frac{1}{j^2-1/4}}\,d\tau_1 d\tau_2 = \frac{-1}{\hbar^2}\,\frac{\varepsilon^2}{4\pi^2}\sum_j\int_{\tau_2=0}^{T} e^{iA(1-j^2)\tau_2}\int_{\tau_1=0}^{\tau_2} e^{iAj^2\tau_1}\cdot\underbrace{\frac{1}{(1-j)^2-1/4}\,\frac{1}{j^2-1/4}}_{B(j)}\,d\tau_1 d\tau_2 =$$

$$= \frac{-\varepsilon^2}{4\hbar^2\pi^2}\sum_j\frac{1}{iAj^2}\int_0^T\left(e^{iAj^2\tau_2}-1\right)e^{iA(1-j^2)\tau_2}\,B(j)\,d\tau_2 =$$

$$= \frac{-\varepsilon^2}{4\hbar^2\pi^2}\sum_j\frac{1}{iAj^2}\,B(j)\left(\frac{1}{iA}\left(e^{iAT}-1\right) - \frac{1}{iA(1-j^2)}\left(e^{iA(1-j^2)T}-1\right)\right)$$

ha $T = \frac{4\Theta\pi}{\hbar}N$

a 2. rend is 0