

1 Гармонический осциллятор

$$V = \frac{1}{2}m\omega^2 x^2, \quad \dot{q}_k = \frac{p_k}{m}, \quad \dot{p}_k = - \left. \frac{\partial V}{\partial x} \right|_{q_k} = -m\omega^2 q_k$$

$$g_k = N \exp \left(\frac{1}{\hbar} \left(-\frac{1}{2}m\omega(x - q_k)^2 + ip_k(x - q_k) \right) \right) = \exp \left(\frac{1}{\hbar} \left(-\frac{1}{2}m\omega x^2 + \xi_k x + \eta_k \right) \right)$$

$$\xi_k = m\omega q_k + ip_k, \quad \eta_k = \hbar \ln N - \frac{1}{2}m\omega q_k^2 - iq_k p_k$$

$$\dot{\xi}_k = m\omega \dot{q}_k + i\dot{p}_k = \omega p_k - im\omega^2 q_k = -i\omega(m\omega q_k + ip_k) = -i\omega \xi_k$$

$$\dot{\eta}_k = -m\omega q_k \dot{q}_k - i(\dot{q}_k p_k + q_k \dot{p}_k) = -\dot{q}_k(m\omega q_k + ip_k) - iq_k \dot{p}_k = -\frac{p_k \xi_k}{m} + im\omega^2 q_k^2$$

$$\mathbb{S}_{mk} = \langle g_m | g_k \rangle = \int \exp \left(\frac{1}{\hbar} (-m\omega x^2 + (\xi_m^* + \xi_k)x + \eta_m^* + \eta_k) \right) dx =$$

$$= \int \exp \left(\frac{1}{\hbar} \left(-m\omega \left[x - \frac{\xi_m^* + \xi_k}{2m\omega} \right]^2 + \frac{(\xi_m^* + \xi_k)^2}{4m\omega} + \eta_m^* + \eta_k \right) \right) dx =$$

$$= \exp \left(\frac{1}{\hbar} \left(\frac{(\xi_m^* + \xi_k)^2}{4m\omega} + \eta_m^* + \eta_k \right) \right) \int \exp \left(-\frac{m\omega}{\hbar} y^2 \right) dy =$$

$$= \exp \left(\frac{1}{\hbar} \left(\frac{(\xi_m^* + \xi_k)^2}{4m\omega} + \eta_m^* + \eta_k \right) \right) \sqrt{\frac{\hbar\pi}{m\omega}}$$

$$\mathbb{S}_{kk} = N^2 \sqrt{\frac{\hbar\pi}{m\omega}} = 1 \Rightarrow N = \left(\frac{m\omega}{\hbar\pi} \right)^{1/4}$$

$$\langle g_m | x | g_k \rangle = \int x \cdot \exp \left(\frac{1}{\hbar} (-m\omega x^2 + (\xi_m^* + \xi_k)x + \eta_m^* + \eta_k) \right) dx =$$

$$= \hbar \int \frac{\partial}{\partial(\xi_m^* + \xi_k)} \exp \left(\frac{1}{\hbar} (-m\omega x^2 + (\xi_m^* + \xi_k)x + \eta_m^* + \eta_k) \right) dx$$

$$= \hbar \frac{\partial \mathbb{S}_{mk}}{\partial(\xi_m^* + \xi_k)} = \frac{(\xi_m^* + \xi_k)}{2m\omega} \mathbb{S}_{mk}$$

$$\langle g_m | x^2 | g_k \rangle = \int x^2 \cdot \exp \left(\frac{1}{\hbar} (-m\omega x^2 + (\xi_m^* + \xi_k)x + \eta_m^* + \eta_k) \right) dx =$$

$$= \hbar^2 \frac{\partial^2 \mathbb{S}_{mk}}{\partial(\xi_m^* + \xi_k)^2} = \frac{\hbar}{2m\omega} + \left(\frac{\xi_m^* + \xi_k}{2m\omega} \right)^2$$

$$\tau_{mk} = \langle g_m | \dot{g}_k \rangle = \frac{1}{\hbar} \mathbb{S}_{mk} \left(\dot{\eta}_k + \dot{\xi}_k \frac{\xi_k + \xi_m^*}{2m\omega} \right) = \frac{1}{\hbar} \mathbb{S}_{mk} \left(im\omega^2 q_k^2 - \frac{p_k \xi_k}{m} - i \frac{\xi_k^2 + \xi_k \xi_m^*}{2m} \right) =$$

$$\begin{aligned}
&= \frac{1}{\hbar} \mathbb{S}_{mk} \left(im\omega^2 q_k^2 - \frac{i\xi_k \xi_m^*}{2m} - \frac{i\xi_k(\xi_k - 2ip_k)}{2m} \right) = \frac{1}{\hbar} \mathbb{S}_{mk} \left(im\omega^2 q_k^2 - \frac{i\xi_k \xi_m^*}{2m} - \frac{i|\xi_k|^2}{2m} \right) = \\
&= \frac{1}{\hbar} \mathbb{S}_{mk} \left(im\omega^2 q_k^2 - \frac{i\xi_k \xi_m^*}{2m} - \frac{i(m^2\omega^2 q_k^2 + p_k^2)}{2m} \right) = \frac{1}{\hbar} \mathbb{S}_{mk} \left(\frac{i}{2} m\omega^2 q_k^2 - \frac{ip_k^2}{2m} - \frac{i\xi_k \xi_m^*}{2m} \right) \\
\mathbb{H}_{mk} &= \langle g_m | \hat{T} | g_k \rangle + \frac{1}{2} m\omega^2 \langle g_m | x^2 | g_k \rangle = -\frac{\hbar^2}{2m} \left\langle g_m \left| \frac{\partial^2}{\partial x^2} \right| g_k \right\rangle + \frac{1}{2} m\omega^2 \langle g_m | x^2 | g_k \rangle = \\
&= -\frac{\hbar^2}{2m} \left\langle g_m \left| \frac{1}{\hbar} \frac{\partial}{\partial x} (-m\omega x + \xi_k) \right| g_k \right\rangle + \frac{1}{2} m\omega^2 \langle g_m | x^2 | g_k \rangle = \\
&= \frac{\hbar\omega}{2} \langle g_m | g_k \rangle - \frac{1}{2m} \langle g_m | (-m\omega x + \xi_k)^2 | g_k \rangle + \frac{1}{2} m\omega^2 \langle g_m | x^2 | g_k \rangle = \\
&= \left(\frac{\hbar\omega}{2} - \frac{\xi_k^2}{2m} \right) \langle g_m | g_k \rangle + \omega \xi_k \langle g_m | x | g_k \rangle - \frac{1}{2} m\omega^2 \langle g_m | x^2 | g_k \rangle + \frac{1}{2} m\omega^2 \langle g_m | x^2 | g_k \rangle = \\
&= \left(\left(\frac{\hbar\omega}{2} - \frac{\xi_k^2}{2m} \right) + \omega \xi_k \frac{(\xi_m^* + \xi_k)}{2m\omega} \right) \langle g_m | g_k \rangle = \left(\frac{\hbar\omega}{2} + \frac{\xi_m^* \xi_k}{2m} \right) \langle g_m | g_k \rangle \\
\mathbb{H}_{mk} - i\hbar\boldsymbol{\tau}_{mk} &= \left(\frac{\hbar\omega}{2} + \frac{\xi_m^* \xi_k}{2m} + \frac{1}{2} m\omega^2 q_k^2 - \frac{p_k^2}{2m} - \frac{\xi_m^* \xi_k}{2m} \right) \langle g_m | g_k \rangle = \\
&= \left(\frac{\hbar\omega}{2} + \frac{1}{2} m\omega^2 q_k^2 - \frac{p_k^2}{2m} \right) \mathbb{S}_{mk} \\
(-i\mathbb{S}^{-1}(\mathbb{H} - i\hbar\boldsymbol{\tau}))_{nk} &= -i \sum_m \mathbb{S}_{nm}^{-1} (\mathbb{H}_{mk} - i\hbar\boldsymbol{\tau}_{mk}) = \\
&= -i \left(\frac{\hbar\omega}{2} + \frac{1}{2} m\omega^2 q_k^2 - \frac{p_k^2}{2m} \right) \sum_m \mathbb{S}_{nm}^{-1} \mathbb{S}_{mk} = -i \left(\frac{\hbar\omega}{2} + \frac{1}{2} m\omega^2 q_k^2 - \frac{p_k^2}{2m} \right) \delta_{nk} \\
\dot{C}_n &= -\frac{i}{\hbar} \sum_k \left(\frac{\hbar\omega}{2} + \frac{1}{2} m\omega^2 q_k^2 - \frac{p_k^2}{2m} \right) \delta_{nk} C_k = -\frac{i}{\hbar} \left(\frac{\hbar\omega}{2} + \frac{1}{2} m\omega^2 q_n^2 - \frac{p_n^2}{2m} \right) C_n \\
C_n(t) &= C_n(0) \exp \left(-\frac{i}{\hbar} \int_0^t \left(\frac{\hbar\omega}{2} + \frac{1}{2} m\omega^2 q_n^2 - \frac{p_n^2}{2m} \right) dt' \right) \\
L_n &= \frac{p_n^2}{2m} - \frac{1}{2} m\omega^2 q_n^2 \\
L &= \vec{C}^\dagger (\mathbb{T} - \mathbb{V}) \vec{C} = \sum_{m,k} C_m^* C_k \left(-\frac{\hbar^2}{2m} \left\langle g_m \left| \frac{\partial^2}{\partial x^2} \right| g_k \right\rangle - \frac{1}{2} m\omega^2 \langle g_m | x^2 | g_k \rangle \right) = \\
&= \sum_{m,k} C_m^* C_k \left(\left(\frac{\hbar\omega}{2} - \frac{\xi_k^2}{2m} \right) \mathbb{S}_{mk} + \omega \xi_k \langle g_m | x | g_k \rangle - \right. \\
&\quad \left. - \frac{1}{2} m\omega^2 \langle g_m | x^2 | g_k \rangle - \frac{1}{2} m\omega^2 \langle g_m | x^2 | g_k \rangle \right)
\end{aligned}$$

$$\begin{aligned}
&= \sum_{m,k} C_m^* C_k \left(\left(\frac{\hbar\omega}{2} - \frac{\xi_k^2}{2m} \right) \mathbb{S}_{mk} + \omega \xi_k \langle g_m | x | g_k \rangle - m\omega^2 \langle g_m | x^2 | g_k \rangle \right) = \\
&= \sum_{m,k} C_m^* C_k \left(\frac{\hbar\omega}{2} - \frac{\xi_k^2}{2m} + \frac{\omega \xi_k (\xi_m^* + \xi_k)}{2m\omega} - m\omega^2 \left(\frac{\hbar}{2m\omega} + \left(\frac{\xi_m^* + \xi_k}{2m\omega} \right)^2 \right) \right) \mathbb{S}_{mk} \\
&= \sum_{m,k} C_m^* C_k \mathbb{S}_{mk} \left(\frac{2\xi_k \xi_m^* - (\xi_m^* + \xi_k)^2}{4m} \right) = - \sum_{m,k} C_m^* C_k \mathbb{S}_{mk} \frac{(\xi_m^*)^2 + \xi_k^2}{4m} = \\
&= -\frac{1}{4m} \left(\sum_{m,k} C_m^* C_k \mathbb{S}_{mk} \xi_k^2 + \sum_{m,k} C_m^* C_k \mathbb{S}_{mk} (\xi_m^2)^* \right) = \\
&= -\frac{1}{4m} \left(\sum_{m,k} C_m^* C_k \mathbb{S}_{mk} \xi_k^2 + \sum_{m,k} (C_m C_k^* \mathbb{S}_{km} \xi_m^2)^* \right) = \\
&= -\frac{1}{2m} \sum_{m,k} \text{Re}(C_m^* C_k \mathbb{S}_{mk} \xi_k^2) = -\frac{1}{2m} \sum_{m,k} (m^2 \omega^2 q_k^2 - p_k^2) \text{Re}(C_m^* \mathbb{S}_{mk} C_k) = \\
&= \sum_{m,k} \left(\frac{p_k^2}{2m} - \frac{1}{2} m \omega^2 q_k^2 \right) \text{Re}(C_m^* \mathbb{S}_{mk} C_k) = \\
&= \sum_{m,k} L_k \text{Re} \left(C_m^*(0) C_k(0) \exp \left(-\frac{i}{\hbar} \int_0^t (L_m - L_k) dt' \right) \mathbb{S}_{mk} \right) = \\
&= \sum_{m,k} L_k \cos \left(\frac{1}{\hbar} \int_0^t (L_m - L_k) dt' \right) \text{Re}(C_m^*(0) \mathbb{S}_{mk} C_k(0)) \\
C(t) &= C(0) \exp \left(-\frac{i}{\hbar} \int_0^t \left(\frac{\hbar\omega}{2} - \frac{p^2}{2m} + \frac{1}{2} m \omega^2 q^2 \right) dt \right) \\
\dot{q} &= \frac{p}{m} \\
\dot{p} &= -m\omega^2 q \\
\ddot{q} &= \frac{\dot{p}}{m} = -\omega^2 q \\
q(t) &= A_1 e^{i\omega t} + A_2 e^{-i\omega t} \\
q(0) &= A_1 + A_2 \\
\dot{q}(0) &= \frac{p(0)}{m} = i\omega(A_1 - A_2) \\
A_1 &= \frac{1}{2} \left(q(0) - \frac{ip(0)}{m\omega} \right)
\end{aligned}$$

$$\begin{aligned}
A_2 &= \frac{1}{2} \left(q(0) + \frac{ip(0)}{m\omega} \right) \\
q(t) &= \frac{1}{2} \left(\left(q(0) - \frac{ip(0)}{m\omega} \right) e^{i\omega t} + \left(q(0) + \frac{ip(0)}{m\omega} \right) e^{-i\omega t} \right) = \\
&= \frac{1}{2} \left(q(0) (e^{i\omega t} + e^{-i\omega t}) - \frac{ip(0)}{m\omega} (e^{i\omega t} - e^{-i\omega t}) \right) = \\
&= q(0) \cos(\omega t) + \frac{p(0)}{m\omega} \sin(\omega t) \\
p(t) &= m\dot{q}(t) = -m\omega q(0) \sin(\omega t) + p(0) \cos(\omega t) \\
\int_0^t \frac{p(t')^2}{2m} dt' &= \frac{1}{2m} \left(p(0)^2 \int_0^t \cos^2(\omega t') dt' + m^2 \omega^2 q(0)^2 \int_0^t \sin^2(\omega t') dt' - \right. \\
&\quad \left. - m\omega q(0)p(0) \int_0^t 2 \sin(\omega t') \cos(\omega t') dt' \right) = \\
&= \frac{p(0)^2}{4m} \int_0^t (1 + \cos(2\omega t')) dt' + \frac{m\omega^2 q(0)^2}{4} \int_0^t (1 - \cos(2\omega t')) dt' + \\
&\quad + \frac{\omega q(0)p(0)}{2} \int_0^t \sin(2\omega t') dt' = \\
&= \frac{1}{2} \left(\frac{p(0)^2}{2m} + \frac{1}{2} m\omega^2 q(0)^2 \right) t + \frac{1}{4\omega} \left(\frac{p(0)^2}{2m} - \frac{1}{2} m\omega^2 q(0)^2 \right) \sin(2\omega t) - \\
&\quad - \frac{q(0)p(0)}{4} (\cos(2\omega t) - 1) \\
\frac{1}{2} m\omega^2 \int_0^t q(t')^2 dt' &= \frac{1}{2} m\omega^2 \left(q(0)^2 \int_0^t \cos^2(\omega t') dt' + \frac{p(0)^2}{m^2 \omega^2} \int_0^t \sin^2(\omega t') dt' + \right. \\
&\quad \left. + \frac{q(0)p(0)}{m\omega} \int_0^t 2 \sin(\omega t') \cos(\omega t') dt' \right) = \\
&= \frac{1}{4} m\omega^2 q(0)^2 \int_0^t (1 + \cos(2\omega t')) dt' + \frac{p(0)^2}{4m} \int_0^t (1 - \cos(2\omega t')) dt' + \\
&\quad + \frac{\omega q(0)p(0)}{2} \int_0^t \sin(2\omega t') dt' = \\
&= \frac{t}{2} \left(\frac{p(0)^2}{2m} + \frac{1}{2} m\omega^2 q(0)^2 \right) - \frac{1}{4\omega} \left(\frac{p(0)^2}{2m} - \frac{1}{2} m\omega^2 q(0)^2 \right) \sin(2\omega t) - \\
&\quad - \frac{q(0)p(0)}{4} (\cos(2\omega t) - 1) \\
\int_0^t \left(\frac{p(t')^2}{2m} - \frac{1}{2} m\omega^2 q(t')^2 \right) dt' &= \left(\frac{p(0)^2}{2m} - \frac{1}{2} m\omega^2 q(0)^2 \right) \frac{\sin(2\omega t)}{2\omega}
\end{aligned}$$

$$C(t) = C(0) \exp \left(-\frac{i\omega t}{2} + \left(\frac{p(0)^2}{2m} - \frac{1}{2}m\omega^2 q(0)^2 \right) \frac{i \sin(2\omega t)}{2\hbar\omega} \right)$$

$$C(t) = C(0) \exp \left(-\frac{i}{\hbar} \left(\frac{\hbar\omega}{2} - L(0) \frac{\sin(2\omega t)}{2\omega t} \right) t \right) \quad (1)$$

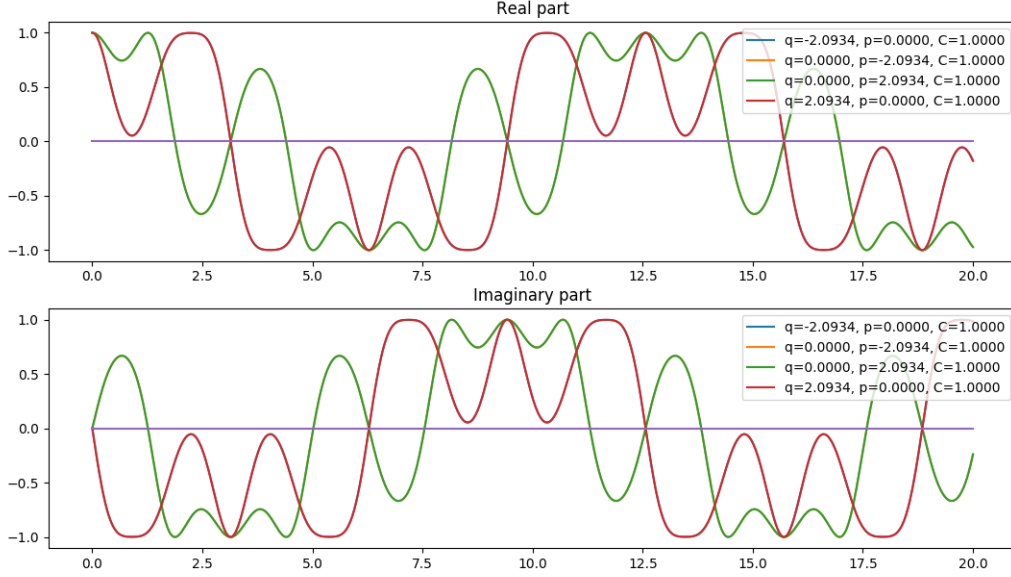


Рис. 1: Вид коэффициентов (уравнение 1), описываем состояние с энергией 2.5 с помощью подогнанного базиса, можем использовать базисные функции с параметром ~ 0.25 и коэффициентами $[-1.0, 1.0, 1.0, -1.0]$. Но такой сигнатуры не получаем.

$$g_k = N \exp \left(\frac{1}{\hbar} \left(-\frac{1}{2}m\omega(x - q)^2 + ipx \right) \right) = \exp \left(\frac{1}{\hbar} \left(-\frac{1}{2}m\omega x^2 + \xi_k x + \eta_k \right) \right)$$

$$\xi_k = m\omega q_k + ip_k, \quad \eta_k = -\frac{1}{2}m\omega q^2$$

$$\dot{\xi}_k = m\omega \dot{q}_k + i\dot{p}_k = \omega p_k - im\omega^2 q_k = -\omega(im\omega q_k - p_k) = -i\omega(m\omega q_k + ip_k) = -i\omega \xi_k$$

$$\dot{\eta}_k = -m\omega q_k \dot{q}_k = -\omega q_k p_k$$

$$\tau_{mk} = \frac{1}{\hbar} \langle g_m | \dot{g}_k \rangle = \frac{1}{\hbar} \mathbb{S}_{mk} \left(\dot{\eta}_k + \dot{\xi}_k \frac{\xi_m^* + \xi_k}{2m\omega} \right) = \frac{1}{\hbar} \mathbb{S}_{mk} \left(-\omega q_k p_k - i\omega \xi_k \frac{\xi_m^* + \xi_k}{2m\omega} \right) =$$

$$= \frac{1}{\hbar} \mathbb{S}_{mk} \left(-\omega q_k p_k - \frac{i\xi_k^2}{2m} - \frac{i\xi_m^* \xi_k}{2m} \right) =$$

$$= \frac{1}{\hbar} \mathbb{S}_{mk} \left(-\omega q_k p_k - \frac{i}{2m} (m^2 \omega^2 q_k^2 - p_k^2 + 2im\omega q_k p_k) - \frac{i\xi_m^* \xi_k}{2m} \right) = \frac{1}{\hbar} \mathbb{S}_{mk} \left(iL_k - \frac{i\xi_m^* \xi_k}{2m} \right)$$

$$\begin{aligned}
\mathbb{H}_{mk} &= \mathbb{S}_{mk} \left(\frac{\hbar\omega}{2} + \frac{\xi_m^* \xi_k}{2m} \right) \\
\mathbb{H}_{mk} - i\hbar\tau_{mk} &= \mathbb{S}_{mk} \left(\frac{\hbar\omega}{2} + L_k \right) \\
\dot{C}_n &= -\frac{i}{\hbar} \sum_{m,k} \mathbb{S}_{nm}^{-1} \mathbb{S}_{mk} \left(\frac{\hbar\omega}{2} + L_k \right) C_k = -\frac{i}{\hbar} \sum_k \left(\sum_m \mathbb{S}_{nm}^{-1} \mathbb{S}_{mk} \right) \left(\frac{\hbar\omega}{2} + L_k \right) C_k \\
\dot{C}_n &= -\frac{i}{\hbar} \sum_k \left(\frac{\hbar\omega}{2} + L_k \right) \delta_{nk} C_k = -\frac{i}{\hbar} \left(\frac{\hbar\omega}{2} + L_n \right) C_n \\
C(t) &= C(0) \exp \left(-\frac{i}{\hbar} \left(\frac{\hbar\omega}{2} + L(0) \frac{\sin(2\omega t)}{2\omega t} \right) t \right) \quad (2)
\end{aligned}$$

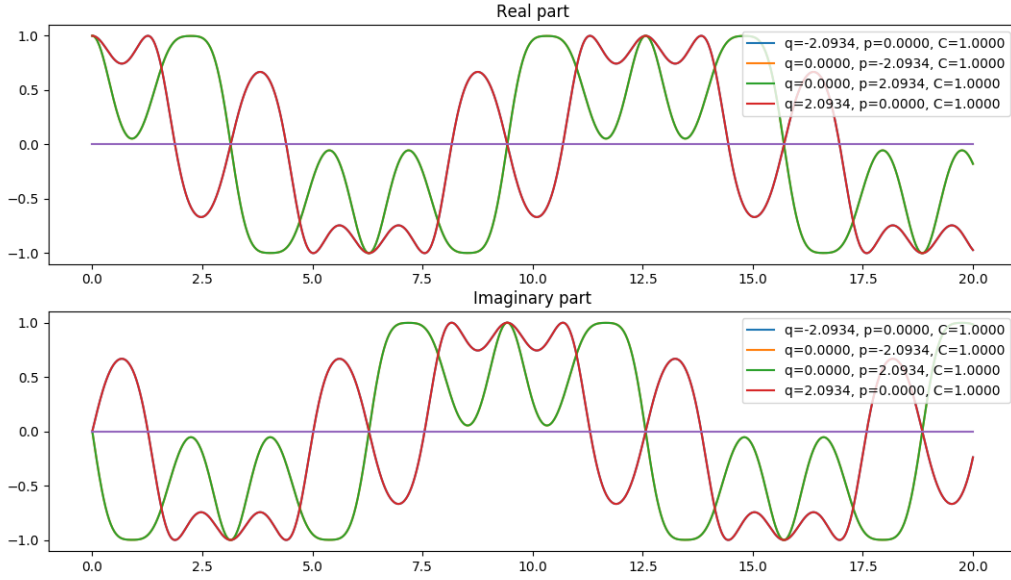


Рис. 2: Вид коэффициентов (уравнение 1), описываем состояние с энергией 2.5 с помощью подогнанного базиса, можем использовать базисные функции с параметром ~ 0.25 и коэффициентами $[-1.0, 1.0, 1.0, -1.0]$. Но такой сигнатуры не получаем.