

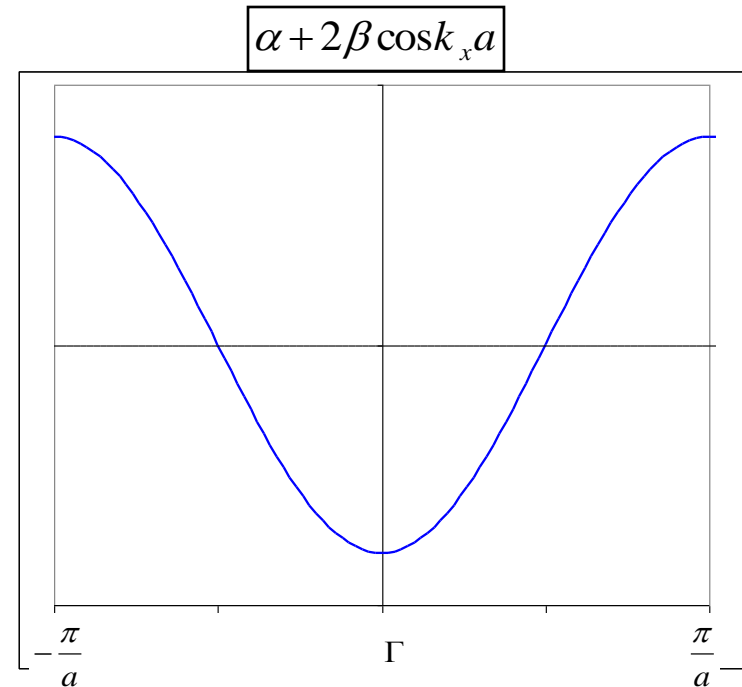
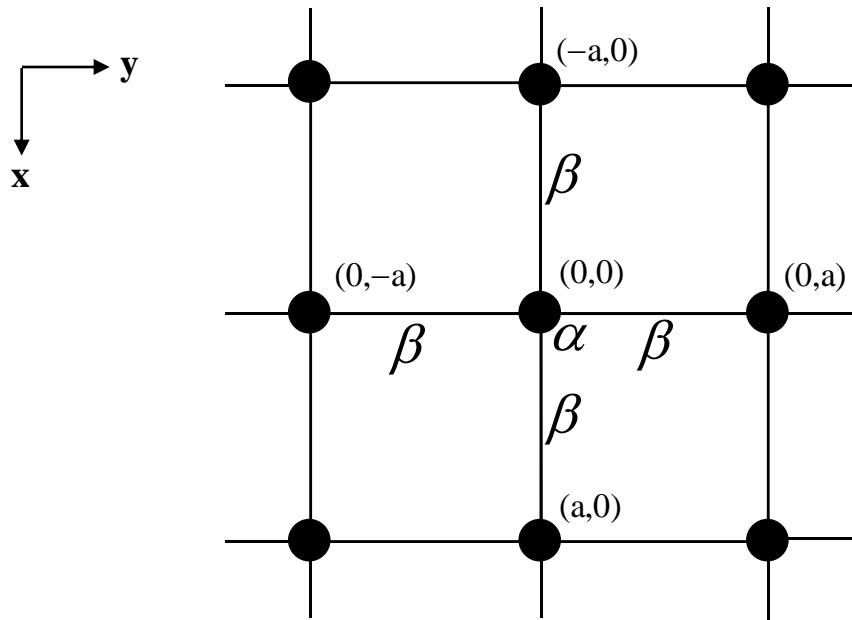
Uvažujeme jen interakce s nejbližšími sousedy:  
jen výměnný integrál  $\beta$  s nejbližším sousedem

$$(E \sim \alpha, t \sim \beta, S \ll 1)$$

$$H(\vec{k}) = \alpha + \beta e^{ik_x a} + \beta e^{-ik_x a} = \alpha + 2\beta \cos k_x a$$

$$H(\vec{k}) = \alpha + \beta e^{ik_x a} + \beta e^{-ik_x a} + \beta e^{ik_y a} + \beta e^{-ik_y a} + \beta e^{ik_z a} + \beta e^{-ik_z a} =$$

$$= \alpha + 2\beta(\cos k_x a + \cos k_y a + \cos k_z a)$$



$$\begin{aligned} + \beta e^{-ika/2} + \beta e^{ika/2} &= \beta(\cos ka/2 - i \sin ka/2) + \beta(\cos ka/2 + i \sin ka/2) = \\ &= \beta(\cos ka/2 + \cos ka/2 - i \sin ka/2 + i \sin ka/2) = 2\beta \cos ka/2 \end{aligned}$$

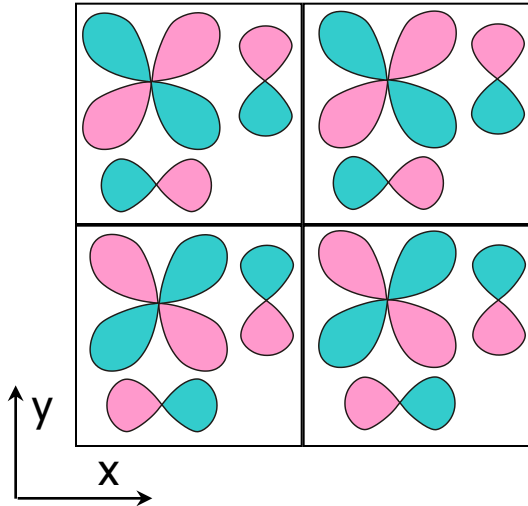
$$\begin{aligned} - \beta e^{-ika/2} - \beta e^{ika/2} &= -\beta(\cos ka/2 - i \sin ka/2) - \beta(\cos ka/2 + i \sin ka/2) = \\ &= -\beta(\cos ka/2 + \cos ka/2 - i \sin ka/2 + i \sin ka/2) = -2\beta \cos ka/2 \end{aligned}$$

$$\begin{aligned} - \beta e^{-ika/2} + \beta e^{ika/2} &= -\beta(\cos ka/2 - i \sin ka/2) + \beta(\cos ka/2 + i \sin ka/2) = \\ &= \beta(-\cos ka/2 + \cos ka/2 + i \sin ka/2 + i \sin ka/2) = 2i\beta \sin ka/2 \end{aligned}$$

$$\begin{aligned} + \beta e^{-ika/2} - \beta e^{ika/2} &= +\beta(\cos ka/2 - i \sin ka/2) - \beta(\cos ka/2 + i \sin ka/2) = \\ &= \beta(\cos ka/2 - \cos ka/2 - i \sin ka/2 - i \sin ka/2) = -2i\beta \sin ka/2 \end{aligned}$$

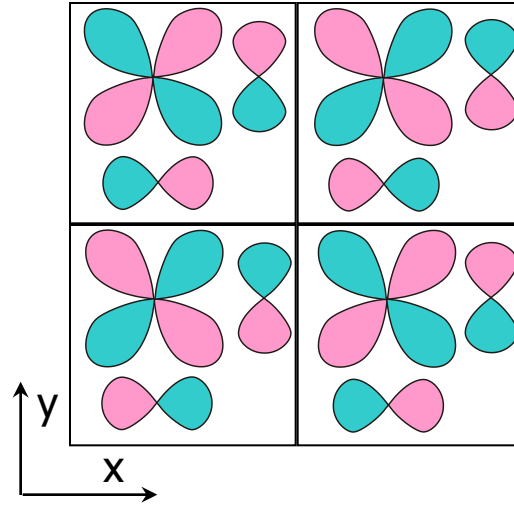
$d_{xy}, p_x, p_y$

$$\begin{vmatrix} \alpha_{d_{xy}} & -i2\beta_{dp} \sin k_y a/2 & i2\beta_{dp} \sin k_x a/2 \\ H_{12}^* & \alpha_{p_x} & -i2\beta_{pp} \sin k_x a/2 - i2\beta_{pp} \sin k_y a/2 \\ H_{13}^* & H_{23}^* & \alpha_{p_y} \end{vmatrix}$$



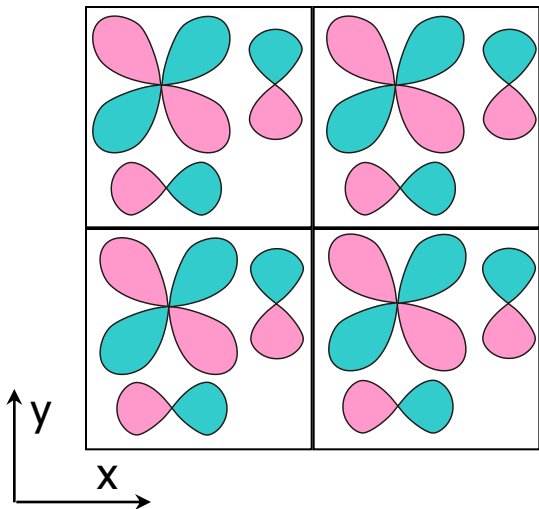
Y

$$\begin{bmatrix} k_x & k_y \\ 0 & \frac{\pi}{a} \\ -1 & -1 \\ 1 & 1 \end{bmatrix}$$



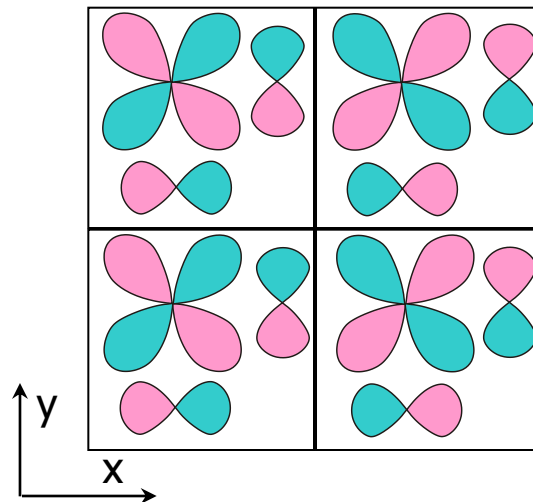
S

$$\begin{bmatrix} k_x & k_y \\ \frac{\pi}{a} & \frac{\pi}{a} \\ -1 & 1 \\ 1 & -1 \end{bmatrix}$$



Gamma

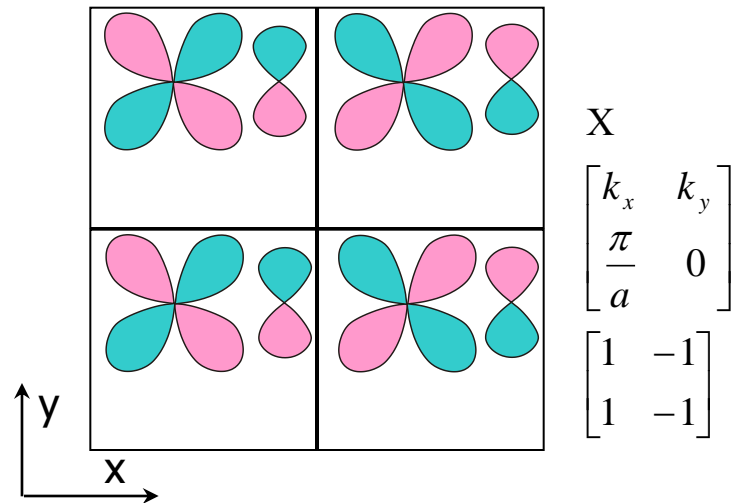
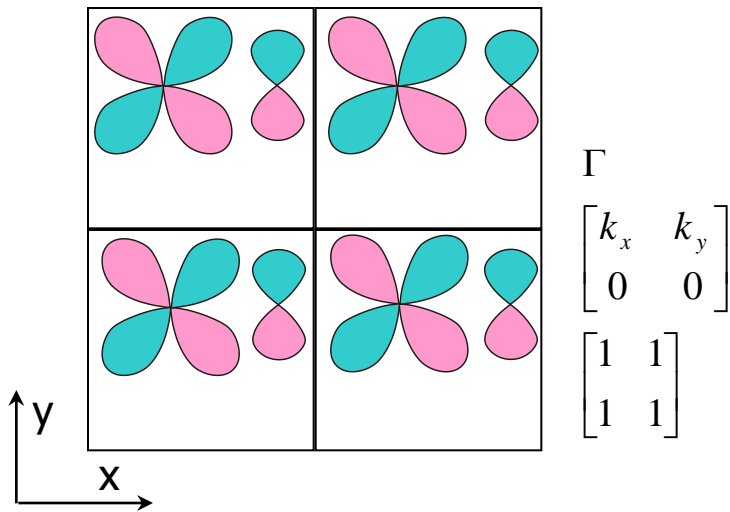
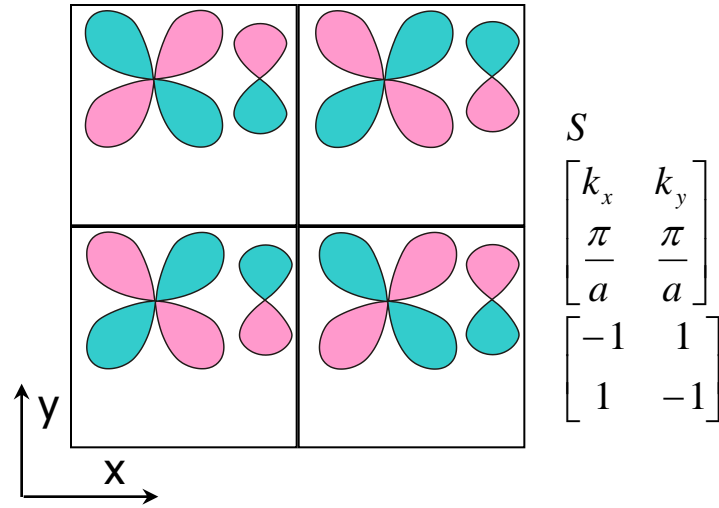
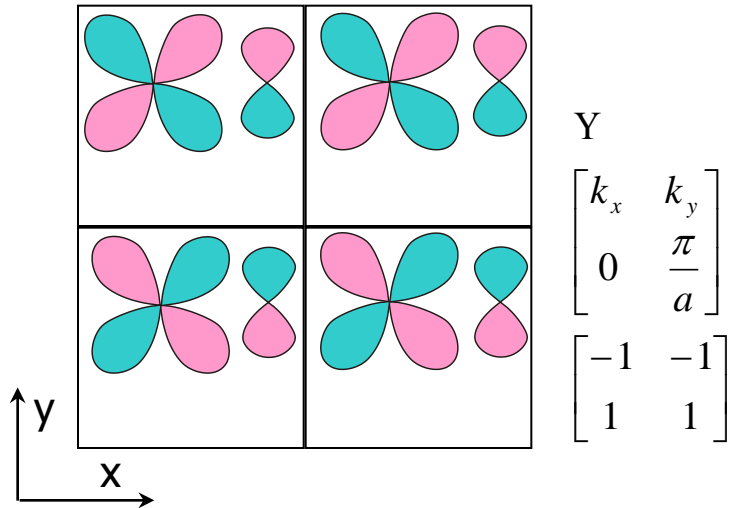
$$\begin{bmatrix} k_x & k_y \\ 0 & 0 \\ 1 & 1 \\ 1 & 1 \end{bmatrix}$$



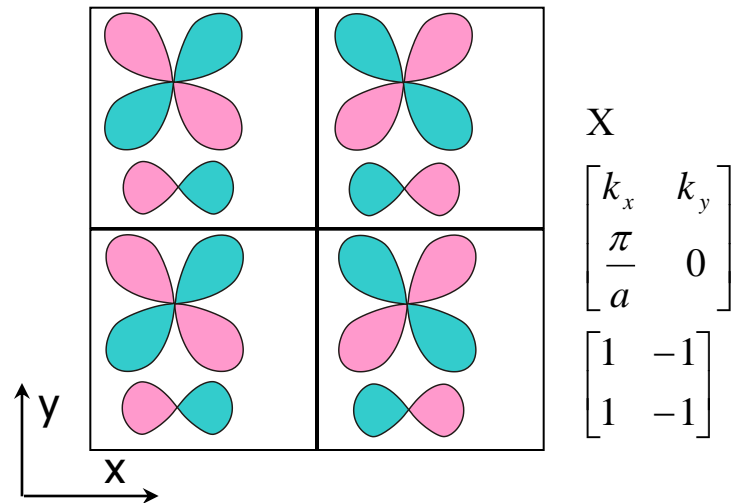
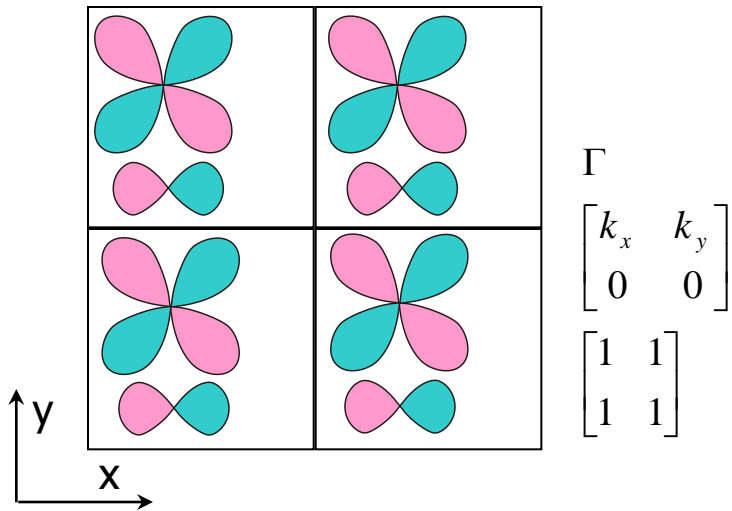
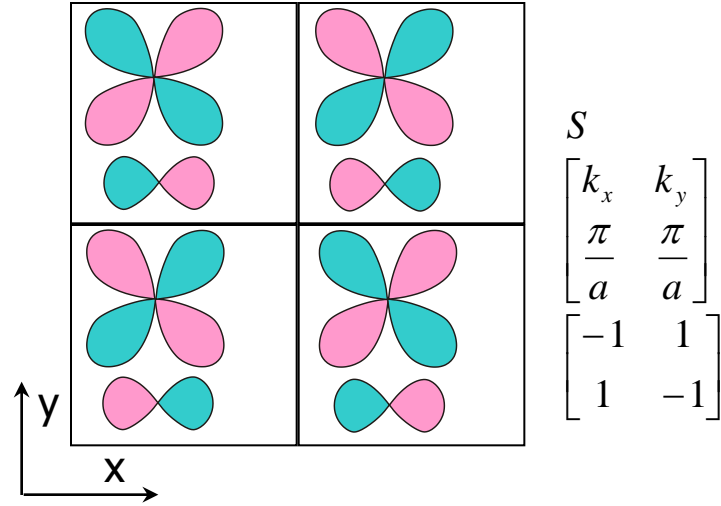
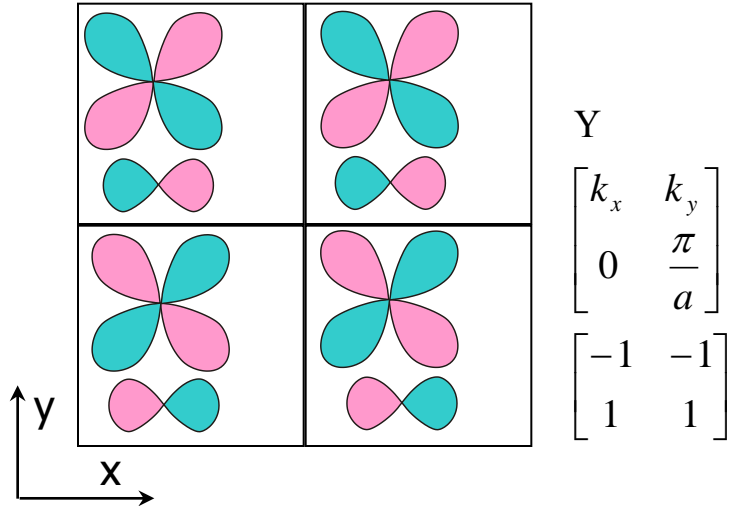
X

$$\begin{bmatrix} k_x & k_y \\ \frac{\pi}{a} & 0 \\ 1 & -1 \\ 1 & -1 \end{bmatrix}$$

$$\Gamma: -\beta_{dp}e^{-ik_x a/2} + \beta_{dp}e^{ik_x a/2} = 2i\beta_{dp} \sin k_x a/2$$

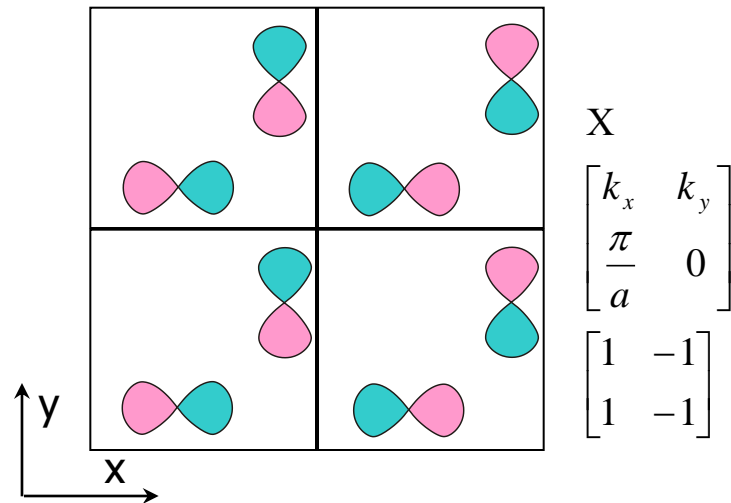
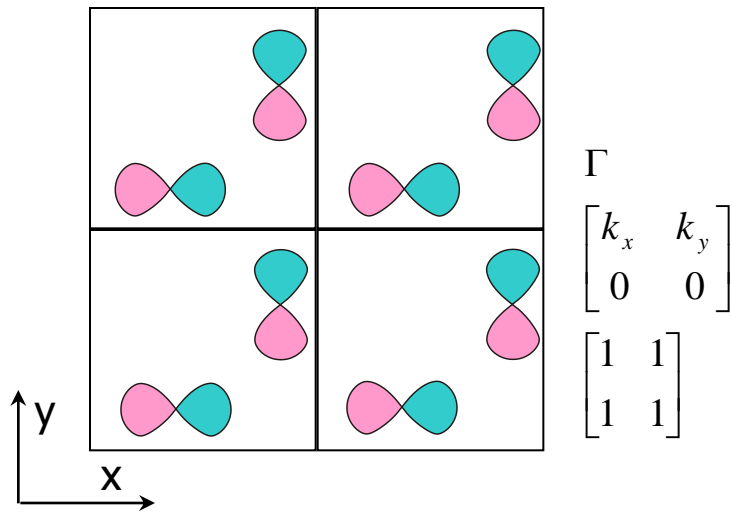
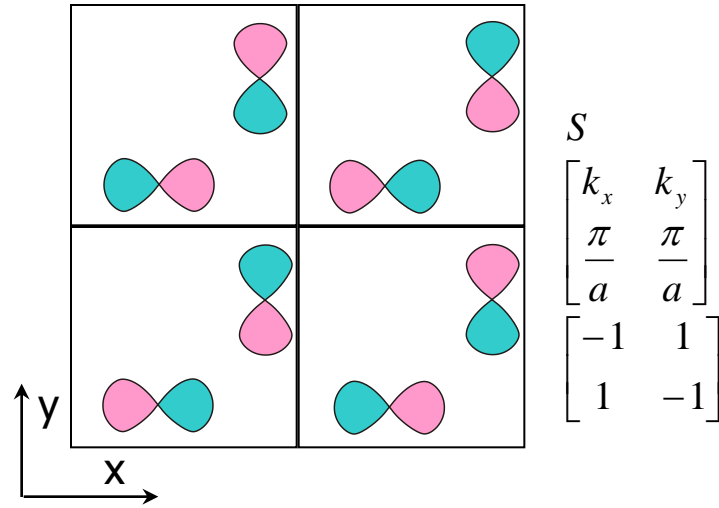
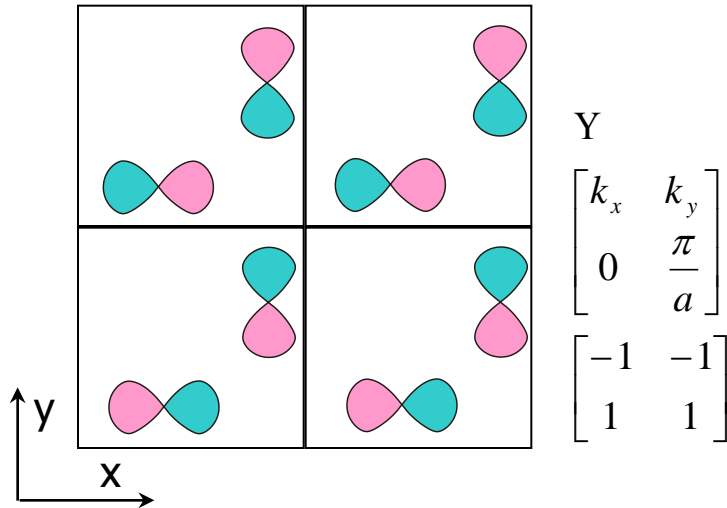


$$\Gamma: \beta_{dp} e^{-ik_y a/2} - \beta_{dp} e^{ik_y a/2} = -2i\beta_{dp} \sin k_y a/2$$



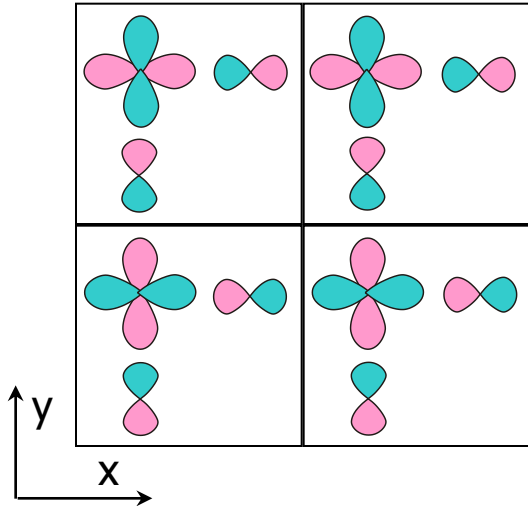
$$\Gamma: \beta_{pp} e^{-ik_x a/2} - \beta_{pp} e^{ik_x a/2} + \beta_{pp} e^{-ik_y a/2} - \beta_{pp} e^{ik_y a/2} =$$

$$-2i\beta_{pp} \sin k_x a/2 - 2i\beta_{pp} \sin k_y a/2$$

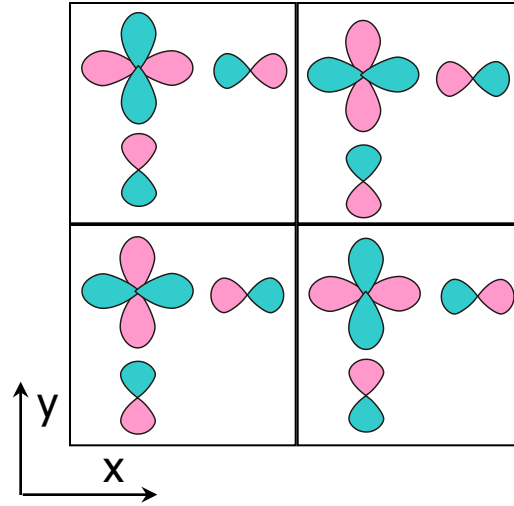


$d_{x^2-y^2}, p_x, p_y$   
 $\beta_{pp}^\pi > \beta_{pp}^\sigma$   
 $\alpha$ 

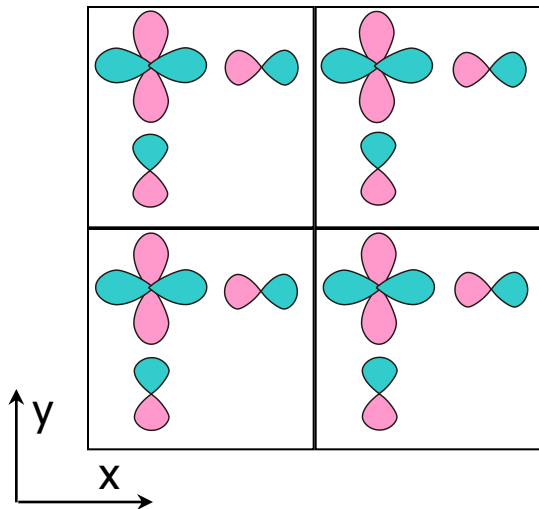
$$\begin{vmatrix} \alpha_{d_{x^2-y^2}} & -i2\beta_{dp} \sin k_y a / 2 & i2\beta_{dp} \sin k_x a / 2 \\ H_{12}^* & \alpha_{p_x} & -i2\beta_{pp} \sin k_x a / 2 - i2\beta_{pp} \sin k_y a / 2 \\ H_{13}^* & H_{23}^* & \alpha_{p_y} \end{vmatrix}$$



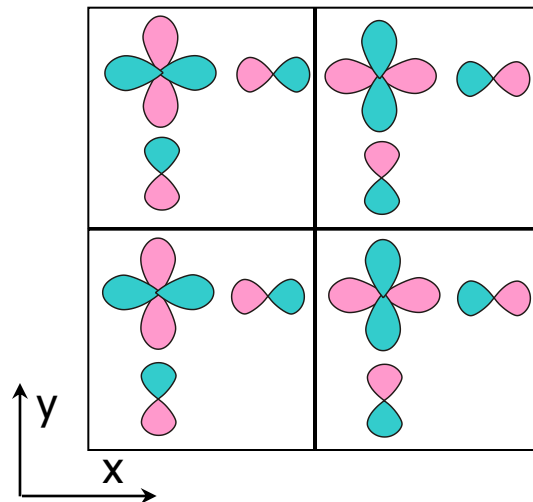
$$Y \begin{bmatrix} k_x & k_y \\ 0 & \frac{\pi}{a} \\ -1 & -1 \\ 1 & 1 \end{bmatrix}$$



$$S \begin{bmatrix} k_x & k_y \\ \frac{\pi}{a} & \frac{\pi}{a} \\ -1 & 1 \\ 1 & -1 \end{bmatrix}$$



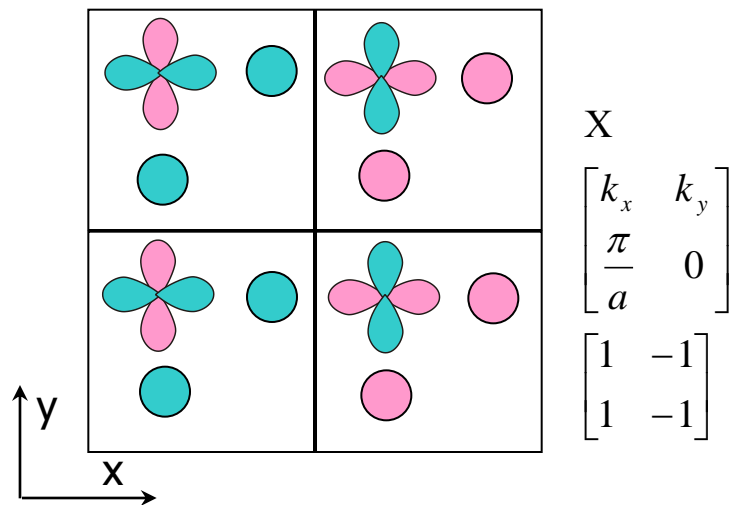
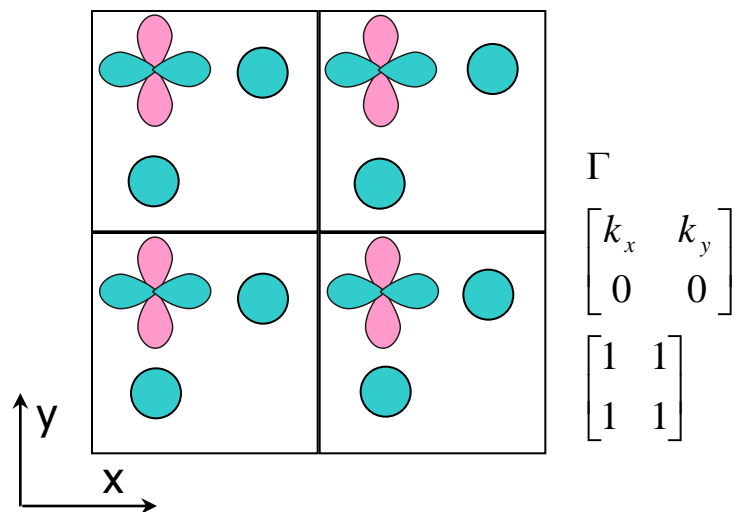
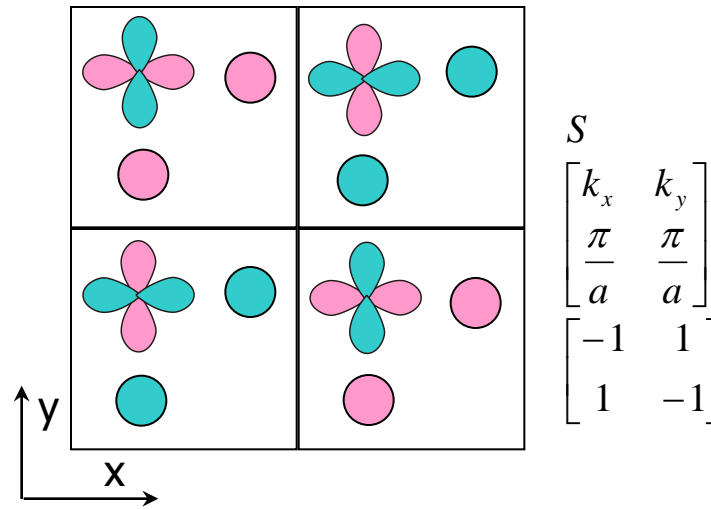
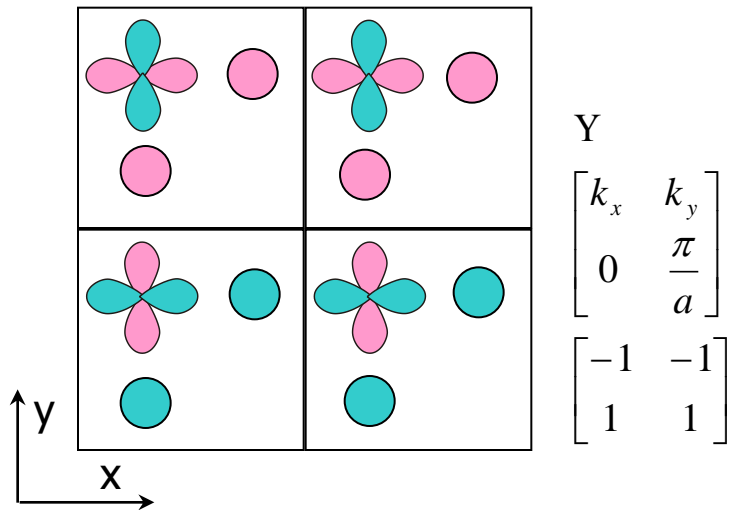
$$\Gamma \begin{bmatrix} k_x & k_y \\ 0 & 0 \\ 1 & 1 \\ 1 & 1 \end{bmatrix}$$



$$X \begin{bmatrix} k_x & k_y \\ \frac{\pi}{a} & 0 \\ 1 & -1 \\ 1 & -1 \end{bmatrix}$$

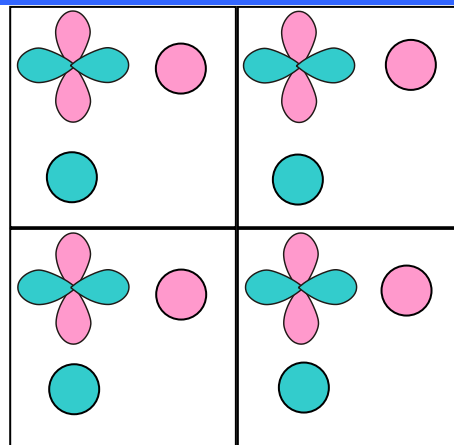
$s + d_{x^2-y^2}$

$$\begin{vmatrix} \alpha_{d_{x^2-y^2}} & 2\beta \cos k_x a / 2 & -2\beta \cos k_y a / 2 \\ H_{12}^* & \alpha_s & 0 \\ H_{13}^* & H_{23}^* & \alpha_s \end{vmatrix}$$

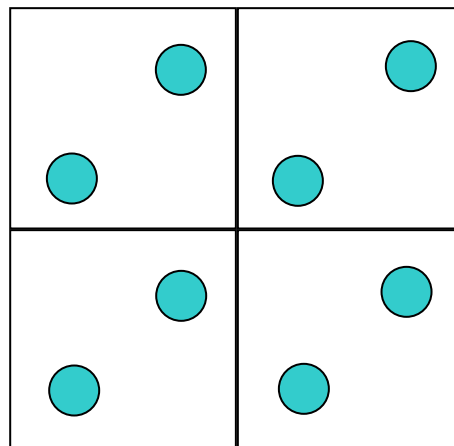




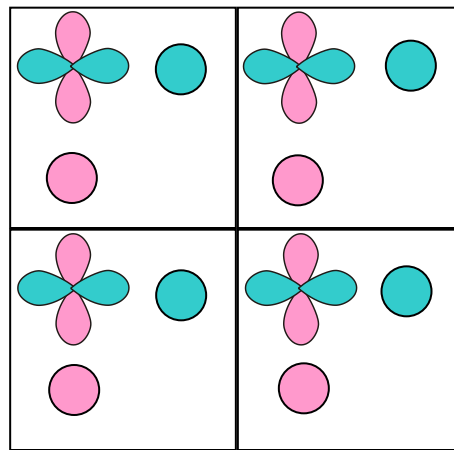
antivazebný



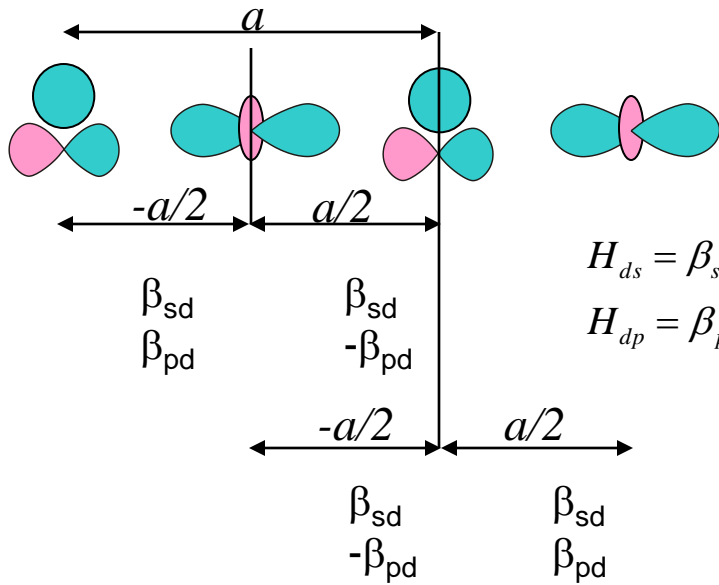
nevazebný



vazebný



Lineární řetěz ve směru  $z$ , poloha A:  $s, p_z$ ; poloha B:  $d_{z2}$ ;



$$H_{ds} = \beta_{sd}e^{-ik_x a/2} + \beta_{sd}e^{ik_x a/2} = 2\beta \cos k_x a/2$$

$$H_{dp} = \beta_{pd}e^{-ik_x a/2} - \beta_{pd}e^{ik_x a/2} = -i2\beta \sin k_x a/2$$

$$H_{sd} = \beta_{sd}e^{-ik_x a/2} + \beta_{sd}e^{ik_x a/2} = 2\beta \cos k_x a/2$$

$$H_{pd} = -\beta_{pd}e^{-ik_x a/2} + \beta_{pd}e^{ik_x a/2} = i2\beta \sin k_x a/2$$

$$\begin{vmatrix} \alpha_s & 0 & 2\beta \cos k_x a/2 \\ 0 & \alpha_p & i2\beta \sin k_x a/2 \\ 2\beta \cos k_x a/2 & -i2\beta \sin k_x a/2 & \alpha_d \end{vmatrix}$$