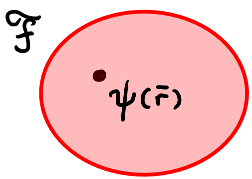
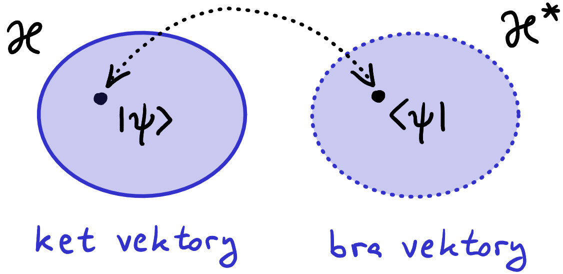
Stavy

1) prostor vlnových funkcí



2) abstraktní Hilbertův prostor



3) reprezentace v bázi

$$\begin{pmatrix} c_1 \\ c_2 \\ c_3 \\ \vdots \end{pmatrix}$$

• skalární součin

$$(\psi,\eta) = \underbrace{\int d^3\vec{r}\ \psi^*(\vec{r})}\ \underbrace{\eta(\vec{r})} \qquad \underbrace{\langle\psi|}\underbrace{\eta\rangle} \qquad \underbrace{(c_1^*\ c_2^*\ c_3^* \dots)}\ \underbrace{\begin{pmatrix} d_1 \\ d_2 \\ d_3 \\ \vdots \end{pmatrix}}$$

• rozklad do ortonormální báze

(pro ON báze)

$$\{\varphi_n(\vec{r})\} \qquad (\varphi_n,\varphi_{n'}) = \delta_{nn'} \qquad \{|n\rangle\} \qquad \langle n|n'\rangle = \delta_{nn'}$$

$$\psi(\vec{r}) = \sum_n c_n \varphi_n(\vec{r}) \qquad |\psi\rangle = \sum_n c_n |n\rangle$$

$$c_n = (\varphi_n,\psi) = \int d^3\vec{r}\ \varphi_n^*(\vec{r})\,\psi(\vec{r}) \qquad c_n = \langle n|\psi\rangle$$

Lineární operátory

1) prostor vlnových funkcí

$$\hat{x}\,\psi(\bar{r},t) = x\,\psi(\bar{r},t)$$

$$\hat{p}_x\,\psi(\bar{r},t) = \frac{\hbar}{i}\frac{\partial}{\partial x}\psi(\bar{r},t)$$

$$\hat{T}\,\psi(\bar{r},t) = -\frac{\hbar^2}{2m}\nabla^2\psi(\bar{r},t)$$

2) abstraktní Hilbertův prostor

$$\hat{A}\,|\psi\rangle$$

3) reprezentace v bázi

$$\begin{pmatrix} A_{11} & A_{12} & \cdots \\ A_{21} & A_{22} & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix}\begin{pmatrix} c_1 \\ c_2 \\ \vdots \end{pmatrix}$$

$$A_{mn} = \int d^3\bar{r}\,\varphi_m^*(\bar{r})\,\hat{A}\,\varphi_n(\bar{r}) = \langle m|\hat{A}|n\rangle$$

- linearita $\hat{A}(c_1\psi + c_2\eta) = c_1\hat{A}\psi + c_2\hat{A}\eta$

- střední hodnota $\langle\hat{A}\rangle = \int d^3\bar{r}\,\psi^*(\bar{r})\,\hat{A}\,\psi(\bar{r}) = \langle\psi|\hat{A}|\psi\rangle = (c_1^*\,c_2^*\,\ldots)\begin{pmatrix} & & \\ & A & \\ & & \end{pmatrix}\begin{pmatrix} c_1 \\ c_2 \\ \vdots \end{pmatrix}$

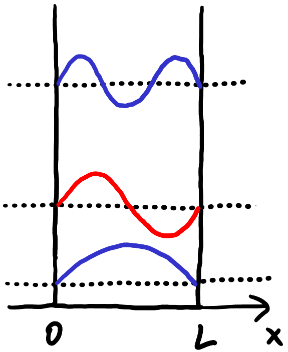
- hermitovské sdružení $(\hat{A}^+\psi,\eta) = (\psi,\hat{A}\eta)$ $\qquad A^{T*}$

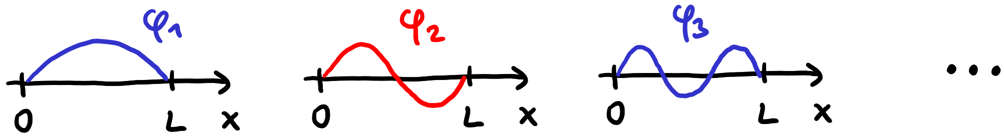
- hermitovský op. $\hat{A}^+ = \hat{A}$

  unitární op. $\hat{A}^+ = \hat{A}^{-1}$ $\longrightarrow$ $A^{T*} = A \qquad A^{T*} = A^{-1}$

  hermitovská / unitární matice

Báze Hilbertova prostoru nekonečně hluboké jámy





vlnové funkce vlastních stavů: $\varphi_n(x) = \sqrt{\frac{2}{L}}\,\sin\frac{n\pi x}{L}$

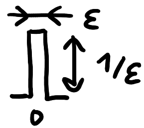
- ortonormalita

$$\int \varphi_m^*(x)\,\varphi_n(x) = \delta_{mn} \qquad \int_0^L \sqrt{\frac{2}{L}}\,\sin\frac{m\pi x}{L}\,\sqrt{\frac{2}{L}}\,\sin\frac{n\pi x}{L} = \begin{cases} 1 & m=n \\ 0 & m\neq n \end{cases}$$

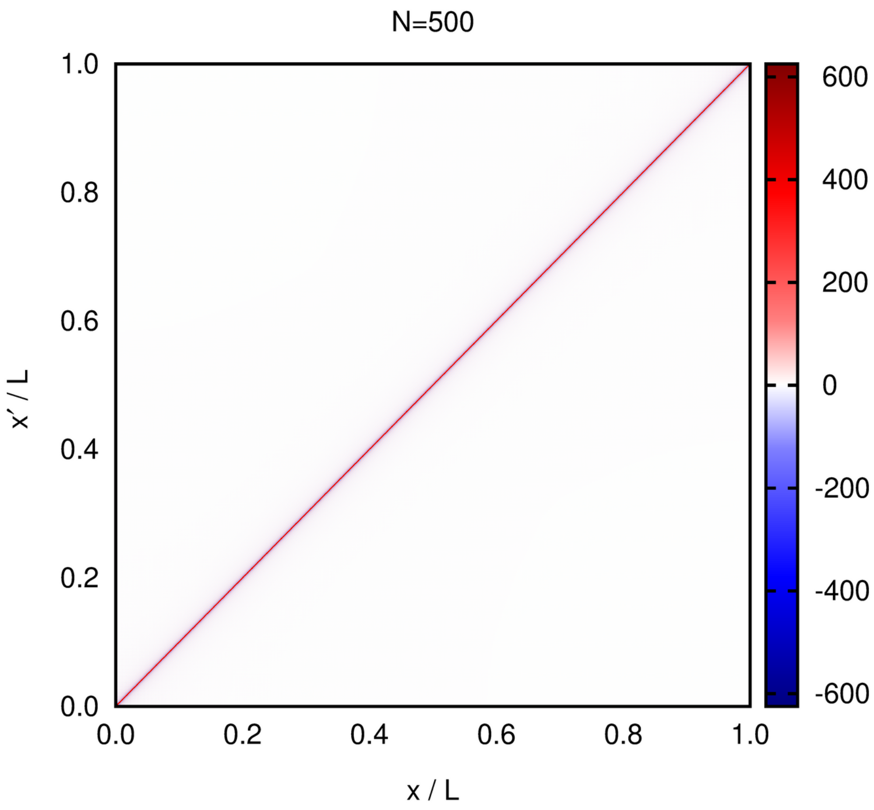
- úplnost – vyjádření pomocí Diracovy δ-funkce

$$\sum_{n=1}^{\infty} \varphi_n(x)\,\varphi_n^*(x') = \delta(x-x')$$

Diracova δ-funkce $\delta(x)$:

limita  pro $\varepsilon \to 0$

$$\lim_{N\to\infty} \sum_{n=1}^{N} \sqrt{\frac{2}{L}} \sin\frac{n\pi x}{L} \sqrt{\frac{2}{L}} \sin\frac{n\pi x'}{L} = \delta(x-x')$$



Alternativní ortonormální báze vystavěná z polynomů

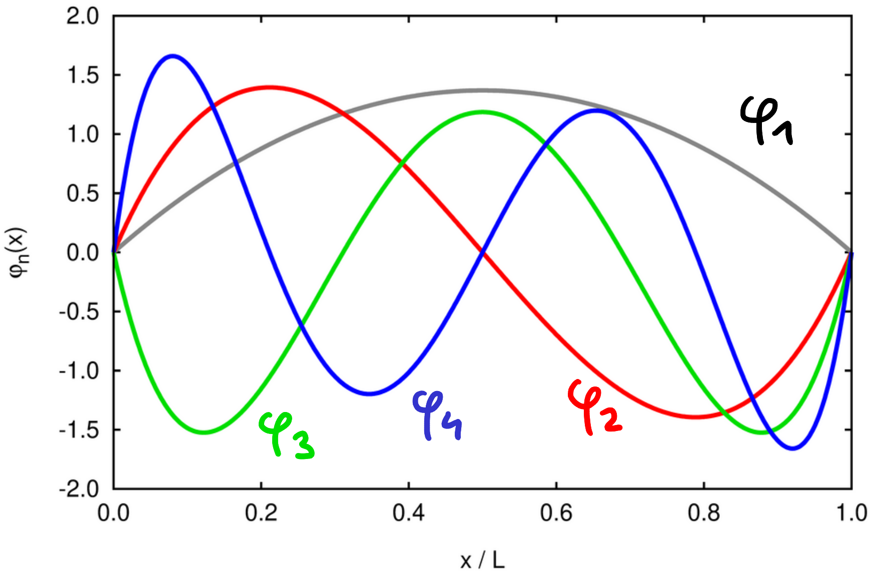
$$\varphi_1(x) = \sqrt{30}\; x(1-x)$$

$$\varphi_2(x) = 2\sqrt{210}\; x(1-x)\left(\tfrac{1}{2}-x\right)$$

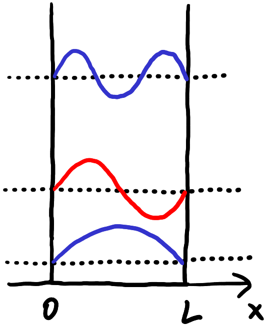
$$\varphi_3(x) = 3\sqrt{\tfrac{5}{2}}\; x(1-x)\left[1-28\left(\tfrac{1}{2}-x\right)^2\right]$$

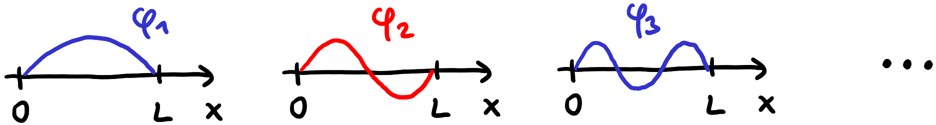
$$\varphi_4(x) = \sqrt{2310}\; x(1-x)\left(\tfrac{1}{2}-x\right)\left[12\left(\tfrac{1}{2}-x\right)^2-1\right]$$

...



Matice operátorů v ortonormální bázi vlastních stavů





$$\varphi_n(x) = \sqrt{\frac{2}{L}}\,\sin\frac{n\pi x}{L} \qquad \int \varphi_m^*(x)\,\varphi_n(x) = \delta_{mn}$$

maticové prvky

$$X_{mn} = \left(\varphi_m, \left(\hat{x} - \frac{L}{2}\right)\varphi_n\right) = \int_0^L \varphi_m^*(x)\left(x - \frac{L}{2}\right)\varphi_n(x)\,dx = \frac{2}{L}\int_0^L \sin\frac{m\pi x}{L}\left(x - \frac{L}{2}\right)\sin\frac{n\pi x}{L}\,dx$$

$$P_{mn} = \left(\varphi_m, \hat{p}\,\varphi_n\right) = \int_0^L \varphi_m^*(x)\left(\frac{\hbar}{i}\frac{d}{dx}\right)\varphi_n(x)\,dx = \frac{2}{L}\int_0^L \sin\frac{m\pi x}{L}\left(\frac{\hbar}{i}\frac{d}{dx}\right)\sin\frac{n\pi x}{L}\,dx$$

explicitně

$$X_{mn} = \begin{cases} \dfrac{4L}{\pi^2}\,\dfrac{mn\left[(-1)^{m+n} - 1\right]}{(m^2 - n^2)^2} & \\[2ex] 0 & \text{pro } m = n \end{cases} \qquad P_{mn} = \begin{cases} \dfrac{2i\hbar}{L}\,\dfrac{mn\left[(-1)^{m+n} - 1\right]}{m^2 - n^2} & \\[2ex] 0 & \text{pro } m = n \end{cases}$$

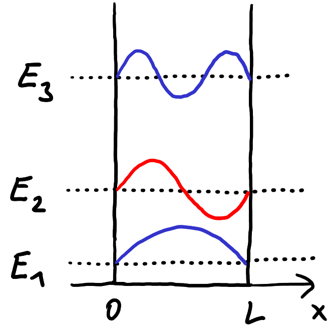
- matice reprezentující $\hat{x} - \frac{L}{2}$ a $\hat{p}$ v bázi $\varphi_n(x) = \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L}$ $n = 1, 2, 3 \ldots$

$$\hat{x} - \frac{L}{2} : \quad -\frac{L}{\pi^2} \begin{pmatrix} 0 & 16/9 & 0 & \cdots \\ 16/9 & 0 & 48/25 & \cdots \\ 0 & 48/25 & 0 & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

$$\hat{p} : \quad \frac{2i\hbar}{L} \begin{pmatrix} 0 & +4/3 & 0 & \cdots \\ -4/3 & 0 & +12/5 & \cdots \\ 0 & -12/5 & 0 & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

- aplikace – spektrum vlastních energií

– matice H reprezentující $\hat{H}$ v bázi vlastních stavů by měla být rovna $H = \mathrm{diag}(E_1, E_2, E_3, \dots)$



– Hamiltonián nekonečně hluboké jámy s potenciálem $V(x) = 0$ na dně je $\hat{H} = \hat{T} = \dfrac{\hat{p}^2}{2m}$

(operuje jen v prostoru jámy, jinde je nulové ψ)

– matici reprezentující $\hat{H}$ získáme pomocí druhé mocniny matice P reprezentující operátor $\hat{p}$

$$H = \frac{1}{2m} P \cdot P = \frac{1}{2m} \left[\frac{2i\hbar}{L} \begin{pmatrix} 0 & +4/3 & 0 & \cdots \\ -4/3 & 0 & +12/5 & \cdots \\ 0 & -12/5 & 0 & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix} \right]^2 = \frac{\pi^2 \hbar^2}{2mL^2} \begin{pmatrix} 1 & 0 & 0 & \cdots \\ 0 & 4 & 0 & \cdots \\ 0 & 0 & 9 & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

řešení pomocí vlnových funkcí: $E_n = \dfrac{\pi^2 \hbar^2}{2mL^2} n^2 \rightarrow$ na diagonále n^2 s $n = 1, 2, 3, \dots$

$N = 20$

$$\hat{P}^2 = \frac{\hbar^2\pi^2}{L^2}\begin{pmatrix} 0.961 & 0.000 & -0.117 & 0.000 & -0.197 & 0.000 & -0.281 & 0.000 & -0.371 & 0.000 & \cdots \\ 0.000 & 3.837 & 0.000 & -0.329 & 0.000 & -0.503 & 0.000 & -0.688 & 0.000 & -0.893 & \cdots \\ -0.117 & 0.000 & 8.648 & 0.000 & -0.594 & 0.000 & -0.848 & 0.000 & -1.121 & 0.000 & \cdots \\ 0.000 & -0.329 & 0.000 & 15.334 & 0.000 & -1.017 & 0.000 & -1.392 & 0.000 & -1.805 & \cdots \\ -0.197 & 0.000 & -0.594 & 0.000 & 23.998 & 0.000 & -1.432 & 0.000 & -1.893 & 0.000 & \cdots \\ 0.000 & -0.503 & 0.000 & -1.017 & 0.000 & 34.447 & 0.000 & -2.126 & 0.000 & -2.759 & \cdots \\ -0.281 & 0.000 & -0.848 & 0.000 & -1.432 & 0.000 & 46.955 & 0.000 & -2.705 & 0.000 & \cdots \\ 0.000 & -0.688 & 0.000 & -1.392 & 0.000 & -2.126 & 0.000 & 61.087 & 0.000 & -3.783 & \cdots \\ -0.371 & 0.000 & -1.121 & 0.000 & -1.893 & 0.000 & -2.705 & 0.000 & 77.419 & 0.000 & \cdots \\ 0.000 & -0.893 & 0.000 & -1.805 & 0.000 & -2.759 & 0.000 & -3.783 & 0.000 & 95.082 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

$N = 200$

$$\hat{P}^2 = \frac{\hbar^2\pi^2}{L^2}\begin{pmatrix} 0.996 & 0.000 & -0.012 & 0.000 & -0.020 & 0.000 & -0.028 & 0.000 & -0.036 & 0.000 & \cdots \\ 0.000 & 3.984 & 0.000 & -0.032 & 0.000 & -0.049 & 0.000 & -0.065 & 0.000 & -0.081 & \cdots \\ -0.012 & 0.000 & 8.964 & 0.000 & -0.061 & 0.000 & -0.085 & 0.000 & -0.109 & 0.000 & \cdots \\ 0.000 & -0.032 & 0.000 & 15.935 & 0.000 & -0.097 & 0.000 & -0.130 & 0.000 & -0.162 & \cdots \\ -0.020 & 0.000 & -0.061 & 0.000 & 24.899 & 0.000 & -0.141 & 0.000 & -0.182 & 0.000 & \cdots \\ 0.000 & -0.049 & 0.000 & -0.097 & 0.000 & 35.854 & 0.000 & -0.195 & 0.000 & -0.243 & \cdots \\ -0.028 & 0.000 & -0.085 & 0.000 & -0.141 & 0.000 & 48.802 & 0.000 & -0.254 & 0.000 & \cdots \\ 0.000 & -0.065 & 0.000 & -0.130 & 0.000 & -0.195 & 0.000 & 63.740 & 0.000 & -0.325 & \cdots \\ -0.036 & 0.000 & -0.109 & 0.000 & -0.182 & 0.000 & -0.254 & 0.000 & 80.673 & 0.000 & \cdots \\ 0.000 & -0.081 & 0.000 & -0.162 & 0.000 & -0.243 & 0.000 & -0.325 & 0.000 & 99.594 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

$N = 2000$

$$\hat{P}^2 = \frac{\hbar^2\pi^2}{L^2}\begin{pmatrix} 1.000 & 0.000 & -0.001 & 0.000 & -0.002 & 0.000 & -0.003 & 0.000 & -0.004 & 0.000 & \cdots \\ 0.000 & 3.998 & 0.000 & -0.003 & 0.000 & -0.005 & 0.000 & -0.006 & 0.000 & -0.008 & \cdots \\ -0.001 & 0.000 & 8.996 & 0.000 & -0.006 & 0.000 & -0.009 & 0.000 & -0.011 & 0.000 & \cdots \\ 0.000 & -0.003 & 0.000 & 15.994 & 0.000 & -0.010 & 0.000 & -0.013 & 0.000 & -0.016 & \cdots \\ -0.002 & 0.000 & -0.006 & 0.000 & 24.990 & 0.000 & -0.014 & 0.000 & -0.018 & 0.000 & \cdots \\ 0.000 & -0.005 & 0.000 & -0.010 & 0.000 & 35.985 & 0.000 & -0.019 & 0.000 & -0.024 & \cdots \\ -0.003 & 0.000 & -0.009 & 0.000 & -0.014 & 0.000 & 48.980 & 0.000 & -0.026 & 0.000 & \cdots \\ 0.000 & -0.006 & 0.000 & -0.013 & 0.000 & -0.019 & 0.000 & 63.974 & 0.000 & -0.032 & \cdots \\ -0.004 & 0.000 & -0.011 & 0.000 & -0.018 & 0.000 & -0.026 & 0.000 & 80.967 & 0.000 & \cdots \\ 0.000 & -0.008 & 0.000 & -0.016 & 0.000 & -0.024 & 0.000 & -0.032 & 0.000 & 99.959 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

$N = 20000$

$$\hat{P}^2 = \frac{\hbar^2\pi^2}{L^2}\begin{pmatrix} 1.000 & 0.000 & 0.000 & 0.000 & 0.000 & 0.000 & 0.000 & 0.000 & 0.000 & 0.000 & \cdots \\ 0.000 & 4.000 & 0.000 & 0.000 & 0.000 & 0.000 & 0.000 & -0.001 & 0.000 & -0.001 & \cdots \\ 0.000 & 0.000 & 9.000 & 0.000 & -0.001 & 0.000 & -0.001 & 0.000 & -0.001 & 0.000 & \cdots \\ 0.000 & 0.000 & 0.000 & 15.999 & 0.000 & -0.001 & 0.000 & -0.001 & 0.000 & -0.002 & \cdots \\ 0.000 & 0.000 & -0.001 & 0.000 & 24.999 & 0.000 & -0.001 & 0.000 & -0.002 & 0.000 & \cdots \\ 0.000 & 0.000 & 0.000 & -0.001 & 0.000 & 35.999 & 0.000 & -0.002 & 0.000 & -0.002 & \cdots \\ 0.000 & 0.000 & -0.001 & 0.000 & -0.001 & 0.000 & 48.998 & 0.000 & -0.003 & 0.000 & \cdots \\ 0.000 & -0.001 & 0.000 & -0.001 & 0.000 & -0.002 & 0.000 & 63.997 & 0.000 & -0.003 & \cdots \\ 0.000 & 0.000 & -0.001 & 0.000 & -0.002 & 0.000 & -0.003 & 0.000 & 80.997 & 0.000 & \cdots \\ 0.000 & -0.001 & 0.000 & -0.002 & 0.000 & -0.002 & 0.000 & -0.003 & 0.000 & 99.996 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$