SKEO

Slater-**K**oster LCAO tight-binding method with **E**volutionary **O**ptimization

Load NC algebra library

Load noncommutative algebra library:

In[1]:=
```
If[Length[PacletFind["NCAlgebra"]] == 0, PacletInstall[
o··· długość  znajdź pakiet                zainstaluj pakiet
    "https://github.com/NCAlgebra/NC/blob/master/NCAlgebra-6.0.3.paclet?raw=true
      "]];
<< NCAlgebra`;
SetNonCommutative[s, y, z, x, xy, yz, z2, xz, x2y2];
(*when caclulating SK elements orbitals should not be commutative*)
```

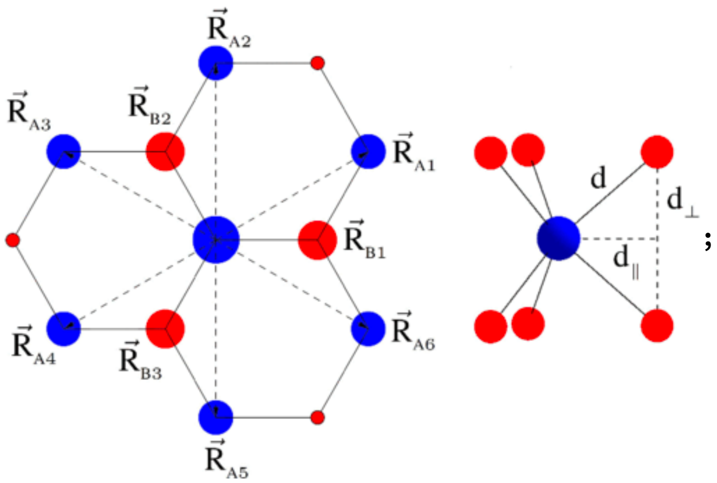
••• NCAlgebra : All lower cap single letter symbols (e.g. a,b,c,...) were set as noncommutative.

Load SKLE library

In[4]:=
```
<< (NotebookDirectory[] <> "SKEO_lib.mx")
    katalog notatnika
NCExpandFunc = NCExpand;(* from NCAlgebra lib *)
```

TMDC monolayer

In this section we follow the model of $M\,X_2$ monolayers introduced in https://journals.aps.org/prb/abstract/10.1103/PhysRevB.97.085153



Now, let's define basis orbitals (we are working in a basis of cubic harmonics: https://en.wikipedia.org/wiki/Cubic_harmonic)

Note that some of basis elements (*PE* and *PO* representing chalcogenide dimer) are composed of orbitals localized on different lattice nodes.

Basis definition

In[6]:=

$$\texttt{Dp2} = \frac{1}{\sqrt{2}}\,(\texttt{x2y2} + \texttt{I xy});\texttt{(*even orbital at M*)}$$

jedność urojona

$$\texttt{Dp1} = \frac{-1}{\sqrt{2}}\,(\texttt{xz} + \texttt{I yz});\texttt{(*odd orbital at M*)}$$

jedność urojona

$$\texttt{D0 = z2;(*even orbital at M*)}$$

$$\texttt{Dm1} = \frac{1}{\sqrt{2}}\,(\texttt{xz} - \texttt{I yz});\texttt{(*odd orbital at M*)}$$

jedność urojona

$$\texttt{Dm2} = \frac{1}{\sqrt{2}}\,(\texttt{x2y2} - \texttt{I xy});\texttt{(*even orbital at M*)}$$

jedność urojona

$$\texttt{PEp1} = \left\{\frac{-1}{2}\,(\texttt{x} + \texttt{I y}),\ \frac{-1}{2}\,(\texttt{x} + \texttt{I y})\right\};$$

jedność urojona jedność urojona

$$\texttt{(*even X2 dimer composed of up and down orbital*)}$$

$$\texttt{PE0} = \left\{\frac{1}{\sqrt{2}}\,\texttt{z},\ \frac{-1}{\sqrt{2}}\,\texttt{z}\right\};\ \texttt{(*even X2 dimer composed of up and down orbital*)}$$

$$\texttt{PEm1} = \left\{\frac{1}{2}\,(\texttt{x} - \texttt{I y}),\ \frac{1}{2}\,(\texttt{x} - \texttt{I y})\right\};$$

jedność urojona jedność urojona

$$\texttt{(*even X2 dimer composed of up and down orbital*)}$$

$$\texttt{POp1} = \left\{\frac{-1}{2}\,(\texttt{x} + \texttt{I y}),\ \frac{1}{2}\,(\texttt{x} + \texttt{I y})\right\};$$

jedność urojona jedność urojona

$$\texttt{(*odd X2 dimer composed of up and down orbital*)}$$

$$\texttt{PO0} = \left\{\frac{1}{\sqrt{2}}\,\texttt{z},\ \frac{1}{\sqrt{2}}\,\texttt{z}\right\};\texttt{(*odd X2 dimer composed of up and down orbital*)}$$

$$\texttt{POm1} = \left\{\frac{1}{2}\,(\texttt{x} - \texttt{I y}),\ \frac{1}{2}\,(-\texttt{x} + \texttt{I y})\right\};$$

jedność urojona jedność urojona

$$\texttt{(*odd X2 dimer composed of up and down orbital*);}$$

Collect all basis elements :

In[17]:=

```
orbitals = {Dm2, D0, Dp2, PEm1, PE0, PEp1, Dm1, Dp1, POm1, PO0, POp1};
```

Hoppings definition

Now define Matrix of hoppings for the each possible bond (we assume Next Nearest Neighbour approximation)

In[18]:=
```
hopMM = {{3/2 dr, Sqrt[3]/2 dr, 0}, {0, Sqrt[3] dr, 0}, {-3/2 dr, Sqrt[3]/2 dr, 0},
   {-3/2 dr, -Sqrt[3]/2 dr, 0}, {0, -Sqrt[3] dr, 0}, {3/2 dr, -Sqrt[3]/2 dr, 0}};
mxu = {{dr, 0, dp}, {-1/2 dr, Sqrt[3]/2 dr, dp}, {-1/2 dr, -Sqrt[3]/2 dr, dp}};
xum = {{-dr, 0, -dp}, {1/2 dr, -Sqrt[3]/2 dr, -dp}, {1/2 dr, Sqrt[3]/2 dr, -dp}};
mxd = {{dr, 0, -dp}, {-1/2 dr, Sqrt[3]/2 dr, -dp}, {-1/2 dr, -Sqrt[3]/2 dr, -dp}};
xdm = {{-dr, 0, dp}, {1/2 dr, -Sqrt[3]/2 dr, dp}, {1/2 dr, Sqrt[3]/2 dr, dp}};
hopMX = {mxu, mxd, {1, 2}};
hopXM = {xum, xdm, {2, 1}};(*last entry, {2,1},
means that hopping is from orbital combined of two nodes to single-noded*)
hopXX = {hopMM, 0, 0, hopMM, {2, 2}};(*0 means that we ommit given hopping;
 (2,2) means that we hop from dimer to dimer*);
```

Hoppings in our basis. Note that hoppings between dimers (consisting of orbitals at different nodes) are combined from multiple possibilities, with the option that some of them may be omitted (using “0” entry). In our case *<up-element, down-element* | *up-element, down-element*> element has 4 possible hoppings to be defined *{<up,up>, <up,down>, <down|up>, <down|down>}*. Here we decided to skip more distant mixed *up-down* and *down-up* hoppings.

In[26]:=
```
Hop = {
    {hopMM, hopMM, hopMM, hopMX, hopMX, hopMX, 0, 0, 0, 0, 0},
    {hopMM, hopMM, hopMM, hopMX, hopMX, hopMX, 0, 0, 0, 0, 0},
    {hopMM, hopMM, hopMM, hopMX, hopMX, hopMX, 0, 0, 0, 0, 0},
    {hopXM, hopXM, hopXM, hopXX, hopXX, hopXX, 0, 0, 0, 0, 0},
    {hopXM, hopXM, hopXM, hopXX, hopXX, hopXX, 0, 0, 0, 0, 0},
    {hopXM, hopXM, hopXM, hopXX, hopXX, hopXX, 0, 0, 0, 0, 0},
    {0, 0, 0, 0, 0, 0, hopMM, hopMM, hopMX, hopMX, hopMX},
    {0, 0, 0, 0, 0, 0, hopMM, hopMM, hopMX, hopMX, hopMX},
    {0, 0, 0, 0, 0, 0, hopXM, hopXM, hopXX, hopXX, hopXX},
    {0, 0, 0, 0, 0, 0, hopXM, hopXM, hopXX, hopXX, hopXX},
    {0, 0, 0, 0, 0, 0, hopXM, hopXM, hopXX, hopXX, hopXX}};
```

We also ommit hoppings between even and odd orbitals (zeros in Hop matrix) .

Tests

Single hoppings

In[27]:=
```
GetHoppingSingle[D0, D0, x, y, z]
```

Out[27]=

$$\frac{3 z^2 \left(\frac{x^2}{x^2+y^2+z^2}+\frac{y^2}{x^2+y^2+z^2}\right) V_{d^2 \pi}}{x^2+y^2+z^2}+\frac{3}{4}\left(\frac{x^2}{x^2+y^2+z^2}+\frac{y^2}{x^2+y^2+z^2}\right)^2 V_{d^2 \delta}+\left(\frac{z^2}{x^2+y^2+z^2}+\frac{1}{2}\left(-\frac{x^2}{x^2+y^2+z^2}-\frac{y^2}{x^2+y^2+z^2}\right)\right)^2 V_{d^2 \sigma}$$

In[28]:=
```
FullSimplify[GetHopping[Dm1, P0p1,
uprość pełniej
    {{{dr, 0, dp}}, {{dr, 0, -dp}}, {1, 2}}, True] /. {dp^2 + dr^2 → d^2}]
                                             prawda
```

Out[28]=

$$-\frac{dp\, dr^2\, e^{i\, dr\, kx}\left(2 V_{d p \pi}-\sqrt{3}\, V_{d p \sigma}\right)}{\sqrt{2}\left(d^2\right)^{3/2}}$$

In[29]:=
```
FullSimplify[GetHopping[Dm2, D0, {{3/2 dr, √3/2 dr, 0}}, True]]
uprość pełniej                                  prawda
```

Out[29]=

$$\frac{\left(3 i+\sqrt{3}\right) e^{\frac{1}{2} i\, dr \left(3 kx+\sqrt{3}\, ky\right)}\left(V_{d^2 \delta}-V_{d^2 \sigma}\right)}{8 \sqrt{2}}$$

Matrix elements

In[30]:=
```
H1v1 = FullSimplify[GetHopping[D0, D0, hopMM, True]]
       uprość pełniej                      prawda
```

Out[30]=

$$\frac{1}{2}\left(\mathrm{Cos}\left[\sqrt{3}\, dr\, ky\right]+\mathrm{Cos}\left[\frac{1}{2} dr\left(3 kx-\sqrt{3}\, ky\right)\right]+\mathrm{Cos}\left[\frac{1}{2} dr\left(3 kx+\sqrt{3}\, ky\right)\right]\right)\left(3 V_{d^2 \delta}+V_{d^2 \sigma}\right)$$

In[31]:=
```
FullSimplify[
uprość pełniej
  H1v1 == 1/2 (3 V_{d² δ} + V_{d² σ}) (2 Cos[3 / 2 kx dr] * Cos[√3 / 2 ky dr] + Cos[√3 ky dr])]
                                        cosinus            cosinus             cosinus
```

Out[31]=
```
True
```

In[32]:=

```
H1v2 = FullSimplify[GetHopping[Dm2, D0, hopMM, True]]
```

uprość pełniej prawda

Out[32]=

$$\frac{1}{4}\sqrt{\frac{3}{2}}\left(-2\,\mathrm{Cos}\left[\sqrt{3}\ \mathrm{dr}\ \mathrm{ky}\right]+\left(1-\mathrm{i}\sqrt{3}\right)\mathrm{Cos}\left[\frac{1}{2}\,\mathrm{dr}\left(3\,\mathrm{kx}-\sqrt{3}\ \mathrm{ky}\right)\right]+\left(1+\mathrm{i}\sqrt{3}\right)\mathrm{Cos}\left[\frac{1}{2}\,\mathrm{dr}\left(3\,\mathrm{kx}+\sqrt{3}\ \mathrm{ky}\right)\right]\right)\left(V_{d^2\,\delta}-V_{d^2\,\sigma}\right)$$

In[33]:=

$$\mathrm{FullSimplify}\left[\mathrm{H1v2}==\frac{-\sqrt{3}}{2\sqrt{2}}\left(V_{d^2\,\sigma}-V_{d^2\,\delta}\right)\left(\mathrm{Cos}\left[3/2\,\mathrm{kx}\,\mathrm{dr}+\sqrt{3}\Big/2\,\mathrm{ky}\,\mathrm{dr}\right]\mathrm{Exp}[\mathrm{I}\,\mathrm{Pi}/3]+\mathrm{Cos}\left[3/2\,\mathrm{kx}\,\mathrm{dr}-\sqrt{3}\Big/2\,\mathrm{ky}\,\mathrm{dr}\right]\mathrm{Exp}[-\mathrm{I}\,\mathrm{Pi}/3]-\mathrm{Cos}\left[\sqrt{3}\ \mathrm{ky}\,\mathrm{dr}\right]\right)\right]$$

uprość pełniej cosinus fu··· ·· pi
cosinus funkc·· ·· pi cosinus

Out[33]=

True

In[34]:=

```
H5v5 = FullSimplify[GetHopping[PE0, PE0, hopXX, True]]
```

uprość pełniej prawda

Out[34]=

$$2\left(\mathrm{Cos}\left[\sqrt{3}\ \mathrm{dr}\ \mathrm{ky}\right]+\mathrm{Cos}\left[\frac{1}{2}\,\mathrm{dr}\left(3\,\mathrm{kx}-\sqrt{3}\ \mathrm{ky}\right)\right]+\mathrm{Cos}\left[\frac{1}{2}\,\mathrm{dr}\left(3\,\mathrm{kx}+\sqrt{3}\ \mathrm{ky}\right)\right]\right)V_{p^2\,\pi}$$

In[35]:=

$$\mathrm{FullSimplify}\left[\mathrm{H5v5}==V_{p^2\,\pi}\left(4\,\mathrm{Cos}[3/2\,\mathrm{kx}\,\mathrm{dr}]*\mathrm{Cos}\left[\sqrt{3}\Big/2\,\mathrm{ky}\,\mathrm{dr}\right]+2\,\mathrm{Cos}\left[\sqrt{3}\ \mathrm{ky}\,\mathrm{dr}\right]\right)\right]$$

uprość pełniej cosinus cosinus cosinus

Out[35]=

True

In[36]:=

```
H4v6 = FullSimplify[GetHopping[PEm1, PEp1, hopXX, True]]
```

uprość pełniej prawda

Out[36]=

$$\frac{1}{2}\left(-2\,\mathrm{Cos}\left[\sqrt{3}\ \mathrm{dr}\ \mathrm{ky}\right]+\left(1-\mathrm{i}\sqrt{3}\right)\mathrm{Cos}\left[\frac{1}{2}\,\mathrm{dr}\left(3\,\mathrm{kx}-\sqrt{3}\ \mathrm{ky}\right)\right]+\left(1+\mathrm{i}\sqrt{3}\right)\mathrm{Cos}\left[\frac{1}{2}\,\mathrm{dr}\left(3\,\mathrm{kx}+\sqrt{3}\ \mathrm{ky}\right)\right]\right)\left(V_{p^2\,\pi}-V_{p^2\,\sigma}\right)$$

In[37]:=

$$\mathrm{FullSimplify}\left[\mathrm{H4v6}==\left(V_{p^2\,\sigma}-V_{p^2\,\pi}\right)\left(\mathrm{Cos}\left[3/2\,\mathrm{kx}\,\mathrm{dr}+\sqrt{3}\Big/2\,\mathrm{ky}\,\mathrm{dr}\right]\mathrm{Exp}[\mathrm{I}\,\mathrm{Pi}/3]+\mathrm{Cos}\left[3/2\,\mathrm{kx}\,\mathrm{dr}-\sqrt{3}\Big/2\,\mathrm{ky}\,\mathrm{dr}\right]\mathrm{Exp}[-\mathrm{I}\,\mathrm{Pi}/3]-\mathrm{Cos}\left[\sqrt{3}\ \mathrm{ky}\,\mathrm{dr}\right]\right)*(-1)\right]$$

uprość pełniej cosinus fu··· ·· pi
cosinus funkc·· ·· pi cosinus

Out[37]=

True

In[38]:=

$$\mathrm{H3v6}=\mathrm{FullSimplify}\left[\mathrm{GetHopping}[\mathrm{Dp2},\mathrm{PEp1},\mathrm{hopMX},\mathrm{True}]\ /.\ \left\{\mathrm{dp}^2+\mathrm{dr}^2\to\mathrm{d}^2\right\}\right]$$

uprość pełniej prawda

Out[38]=

$$\frac{1}{4\sqrt{2}\left(\mathrm{d}^2\right)^{3/2}}\,e^{-\frac{1}{2}\,\mathrm{i}\,\mathrm{dr}\left(\mathrm{kx}+\sqrt{3}\ \mathrm{ky}\right)}\left(2\,\mathrm{dr}\left(-2\,\mathrm{d}^2+\mathrm{dr}^2\right)\left(1-\mathrm{i}\sqrt{3}+\left(1+\mathrm{i}\sqrt{3}\right)e^{\mathrm{i}\sqrt{3}\ \mathrm{dr}\ \mathrm{ky}}-2\,e^{\frac{1}{2}\,\mathrm{i}\,\mathrm{dr}\left(3\,\mathrm{kx}+\sqrt{3}\ \mathrm{ky}\right)}\right)V_{d\,p\,\pi}-\mathrm{dr}^3\left(-3\,\mathrm{i}+\sqrt{3}+\left(3\,\mathrm{i}+\sqrt{3}\right)e^{\mathrm{i}\sqrt{3}\ \mathrm{dr}\ \mathrm{ky}}-2\sqrt{3}\ e^{\frac{1}{2}\,\mathrm{i}\,\mathrm{dr}\left(3\,\mathrm{kx}+\sqrt{3}\ \mathrm{ky}\right)}\right)V_{d\,p\,\sigma}\right)$$

In[39]:=
$$\texttt{FullSimplify}\left[H3v6 == \frac{dr}{\sqrt{2}\ d}\left(\sqrt{3}\Big/2\,V_{dp\sigma}\left(dp^2/d^2-1\right)-V_{dp\pi}\left(dp^2/d^2+1\right)\right)\left(\texttt{Exp}[I\,kx\,dr]+\texttt{Exp}\left[-I\,kx\,dr\ /2+I\ \sqrt{3}\ ky\,dr/2-2\,I\,Pi\ /3\right]+\texttt{Exp}\left[-I\,kx\,dr\ /2-I\ \sqrt{3}\ ky\,dr/2+2\,I\,Pi\ /3\right]\right)*(-1)\right]$$

uprość pełniej; fu⋯ jedność ur⋯ funkc⋯ jedność urojona jedność urojona · pi; funkc⋯ jedność urojona jedność urojona · pi

Out[39]=
$$\frac{1}{\sqrt{d^2}}\,d\,dr\,e^{-\frac{1}{2}\,i\,dr\,\left(kx+\sqrt{3}\,ky\right)}\left(2\left(-2\,d^3+\sqrt{d^2}\,\left(d^2+dp^2\right)+d\,dr^2\right)\left(-1+i\,\sqrt{3}+\left(-1-i\,\sqrt{3}\right)e^{i\,\sqrt{3}\,dr\,ky}+2\,e^{\frac{1}{2}\,i\,dr\,\left(3\,kx+\sqrt{3}\,ky\right)}\right)V_{dp\pi}-\left(\left(d^2\right)^{3/2}-\sqrt{d^2}\,dp^2-d\,dr^2\right)\left(-3\,i+\sqrt{3}+\left(3\,i+\sqrt{3}\right)e^{i\,\sqrt{3}\,dr\,ky}-2\,\sqrt{3}\,e^{\frac{1}{2}\,i\,dr\,\left(3\,kx+\sqrt{3}\,ky\right)}\right)V_{dp\sigma}\right)==0$$

In[40]:=
```
H7v11 = FullSimplify[GetHopping[Dm1, POp1, hopMX, True] /. {dp^2 + dr^2 → d^2}]
```
uprość pełniej; prawda

Out[40]=
$$\frac{1}{2\,\sqrt{2}\,\left(d^2\right)^{3/2}}\,dp\,dr^2\,e^{-\frac{1}{2}\,i\,dr\,\left(kx+\sqrt{3}\,ky\right)}\left(2\left(1-i\,\sqrt{3}+\left(1+i\,\sqrt{3}\right)e^{i\,\sqrt{3}\,dr\,ky}-2\,e^{\frac{1}{2}\,i\,dr\,\left(3\,kx+\sqrt{3}\,ky\right)}\right)V_{dp\pi}-\left(-3\,i+\sqrt{3}+\left(3\,i+\sqrt{3}\right)e^{i\,\sqrt{3}\,dr\,ky}-2\,\sqrt{3}\,e^{\frac{1}{2}\,i\,dr\,\left(3\,kx+\sqrt{3}\,ky\right)}\right)V_{dp\sigma}\right)$$

In[41]:=
$$\texttt{FullSimplify}\left[H7v11 == -\frac{dp\,dr^2}{\sqrt{2}\ d^3}\left(\sqrt{3}\ V_{dp\sigma}-2\,V_{dp\pi}\right)\left(\texttt{Exp}[I\,kx\,dr]+\texttt{Exp}\left[-I\,kx\,dr\ /2+I\ \sqrt{3}\ ky\,dr/2-2\,I\,Pi/3\right]+\texttt{Exp}\left[-I\,kx\,dr\ /2-I\ \sqrt{3}\ ky\,dr/2+2\,I\,Pi/3\right]\right)*(-1)\right]$$

uprość pełniej; fu⋯ jedność ur⋯ funkc⋯ jedność urojona jedność urojona · pi; funkc⋯ jedność urojona jedność urojona · pi

Out[41]=
$$\frac{1}{d\,\sqrt{d^2}}\left(-d+\sqrt{d^2}\right)dp\,dr\,e^{-\frac{1}{2}\,i\,dr\,\left(kx+\sqrt{3}\,ky\right)}\left(\left(-2+2\,i\,\sqrt{3}+\left(-2-2\,i\,\sqrt{3}\right)e^{i\,\sqrt{3}\,dr\,ky}+4\,e^{\frac{1}{2}\,i\,dr\,\left(3\,kx+\sqrt{3}\,ky\right)}\right)V_{dp\pi}+\left(-3\,i+\sqrt{3}+\left(3\,i+\sqrt{3}\right)e^{i\,\sqrt{3}\,dr\,ky}-2\,\sqrt{3}\,e^{\frac{1}{2}\,i\,dr\,\left(3\,kx+\sqrt{3}\,ky\right)}\right)V_{dp\sigma}\right)==0$$

In[42]:=
```
H7v10 = FullSimplify[GetHopping[Dm1, P00, hopMX, True] /. {dp^2 + dr^2 → d^2}]
```
uprość pełniej prawda

Out[42]=
$$\frac{1}{2\left(d^2\right)^{3/2}} dr\, e^{-\frac{1}{2} i\, dr\, \left(kx+\sqrt{3}\, ky\right)} \left(\left(d^2-2\, dp^2\right)\left(1+i\sqrt{3}+\left(1-i\sqrt{3}\right) e^{i\sqrt{3}\, dr\, ky}-2\, e^{\frac{1}{2} i\, dr\, \left(3\, kx+\sqrt{3}\, ky\right)}\right) V_{d p \pi}+ dp^2\left(3\, i+\sqrt{3}+\left(-3\, i+\sqrt{3}\right) e^{i\sqrt{3}\, dr\, ky}-2\sqrt{3}\, e^{\frac{1}{2} i\, dr\, \left(3\, kx+\sqrt{3}\, ky\right)}\right) V_{d p \sigma}\right)$$

In[43]:=
```
FullSimplify[H7v10 == -dr/d (dp^2/d^2 (√3 Vdpσ - 2 Vdpπ) + Vdpπ)
   (Exp[I kx dr] + Exp[-I kx dr / 2 + I √3 ky dr / 2 + 2 I Pi / 3] +
     Exp[-I kx dr / 2 - I √3 ky dr / 2 - 2 I Pi / 3])]
```
uprość pełniej

fu⋯ jedność ur⋯ funkc⋯ jedność urojona jedność urojona ⋅ pi

funkc⋯ jedność urojona jedność urojona ⋅ pi

Out[43]=
$$\frac{1}{\sqrt{d^2}} d\left(-d+\sqrt{d^2}\right) dr\, e^{-\frac{1}{2} i\, dr\, \left(kx+\sqrt{3}\, ky\right)} \left(\left(d^2-2\, dp^2\right)\left(-1-i\sqrt{3}+i\left(i+\sqrt{3}\right) e^{i\sqrt{3}\, dr\, ky}+2\, e^{\frac{1}{2} i\, dr\, \left(3\, kx+\sqrt{3}\, ky\right)}\right) V_{d p \pi}- dp^2\left(3\, i+\sqrt{3}+\left(-3\, i+\sqrt{3}\right) e^{i\sqrt{3}\, dr\, ky}-2\sqrt{3}\, e^{\frac{1}{2} i\, dr\, \left(3\, kx+\sqrt{3}\, ky\right)}\right) V_{d p \sigma}\right) == 0$$

In[44]:=
```
H8v9 = FullSimplify[GetHopping[Dp1, POm1, hopMX, True] /. {dp^2 + dr^2 → d^2}]
```
uprość pełniej prawda

Out[44]=
$$\frac{1}{2\sqrt{2}\left(d^2\right)^{3/2}} dp\, dr^2\, e^{-\frac{1}{2} i\, dr\, \left(kx+\sqrt{3}\, ky\right)} \left(2\left(1+i\sqrt{3}+\left(1-i\sqrt{3}\right) e^{i\sqrt{3}\, dr\, ky}-2\, e^{\frac{1}{2} i\, dr\, \left(3\, kx+\sqrt{3}\, ky\right)}\right) V_{d p \pi}- \left(3\, i+\sqrt{3}+\left(-3\, i+\sqrt{3}\right) e^{i\sqrt{3}\, dr\, ky}-2\sqrt{3}\, e^{\frac{1}{2} i\, dr\, \left(3\, kx+\sqrt{3}\, ky\right)}\right) V_{d p \sigma}\right)$$

In[45]:=
```
FullSimplify[H8v9 ==
   dp dr^2/(√2 d^3) (√3 Vdpσ - 2 Vdpπ) (Exp[I kx dr] + Exp[-I kx dr / 2 + I √3 ky dr / 2 + 2 I Pi / 3] +
     Exp[-I kx dr / 2 - I √3 ky dr / 2 - 2 I Pi / 3])]
```
uprość pełniej

fu⋯ jedność ur⋯ funkc⋯ jedność urojona jedność urojona ⋅ pi

funkc⋯ jedność urojona jedność urojona ⋅ pi

Out[45]=
$$\frac{1}{d\sqrt{d^2}}\left(-d+\sqrt{d^2}\right) dp\, dr\, e^{-\frac{1}{2} i\, dr\, \left(kx+\sqrt{3}\, ky\right)} \left(\left(-2-2\, i\sqrt{3}+2\, i\left(i+\sqrt{3}\right) e^{i\sqrt{3}\, dr\, ky}+4\, e^{\frac{1}{2} i\, dr\, \left(3\, kx+\sqrt{3}\, ky\right)}\right) V_{d p \pi}+ \left(3\, i+\sqrt{3}+\left(-3\, i+\sqrt{3}\right) e^{i\sqrt{3}\, dr\, ky}-2\sqrt{3}\, e^{\frac{1}{2} i\, dr\, \left(3\, kx+\sqrt{3}\, ky\right)}\right) V_{d p \sigma}\right) == 0$$

In[46]:=

```
H8v10 = FullSimplify[GetHopping[Dp1, P00, hopMX, True] /. {dp^2 + dr^2 → d^2}]
        uprość pełniej                                    prawda
```

Out[46]=

$$\frac{1}{2\left(d^2\right)^{3/2}} dr\, e^{-\frac{1}{2} i\, dr \left(kx+\sqrt{3}\, ky\right)} \left(\left(d^2-2\, dp^2\right)\left(-1+i\sqrt{3}+\left(-1-i\sqrt{3}\right) e^{i\sqrt{3}\, dr\, ky}+2\, e^{\frac{1}{2} i\, dr\left(3\, kx+\sqrt{3}\, ky\right)}\right) V_{d p \pi} - dp^2\left(-3\, i+\sqrt{3}+\left(3\, i+\sqrt{3}\right) e^{i\sqrt{3}\, dr\, ky}-2\sqrt{3}\, e^{\frac{1}{2} i\, dr\left(3\, kx+\sqrt{3}\, ky\right)}\right) V_{d p \sigma}\right)$$

In[47]:=

```
FullSimplify[H8v10 == dr/d (dp^2/d^2 (√3 V_dpσ - 2 V_dpπ) + V_dpπ)
uprość pełniej
  (Exp[I kx dr] + Exp[-I kx dr / 2 + I √3 ky dr / 2 - 2 I Pi / 3] +
  fu···  jednosć ur··  funkc··  jednosć urojona  jednosć urojona   ·  pi
    Exp[-I kx dr / 2 - I √3 ky dr / 2 + 2 I Pi / 3])]
    funkc··  jednosć urojona  jednosć urojona   ·  pi
```

Out[47]=

$$\frac{1}{\sqrt{d^2}} d\left(-d+\sqrt{d^2}\right) dr\, e^{-\frac{1}{2} i\, dr\left(kx+\sqrt{3}\, ky\right)} \left(\left(d^2-2\, dp^2\right)\left(-1+i\sqrt{3}+\left(-1-i\sqrt{3}\right) e^{i\sqrt{3}\, dr\, ky}+2\, e^{\frac{1}{2} i\, dr\left(3\, kx+\sqrt{3}\, ky\right)}\right) V_{d p \pi} - dp^2\left(-3\, i+\sqrt{3}+\left(3\, i+\sqrt{3}\right) e^{i\sqrt{3}\, dr\, ky}-2\sqrt{3}\, e^{\frac{1}{2} i\, dr\left(3\, kx+\sqrt{3}\, ky\right)}\right) V_{d p \sigma}\right) == 0$$

In[48]:=

```
H9v11 = FullSimplify[GetHopping[P0m1, P0p1, hopXX, True] /. {dp^2 + dr^2 → d^2}]
        uprość pełniej                                        prawda
```

Out[48]=

$$\frac{1}{2}\left(-2\, \mathrm{Cos}\left[\sqrt{3}\, dr\, ky\right]+\left(1-i\sqrt{3}\right)\mathrm{Cos}\left[\frac{1}{2} dr\left(3\, kx-\sqrt{3}\, ky\right)\right]+\left(1+i\sqrt{3}\right)\mathrm{Cos}\left[\frac{1}{2} dr\left(3\, kx+\sqrt{3}\, ky\right)\right]\right)\left(V_{p^2 \pi}-V_{p^2 \sigma}\right)$$

In[49]:=

```
FullSimplify[H9v11 == (V_p²σ - V_p²π) (Cos[3/2 kx dr + √3 / 2 ky dr] Exp[I Pi / 3] +
uprość pełniej                          cosinus                          fu···  ·  pi
    Cos[3/2 kx dr - √3 / 2 ky dr] Exp[-I Pi / 3] - Cos[√3 ky dr]) * (-1)]
    cosinus                          funkc··  ·  pi    cosinus
```

Out[49]=

```
True
```

In[50]:=

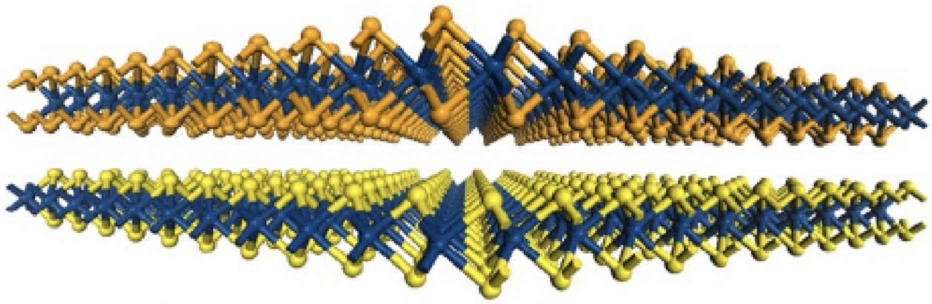
```
H9v10 = FullSimplify[GetHopping[P0m1, P00, hopXX, True] /. {dp^2 + dr^2 → d^2}]
        uprość pełniej                                      prawda
```

Out[50]=

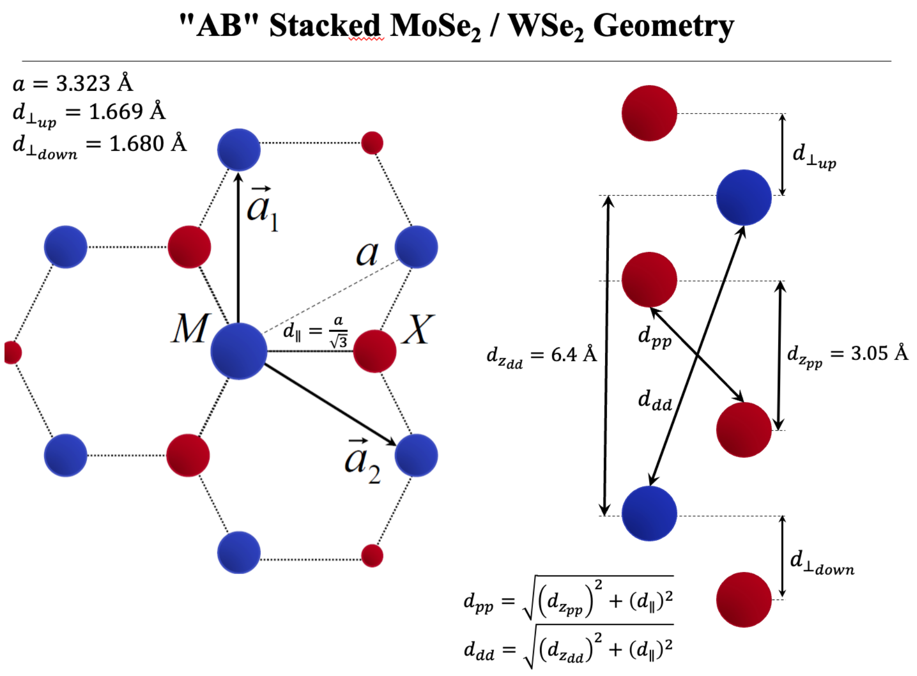
```
0
```

TMDC heterostructure

In this section we introduce TB model for stacked TMDC heterostructure.


;

Interalyer hoppings



;

Let' s define interalyer hoppings (intralayer are the same as in the previous chapter), <top layer | bottom layer>:

In[53]:=

$$\texttt{ihopMM = List}\left[\{-dr, 0, -dzdd\}, \left\{\frac{1}{2}\,dr, -\frac{\sqrt{3}}{2}\,dr, -dzdd\right\}, \left\{\frac{1}{2}\,dr, \frac{\sqrt{3}}{2}\,dr, -dzdd\right\}\right];$$

```
ihopMX = {{{0, 0, -dzdp}}, 0, {1, 2}};
(* M from top layer only coupled with (nearer) up X-atom from bottom layer *)
ihopXM = {0, {{0, 0, -dzdp}}, {2, 1}}; (* only (nearer) down X-
 atom from top layer is coupled with M atom from bottom layer *)
```

$$\texttt{ihopxx = List}\left[\{dr, 0, -dzpp\}, \left\{-\frac{1}{2}\,dr, \frac{\sqrt{3}}{2}\,dr, -dzpp\right\}, \left\{-\frac{1}{2}\,dr, -\frac{\sqrt{3}}{2}\,dr, -dzpp\right\}\right];$$

```
ihopXX = {0, 0, ihopxx, 0, {2, 2}};(* only down X-
 atom from top dimer is coupled with up X-atom from bottom dimer *)
```

```
In[58]:= IHop = {
    {ihopMM, ihopMM, ihopMM, ihopMX, ihopMX, ihopMX},
    {ihopMM, ihopMM, ihopMM, ihopMX, ihopMX, ihopMX},
    {ihopMM, ihopMM, ihopMM, ihopMX, ihopMX, ihopMX},
    {ihopXM, ihopXM, ihopXM, ihopXX, ihopXX, ihopXX},
    {ihopXM, ihopXM, ihopXM, ihopXX, ihopXX, ihopXX},
    {ihopXM, ihopXM, ihopXM, ihopXX, ihopXX, ihopXX}};

In[59]:= Iorbitals = {Dm2, D0, Dp2, PEm1, PE0, PEp1};

In[60]:= HSKinter = HSKHoppings[Iorbitals, IHop, True];
```

prawda

[1,1]

$$\frac{1}{8\left(dr^2+dzdd^2\right)^2} e^{-\frac{1}{2} i\, dr\left(2 kx+\sqrt{3} ky\right)}\left(e^{\frac{3 i\, dr\, kx}{2}}+e^{\frac{1}{2} i \sqrt{3}\, dr\, ky}+e^{\frac{1}{2} i\, dr\left(3 kx+2 \sqrt{3} ky\right)}\right) \left(4\left(dr^4+2 dr^2 dzdd^2\right) V_{d^2\pi}+\left(dr^4+8 dr^2 dzdd^2+8 dzdd^4\right) V_{d^2\delta}+3 dr^4 V_{d^2\sigma}\right)$$

[1,2]

$$\frac{1}{8\left(dr^2+dzdd^2\right)^2} \sqrt{\frac{3}{2}}\, dr^2 e^{-\frac{1}{2} i\, dr\left(2 kx+\sqrt{3} ky\right)}\left(\left(-1-i\sqrt{3}\right) e^{\frac{3 i\, dr\, kx}{2}}+2 e^{\frac{1}{2} i \sqrt{3}\, dr\, ky}+i\left(i+\sqrt{3}\right) e^{\frac{1}{2} i\, dr\left(3 kx+2 \sqrt{3} ky\right)}\right) \left(-4 dzdd^2 V_{d^2\pi}+\left(dr^2+2 dzdd^2\right) V_{d^2\delta}-\left(dr^2-2 dzdd^2\right) V_{d^2\sigma}\right)$$

[1,3]

$$\frac{1}{16\left(dr^2+dzdd^2\right)^2} dr^4 e^{-\frac{1}{2} i\, dr\left(2 kx+\sqrt{3} ky\right)} \left(\left(1-i\sqrt{3}\right) e^{\frac{3 i\, dr\, kx}{2}}-2 e^{\frac{1}{2} i \sqrt{3}\, dr\, ky}+\left(1+i\sqrt{3}\right) e^{\frac{1}{2} i\, dr\left(3 kx+2 \sqrt{3} ky\right)}\right)\left(4 V_{d^2\pi}-V_{d^2\delta}-3 V_{d^2\sigma}\right)$$

[1,4]
0

[1,5]
0

[1,6]
0

[2,1]

$$\frac{1}{8\left(dr^2+dzdd^2\right)^2} \sqrt{\frac{3}{2}}\, dr^2 e^{-\frac{1}{2} i\, dr\left(2 kx+\sqrt{3} ky\right)}\left(i\left(i+\sqrt{3}\right) e^{\frac{3 i\, dr\, kx}{2}}+2 e^{\frac{1}{2} i \sqrt{3}\, dr\, ky}+\left(-1-i\sqrt{3}\right) e^{\frac{1}{2} i\, dr\left(3 kx+2 \sqrt{3} ky\right)}\right) \left(-4 dzdd^2 V_{d^2\pi}+\left(dr^2+2 dzdd^2\right) V_{d^2\delta}-\left(dr^2-2 dzdd^2\right) V_{d^2\sigma}\right)$$

[2,2]

$$\frac{1}{4\left(dr^2+dzdd^2\right)^2} e^{-\frac{1}{2} i\, dr\left(2 kx+\sqrt{3} ky\right)}\left(e^{\frac{3 i\, dr\, kx}{2}}+e^{\frac{1}{2} i \sqrt{3}\, dr\, ky}+e^{\frac{1}{2} i\, dr\left(3 kx+2 \sqrt{3} ky\right)}\right) \left(12 dr^2 dzdd^2 V_{d^2\pi}+3 dr^4 V_{d^2\delta}+\left(dr^2-2 dzdd^2\right)^2 V_{d^2\sigma}\right)$$

[2,3]

$$\frac{1}{8\left(dr^2+dzdd^2\right)^2}\sqrt{\frac{3}{2}}\,dr^2\,e^{-\frac{1}{2}i\,dr\,\left(2\,kx+\sqrt{3}\,ky\right)}\left(\left(-1-i\sqrt{3}\right)e^{\frac{3\,i\,dr\,kx}{2}}+2\,e^{\frac{1}{2}i\sqrt{3}\,dr\,ky}+i\left(i+\sqrt{3}\right)e^{\frac{1}{2}i\,dr\,\left(3\,kx+2\sqrt{3}\,ky\right)}\right)\left(-4\,dzdd^2\,V_{d^2\pi}+\left(dr^2+2\,dzdd^2\right)V_{d^2\delta}-\left(dr^2-2\,dzdd^2\right)V_{d^2\sigma}\right)$$

[2,4]

0

[2,5]

$$\frac{dzdp\,V_{dp\sigma}}{\sqrt{2}\,\sqrt{dzdp^2}}$$

[2,6]

0

[3,1]

$$\frac{1}{16\left(dr^2+dzdd^2\right)^2}dr^4\,e^{-\frac{1}{2}i\,dr\,\left(2\,kx+\sqrt{3}\,ky\right)}\left(\left(1+i\sqrt{3}\right)e^{\frac{3\,i\,dr\,kx}{2}}-2\,e^{\frac{1}{2}i\sqrt{3}\,dr\,ky}+\left(1-i\sqrt{3}\right)e^{\frac{1}{2}i\,dr\,\left(3\,kx+2\sqrt{3}\,ky\right)}\right)\left(4\,V_{d^2\pi}-V_{d^2\delta}-3\,V_{d^2\sigma}\right)$$

[3,2]

$$\frac{1}{8\left(dr^2+dzdd^2\right)^2}\sqrt{\frac{3}{2}}\,dr^2\,e^{-\frac{1}{2}i\,dr\,\left(2\,kx+\sqrt{3}\,ky\right)}\left(i\left(i+\sqrt{3}\right)e^{\frac{3\,i\,dr\,kx}{2}}+2\,e^{\frac{1}{2}i\sqrt{3}\,dr\,ky}+\left(-1-i\sqrt{3}\right)e^{\frac{1}{2}i\,dr\,\left(3\,kx+2\sqrt{3}\,ky\right)}\right)\left(-4\,dzdd^2\,V_{d^2\pi}+\left(dr^2+2\,dzdd^2\right)V_{d^2\delta}-\left(dr^2-2\,dzdd^2\right)V_{d^2\sigma}\right)$$

[3,3]

$$\frac{1}{8\left(dr^2+dzdd^2\right)^2}e^{-\frac{1}{2}i\,dr\,\left(2\,kx+\sqrt{3}\,ky\right)}\left(e^{\frac{3\,i\,dr\,kx}{2}}+e^{\frac{1}{2}i\sqrt{3}\,dr\,ky}+e^{\frac{1}{2}i\,dr\,\left(3\,kx+2\sqrt{3}\,ky\right)}\right)\left(4\left(dr^4+2\,dr^2\,dzdd^2\right)V_{d^2\pi}+\left(dr^4+8\,dr^2\,dzdd^2+8\,dzdd^4\right)V_{d^2\delta}+3\,dr^4\,V_{d^2\sigma}\right)$$

[3,4]

0

[3,5]

0

[3,6]

0

[4,1]

0

[4,2]

0

[4,3]

0

[4,4]

$$\frac{e^{-\frac{1}{2} i\, dr\, (kx+\sqrt{3}\, ky)} \left(1+e^{i \sqrt{3}\, dr\, ky}+e^{\frac{1}{2} i\, dr\, (3\, kx+\sqrt{3}\, ky)}\right) \left(\left(dr^2+2\, dzpp^2\right) V_{p^2\, \pi}+dr^2\, V_{p^2\, \sigma}\right)}{4 \left(dr^2+dzpp^2\right)}$$

[4,5]

$$\frac{dr\, dzpp\, e^{-\frac{1}{2} i\, dr\, (kx+\sqrt{3}\, ky)} \left(-1-i \sqrt{3}+i \left(i+\sqrt{3}\right) e^{i \sqrt{3}\, dr\, ky}+2\, e^{\frac{1}{2} i\, dr\, (3\, kx+\sqrt{3}\, ky)}\right) \left(V_{p^2\, \pi}-V_{p^2\, \sigma}\right)}{4 \sqrt{2} \left(dr^2+dzpp^2\right)}$$

[4,6]

$$\frac{dr^2\, e^{-\frac{1}{2} i\, dr\, (kx+\sqrt{3}\, ky)} \left(-1+i \sqrt{3}+\left(-1-i \sqrt{3}\right) e^{i \sqrt{3}\, dr\, ky}+2\, e^{\frac{1}{2} i\, dr\, (3\, kx+\sqrt{3}\, ky)}\right) \left(V_{p^2\, \pi}-V_{p^2\, \sigma}\right)}{8 \left(dr^2+dzpp^2\right)}$$

[5,1]

0

[5,2]

$$\frac{dzdp\, V_{d\, p\, \sigma}}{\sqrt{2} \sqrt{dzdp^2}}$$

[5,3]

0

[5,4]

$$\frac{dr\, dzpp\, e^{-\frac{1}{2} i\, dr\, (kx+\sqrt{3}\, ky)} \left(1-i \sqrt{3}+\left(1+i \sqrt{3}\right) e^{i \sqrt{3}\, dr\, ky}-2\, e^{\frac{1}{2} i\, dr\, (3\, kx+\sqrt{3}\, ky)}\right) \left(V_{p^2\, \pi}-V_{p^2\, \sigma}\right)}{4 \sqrt{2} \left(dr^2+dzpp^2\right)}$$

[5,5]

$$-\frac{e^{-\frac{1}{2} i\, dr\, (kx+\sqrt{3}\, ky)} \left(1+e^{i \sqrt{3}\, dr\, ky}+e^{\frac{1}{2} i\, dr\, (3\, kx+\sqrt{3}\, ky)}\right) \left(dr^2\, V_{p^2\, \pi}+dzpp^2\, V_{p^2\, \sigma}\right)}{2 \left(dr^2+dzpp^2\right)}$$

[5,6]

$$\frac{dr\, dzpp\, e^{-\frac{1}{2} i\, dr\, (kx+\sqrt{3}\, ky)} \left(-1-i \sqrt{3}+i \left(i+\sqrt{3}\right) e^{i \sqrt{3}\, dr\, ky}+2\, e^{\frac{1}{2} i\, dr\, (3\, kx+\sqrt{3}\, ky)}\right) \left(V_{p^2\, \pi}-V_{p^2\, \sigma}\right)}{4 \sqrt{2} \left(dr^2+dzpp^2\right)}$$

[6,1]

0

[6,2]

0

[6,3]

0

[6,4]

$$\frac{dr^2\, e^{-\frac{1}{2} i\, dr\, (kx+\sqrt{3}\, ky)} \left(-1-i \sqrt{3}+i \left(i+\sqrt{3}\right) e^{i \sqrt{3}\, dr\, ky}+2\, e^{\frac{1}{2} i\, dr\, (3\, kx+\sqrt{3}\, ky)}\right) \left(V_{p^2\, \pi}-V_{p^2\, \sigma}\right)}{8 \left(dr^2+dzpp^2\right)}$$

[6,5]

$$\frac{dr\ dzpp\ e^{-\frac{1}{2} i\, dr\, (kx+\sqrt{3}\, ky)} \left(1 - i\sqrt{3} + \left(1 + i\sqrt{3}\right) e^{i\sqrt{3}\, dr\, ky} - 2\, e^{\frac{1}{2} i\, dr\, (3\, kx+\sqrt{3}\, ky)}\right) \left(V_{p^2\pi} - V_{p^2\sigma}\right)}{4\sqrt{2}\left(dr^2 + dzpp^2\right)}$$

[6,6]

$$\frac{e^{-\frac{1}{2} i\, dr\, (kx+\sqrt{3}\, ky)} \left(1 + e^{i\sqrt{3}\, dr\, ky} + e^{\frac{1}{2} i\, dr\, (3\, kx+\sqrt{3}\, ky)}\right) \left(\left(dr^2 + 2\, dzpp^2\right) V_{p^2\pi} + dr^2\, V_{p^2\sigma}\right)}{4\left(dr^2 + dzpp^2\right)}$$

In[61]:= HSKinter⟦2, 2⟧ (*D0-D0*)

Out[61]=

$$\frac{1}{4\left(dr^2 + dzdd^2\right)^2} e^{-\frac{1}{2} i\, dr\, (2\, kx+\sqrt{3}\, ky)} \left(e^{\frac{3\, i\, dr\, kx}{2}} + e^{\frac{1}{2} i\sqrt{3}\, dr\, ky} + e^{\frac{1}{2} i\, dr\, (3\, kx+2\sqrt{3}\, ky)}\right)$$
$$\left(12\, dr^2\, dzdd^2\, V_{d^2\pi} + 3\, dr^4\, V_{d^2\delta} + \left(dr^2 - 2\, dzdd^2\right)^2 V_{d^2\sigma}\right)$$

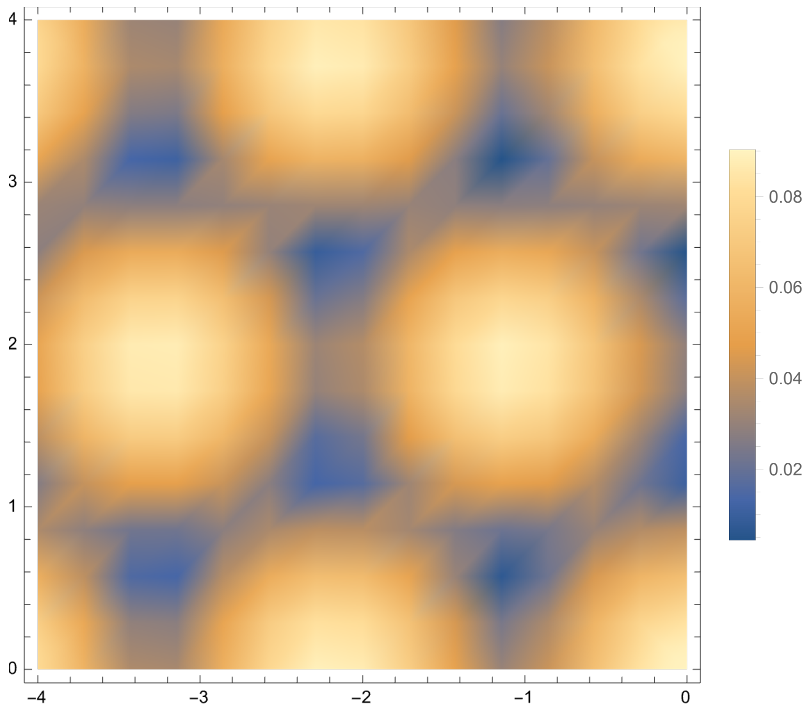
In[62]:= DensityPlot[
wykres gęstości

Abs[HSKinter⟦2, 2⟧ /. {dr → 3.323 / $\sqrt{3}$, dzpp → 3.05, dzdd → 6.4, $V_{d^2\pi}$ → 1.8318,
wartość bezwzględna

$V_{d^2\delta}$ → -0.3299, $V_{d^2\sigma}$ → -0.5, $V_{p^2\pi}$ → -0.1547, $V_{p^2\sigma}$ → -1.1006}],

{kx, -4, 0}, {ky, 0, 4}, PlotLegends → Automatic]
legenda dla grafik automatyczny

Out[62]=



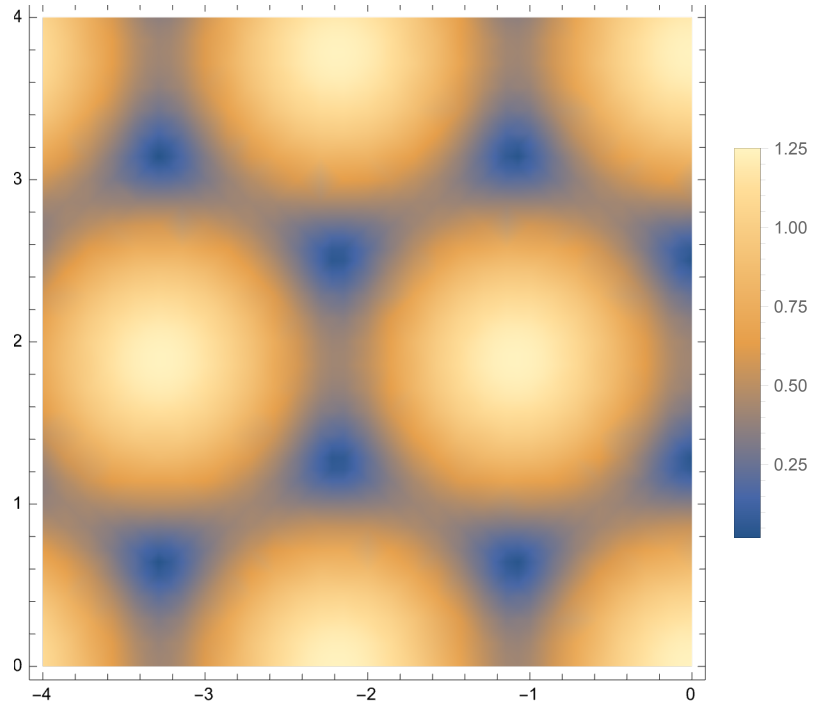
In[63]:= HSKinter⟦5, 5⟧ (*P0-P0*)

Out[63]=

$$-\frac{e^{-\frac{1}{2} i\, dr\, (kx+\sqrt{3}\, ky)} \left(1 + e^{i\sqrt{3}\, dr\, ky} + e^{\frac{1}{2} i\, dr\, (3\, kx+\sqrt{3}\, ky)}\right) \left(dr^2\, V_{p^2\pi} + dzpp^2\, V_{p^2\sigma}\right)}{2\left(dr^2 + dzpp^2\right)}$$

In[64]:=
```
DensityPlot[
  Abs[HSKinter⟦5, 5⟧ /. {dr → 3.323 / √3, dzpp → 3.05, dzdd → 6.4, Vd²π → 1.8318,
      Vd²δ → -0.3299, Vd²σ → -0.5, Vp²π → -0.1547, Vp²σ → -1.1006}],
  {kx, -4, 0}, {ky, 0, 4}, PlotLegends → Automatic]
```
wykres gęstości; wartość bezwzględna; legenda dla grafik; automatyczny

Out[64]=



In[66]:=
```
Abs[HSKinter⟦2, 5⟧ /. {dr → 3.323 / √3, dzpp → 3.05, dzdd → 6.4, dzdp → 4.5,
    Vd²π → 1.8318, Vd²δ → -0.3299, Vd²σ → -0.5, Vp²π → -0.1547, Vp²σ → -1.1006}]
```
wartość bezwzględna

Out[66]=

$0.707107\,\mathrm{Abs}[V_{dp\sigma}]$

In[67]:=
```
DensityPlot[
  Abs[HSKinter[[1, 1]] /. {dr → 3.323/√3, dzpp → 3.05, dzdd → 6.4, Vd²π → 1.8318,
     Vd²δ → -0.3299, Vd²σ → -0.5, Vp²π → -0.1547, Vp²σ → -1.1006}],
  {kx, -4, 0}, {ky, 0, 4}, PlotLegends → Automatic]
```
wykres gęstości; wartość bezwzględna; legenda dla grafik; automatyczny

Out[67]=