Řešení 2D Schrödingerovy rovnice Lanczosovou diagonalizací

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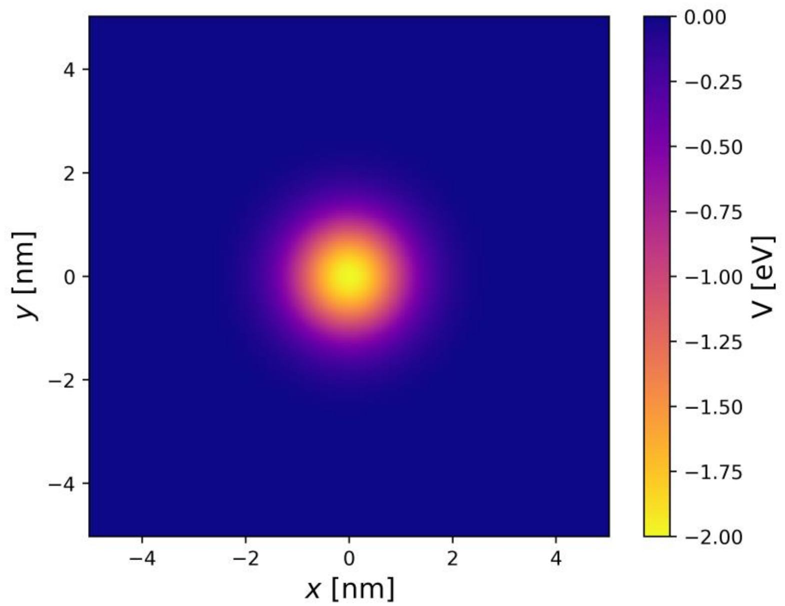
$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right)\Psi(x,y)+V(x,y)\Psi(x,y)=E\Psi(x,y)$$

$$\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right)\Psi(x,y)\approx\frac{\Psi_{i-1,j}+\Psi_{i+1,j}+\Psi_{i,j-1}+\Psi_{i,j+1}-4\Psi_{i,j}}{\Delta^2}$$

- rotačně symetrický gaussovský potenciál s grupou symetrie $O(2)$

$$V(x,y) = -V_0 \exp\left(-\frac{x^2+y^2}{2\sigma^2}\right) \,,$$

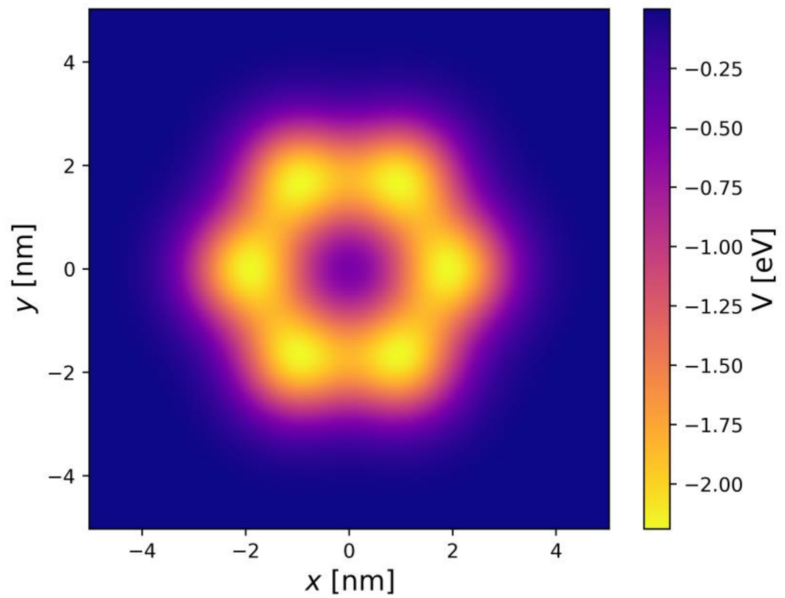
kde $V_0 = 2\,\mathrm{eV}$ a $\sigma = 2\,\mathrm{nm}$



- potenciál s grupou symetrie C_{6v} připomínající molekulu benzenu

$$V(x,y) = -V_0 \sum_{n=1}^{6} \exp\left[-\frac{(x - R\cos\frac{n\pi}{3})^2 + (y - R\sin\frac{n\pi}{3})^2}{2\sigma^2}\right]$$

s parametry $V_0 = 2\,\mathrm{eV}$, $\sigma = 0.8\,\mathrm{nm}$, $R = 2\,\mathrm{nm}$.



Matice $\hat{H}$ s rozměry $N \times N$

1. Úvodní část postupu

   (a) $\mathbf{v}_1$ je náhodný normovaný vektor délky N
   (b) $\mathbf{w}'_1 = \hat{H}\mathbf{v}_1$
   (c) $\alpha_1 = \mathbf{w}'_1 \cdot \mathbf{v}_1$
   (d) $\mathbf{w}_1 = \mathbf{w}'_1 - \alpha_1 \mathbf{v}_1$

2. Iterační část postupu, for $j = 2, \ldots, m$

   (a) $\beta_j = |\mathbf{w}_{j-1}|$
   (b) $\mathbf{v}_j = \mathbf{w}_{j-1}/\beta_j$
   (c) $\mathbf{w}'_j = \hat{H}\mathbf{v}_j$
   (d) $\alpha_j = \mathbf{w}'_j \cdot \mathbf{v}_j$
   (e) $\mathbf{w}_j = \mathbf{w}'_j - \alpha_j \mathbf{v}_j - \beta_{j-1}\mathbf{v}_{j-1}$

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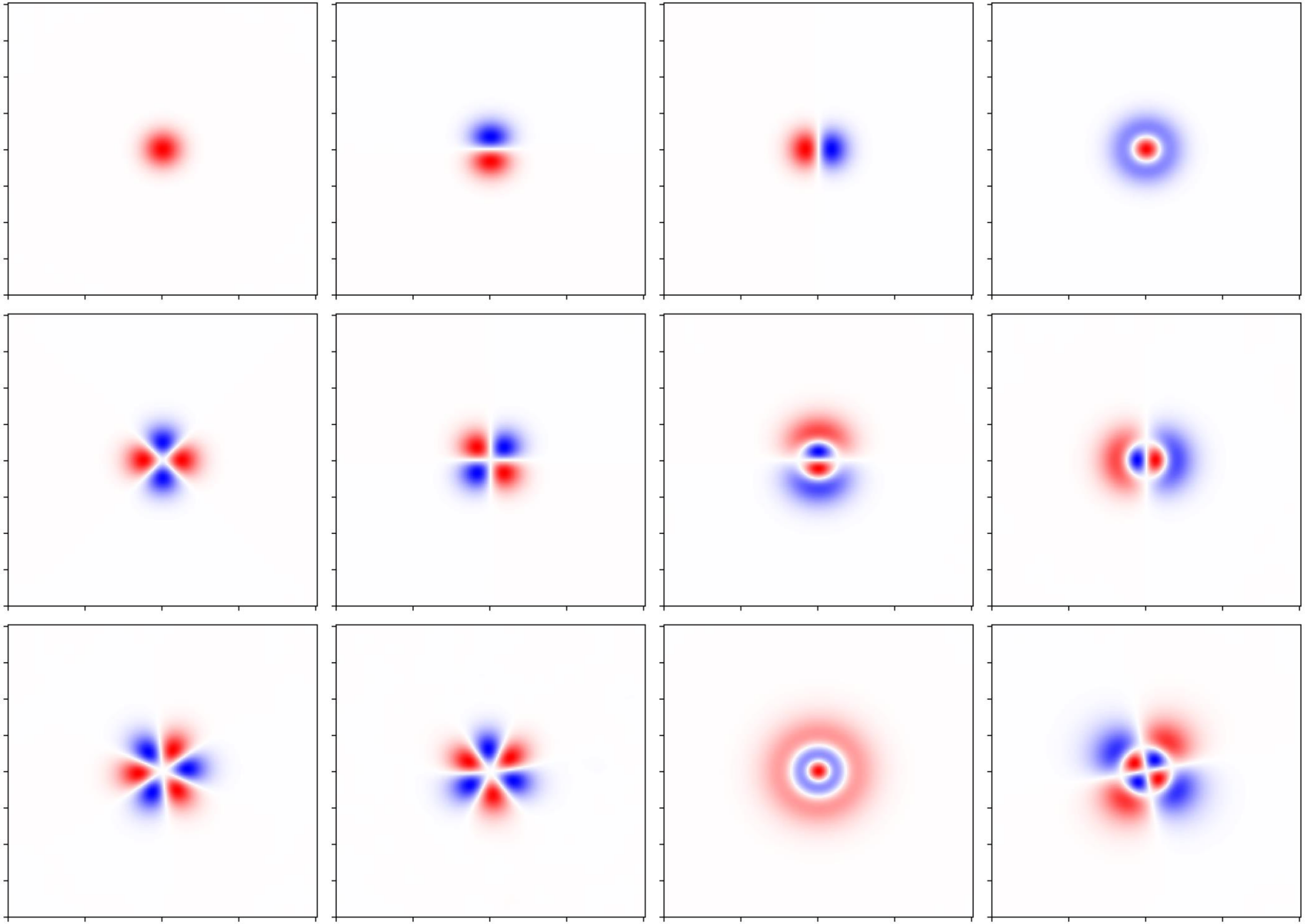
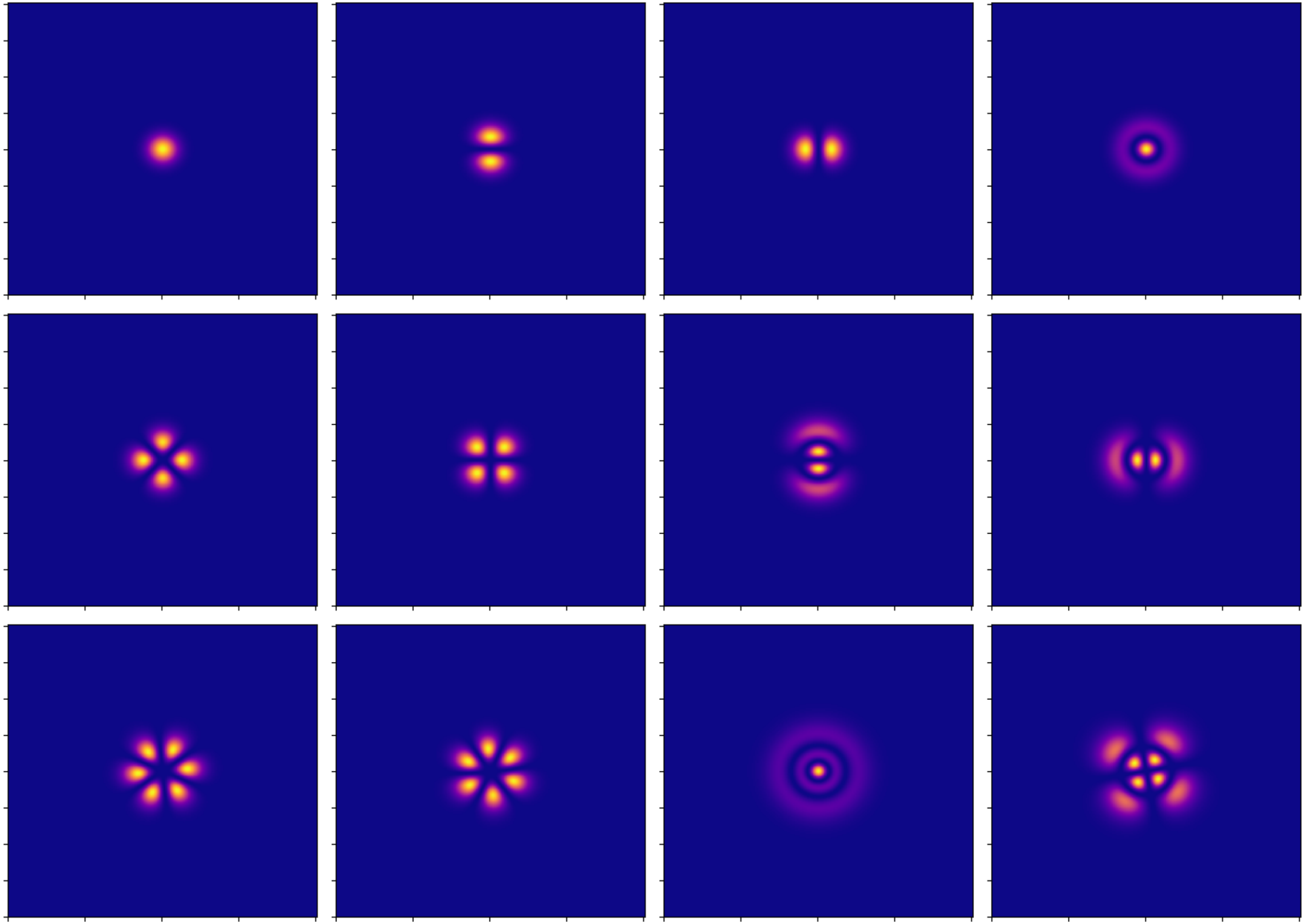
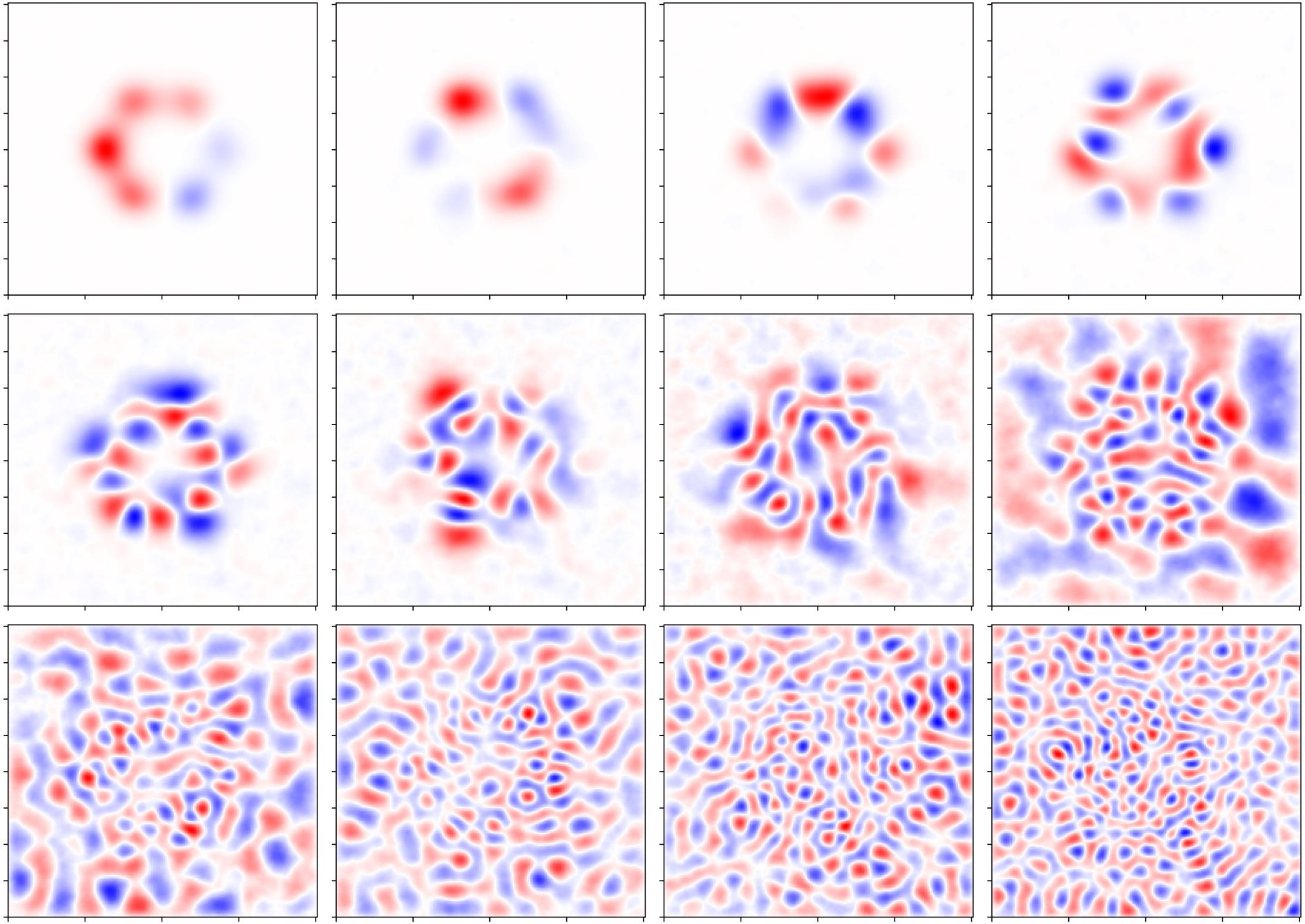
$$T = \begin{pmatrix} \alpha_1 & \beta_2 & & & & 0 \\ \beta_2 & \alpha_2 & \beta_3 & & & \\ & \beta_3 & \alpha_3 & \ddots & & \\ & & \ddots & \ddots & \beta_{m-1} & \\ & & & \beta_{m-1} & \alpha_{m-1} & \beta_m \\ 0 & & & & \beta_m & \alpha_m \end{pmatrix}$$

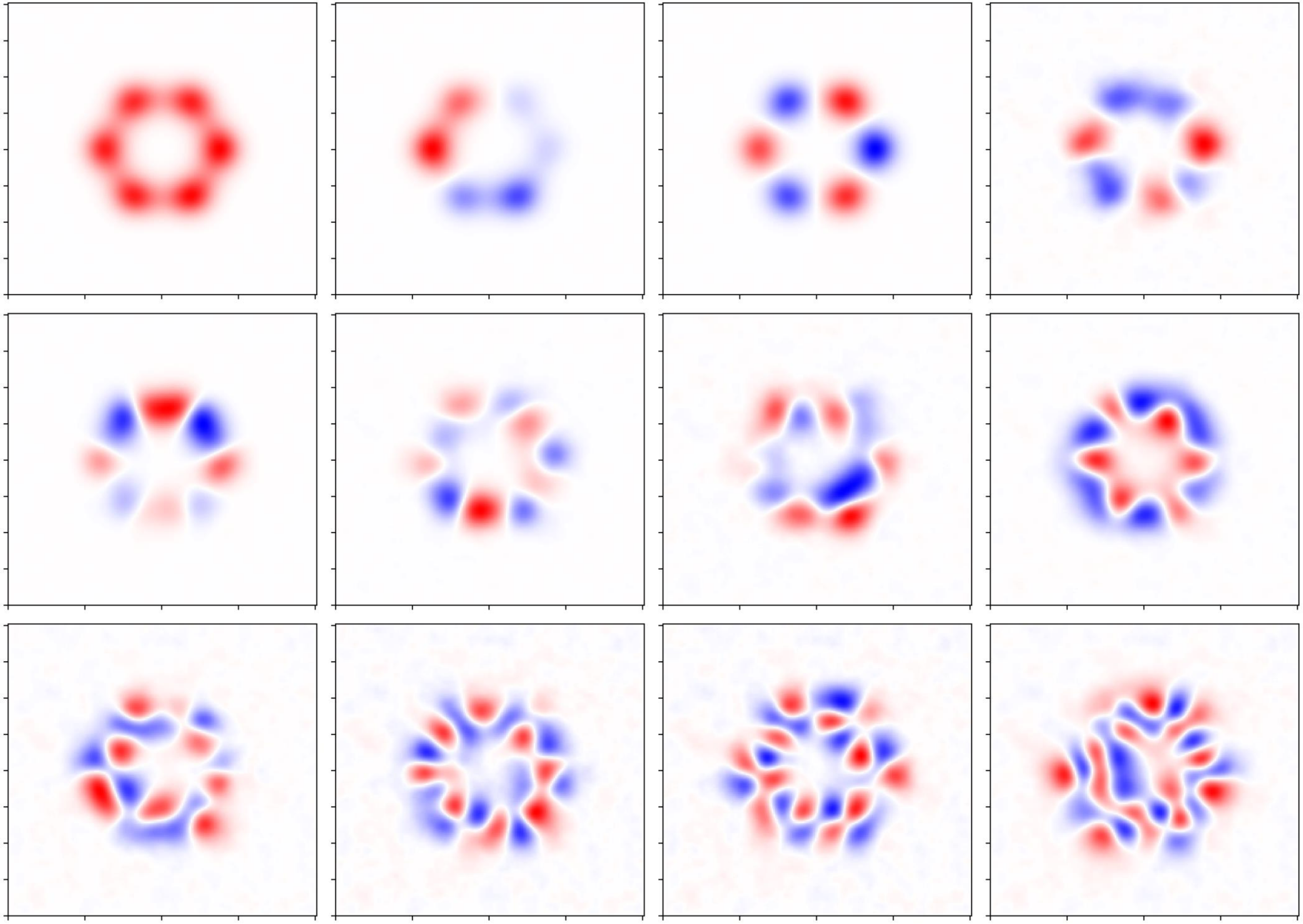
Matice $\hat{V}$: ortonormální sloupce

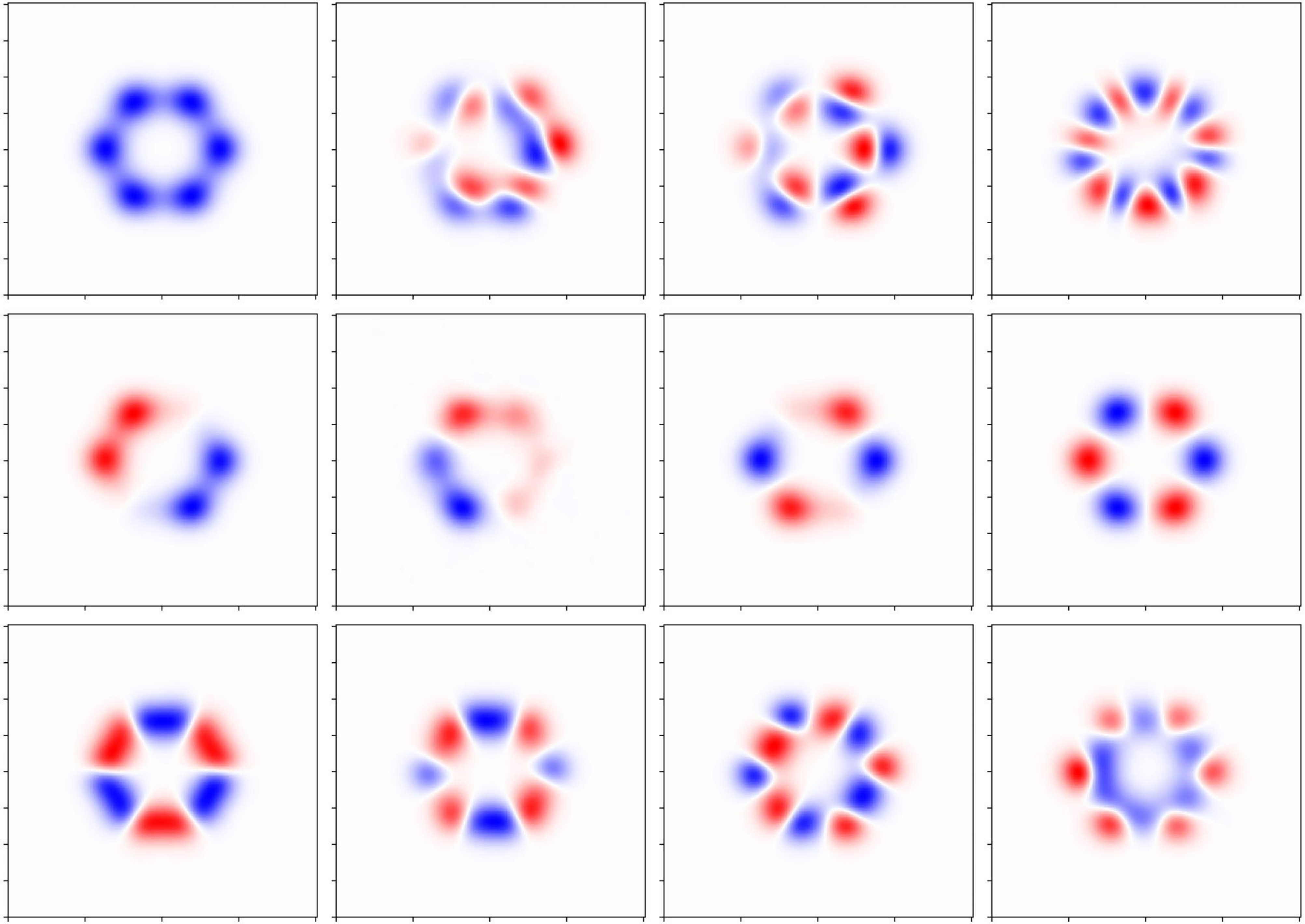
$$\hat{T}\mathbf{t_i} = \lambda_i \mathbf{t}_i$$
$$\psi_i = \hat{V}\mathbf{t_i}$$

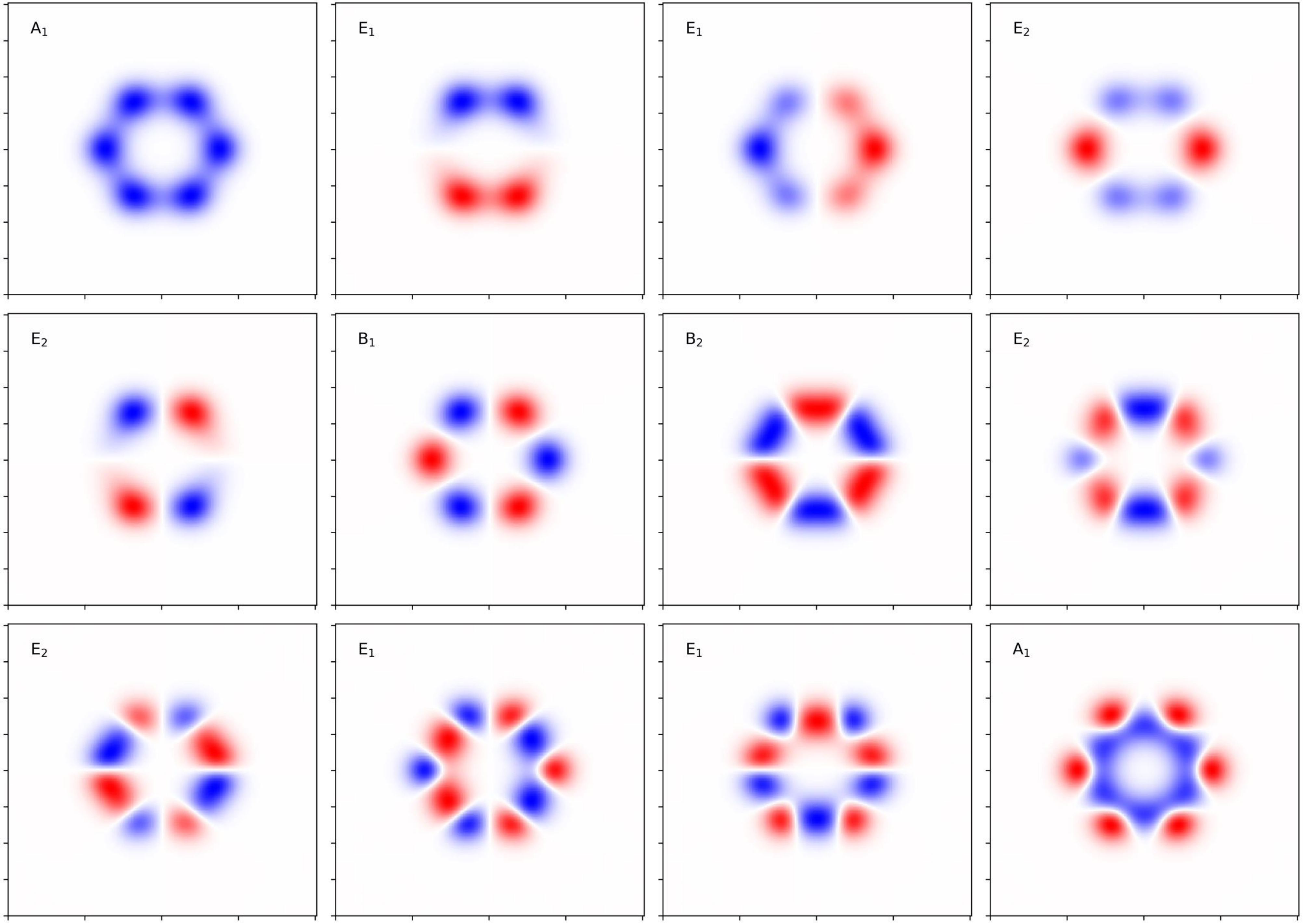




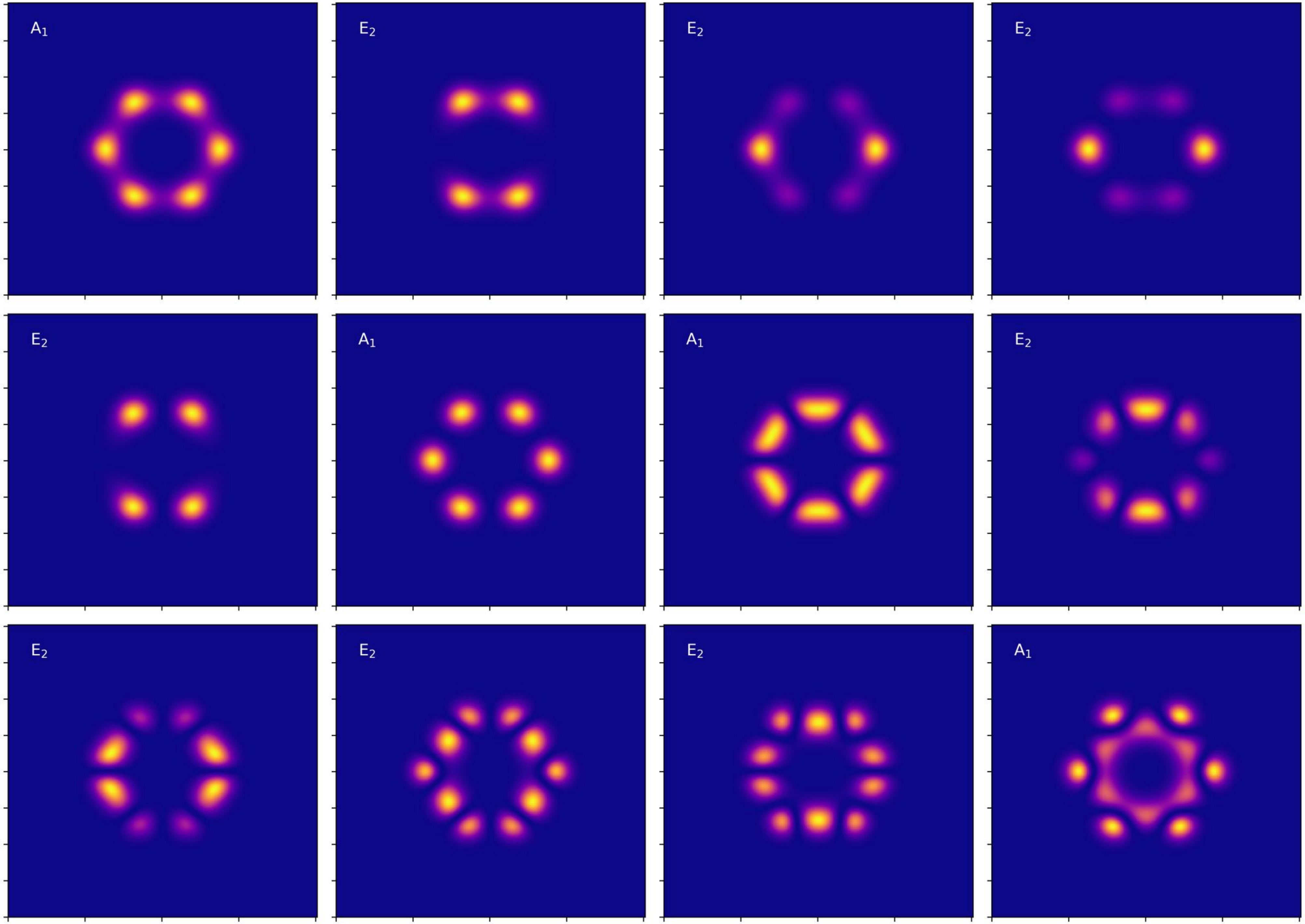


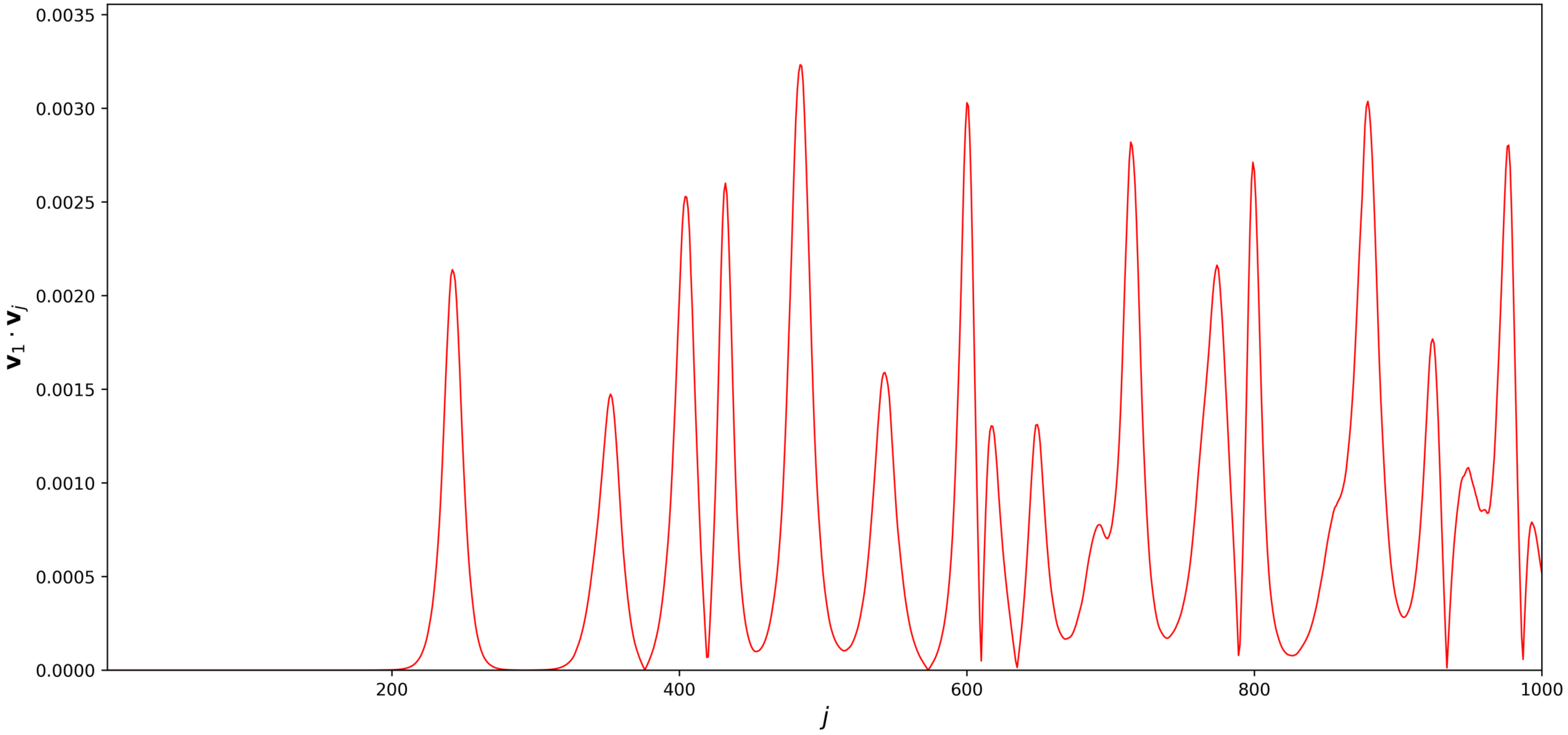






A1
E1
E1
E2
E2
B1
B2
E2
E2
E1
E1
A1


A1
E2
E2
E2
E2
A1
A1
E2
E2
E2
E2
A1


0.0035
0.0030
0.0025
0.0020
0.0015
0.0010
0.0005
0.0000
$\mathbf{v}_1 \cdot \mathbf{v}_j$
200
400
600
800
1000
j