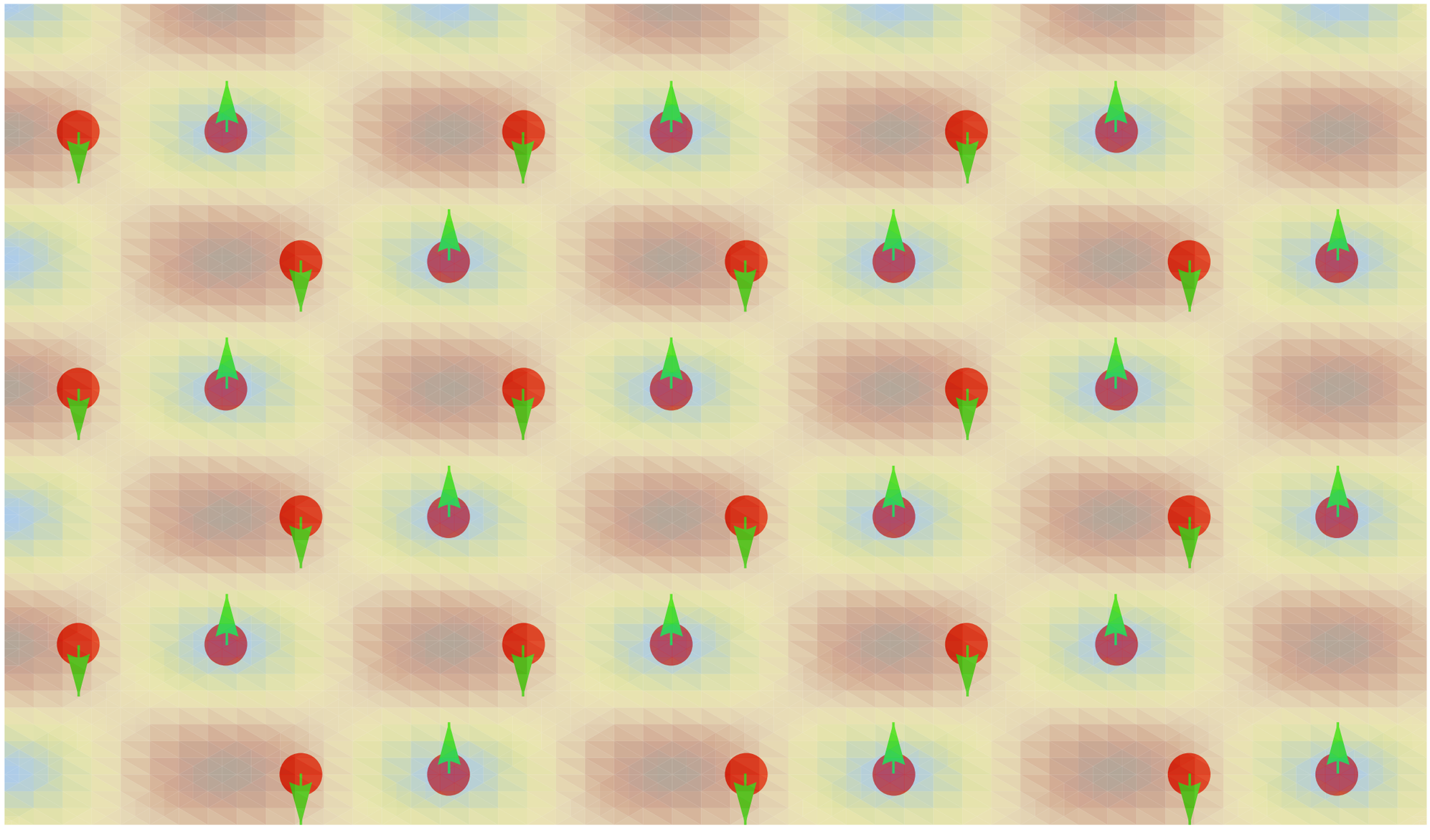
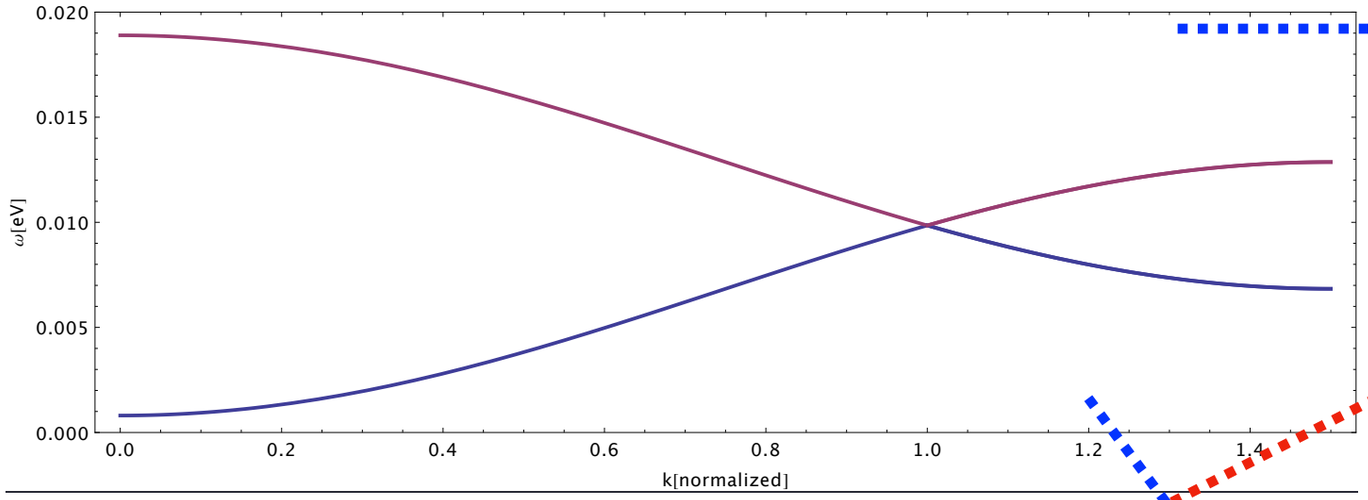
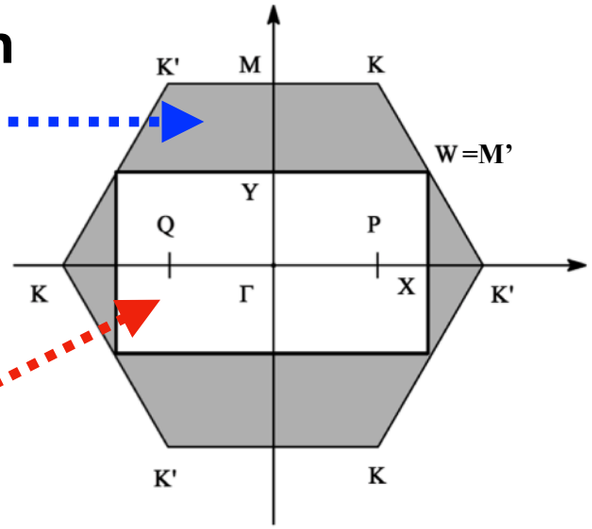
# $CrI_3$

## Dispersion relation



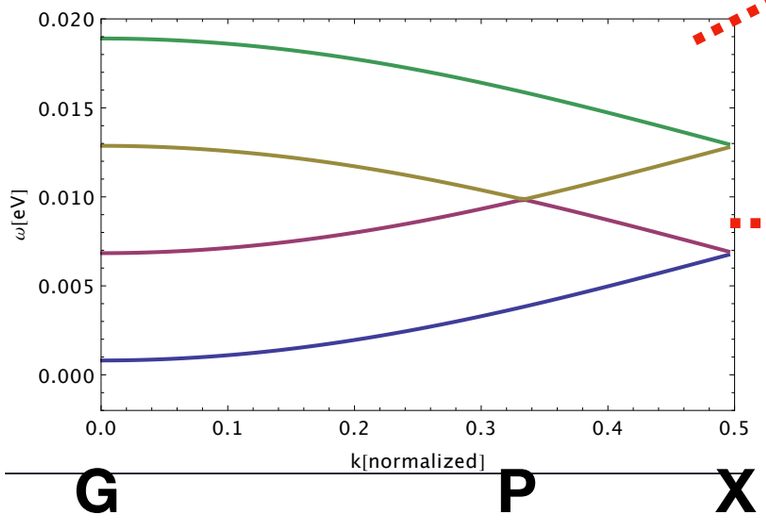
# Analytic expression from Kartsev's paper - HP transformation



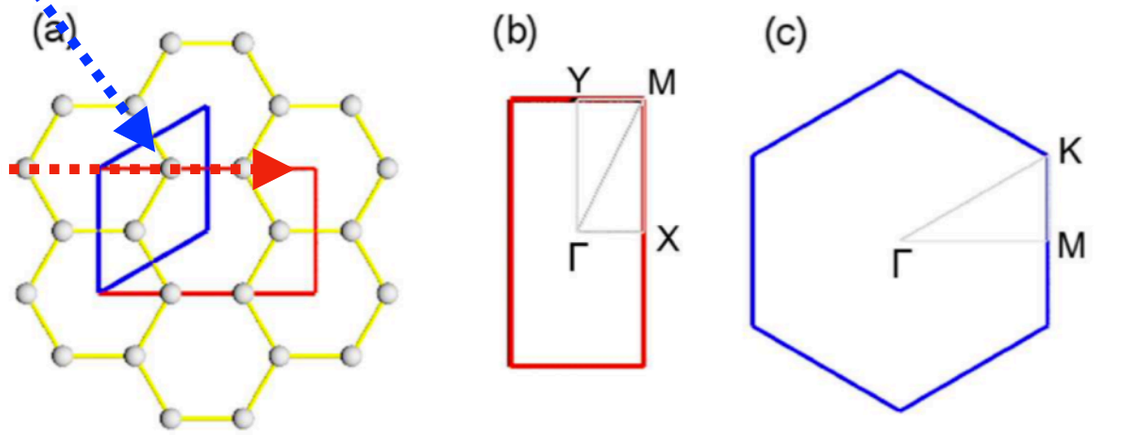




**G** **K** **2X (M)**

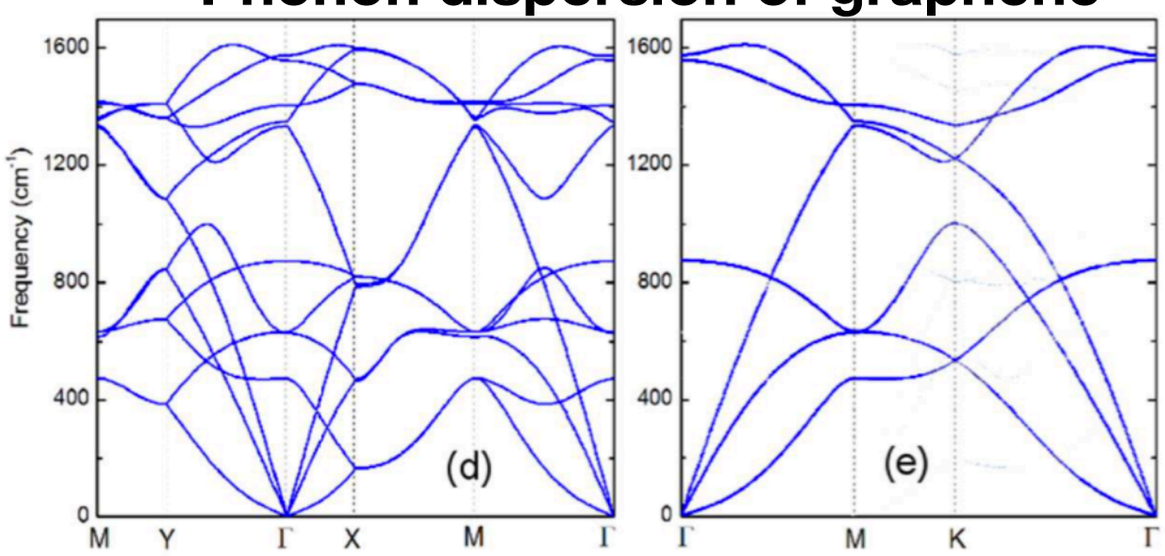
# Dynamical Matrix Method - Bloch waves

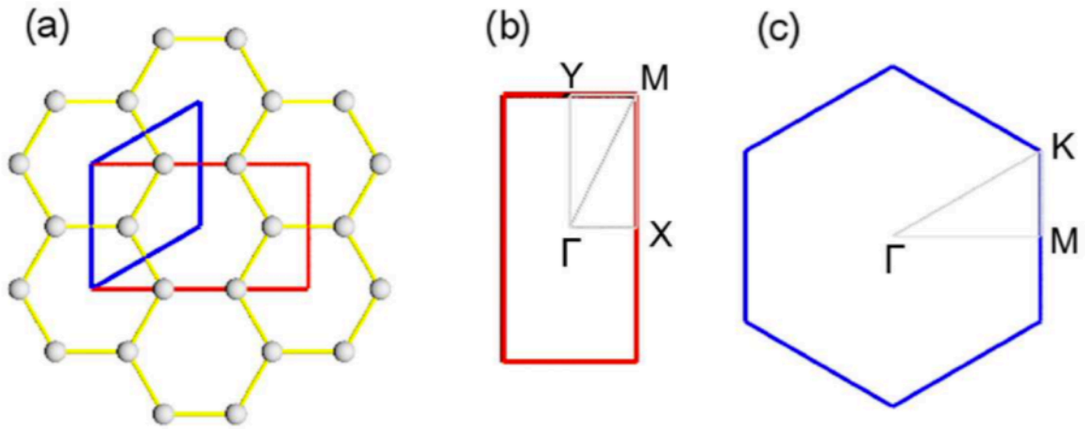


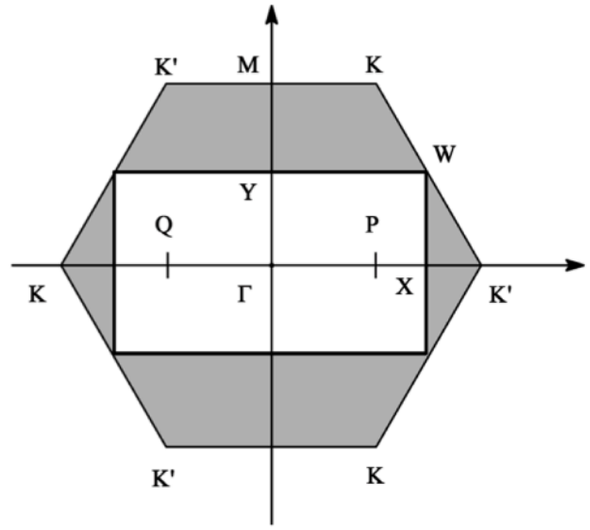

**G** **P** **X**

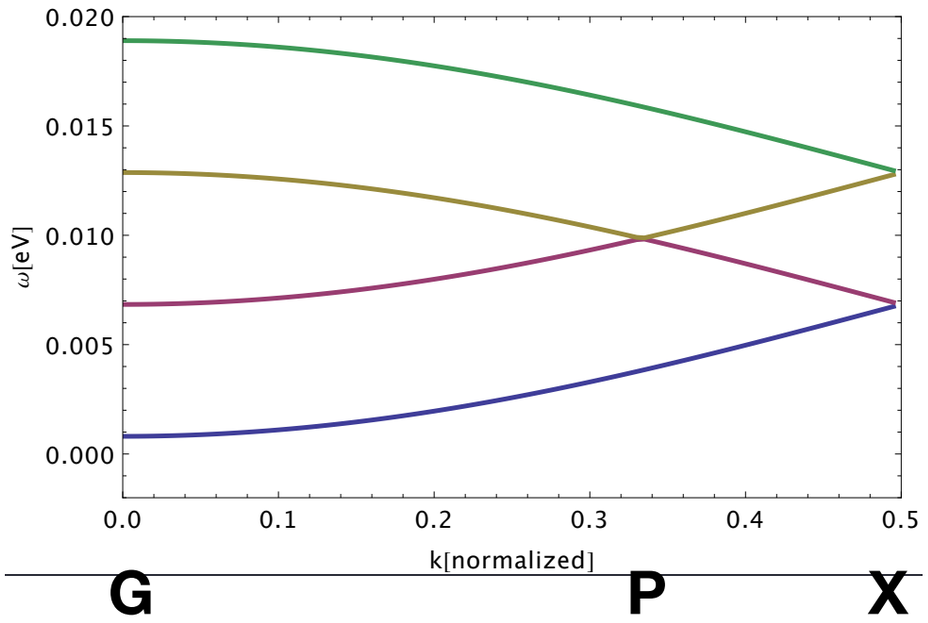



# Phonon dispersion of graphene






$$X=(\frac{1}{2},0,0)$$

$$Y=(\frac{1}{2},0,0)$$

$$W=(\frac{1}{2},\frac{1}{2},0)$$

$$P=(\frac{1}{3},0,0)$$

$$\Gamma=(0,0,0)$$

$$K=(\frac{2}{3},\frac{1}{3},0)$$

$$M=(\frac{1}{2},0,0)$$

## Rectangular lattice

Real space

$a_0 = 0.7079$ nm

$\vec{a}_{1r} = a_0(1,0,0)$

$\vec{a}_{2r} = a_0(0,\sqrt{3},0)$

$\vec{a}_{3r} = a_0(0,0,1)$

Reciprocal space

$$\vec{b}_{1r} = \frac{2\pi}{a_0}(1,0,0)$$

$$\vec{b}_{2r} = \frac{2\pi}{a_0}(1,\frac{1}{\sqrt{3}},0)$$

$$\vec{b}_{3r} = \frac{2\pi}{a_0}(0,0,1)$$

## Hexagonal lattice

Real space

$a_0 = 0.7079$ nm

$\vec{a}_{1h} = a_0(1,0,0)$

$\vec{a}_{2h} = a_0(\frac{1}{2},\frac{\sqrt{3}}{2},0)$

$\vec{a}_{3h} = a_0(0,0,1)$

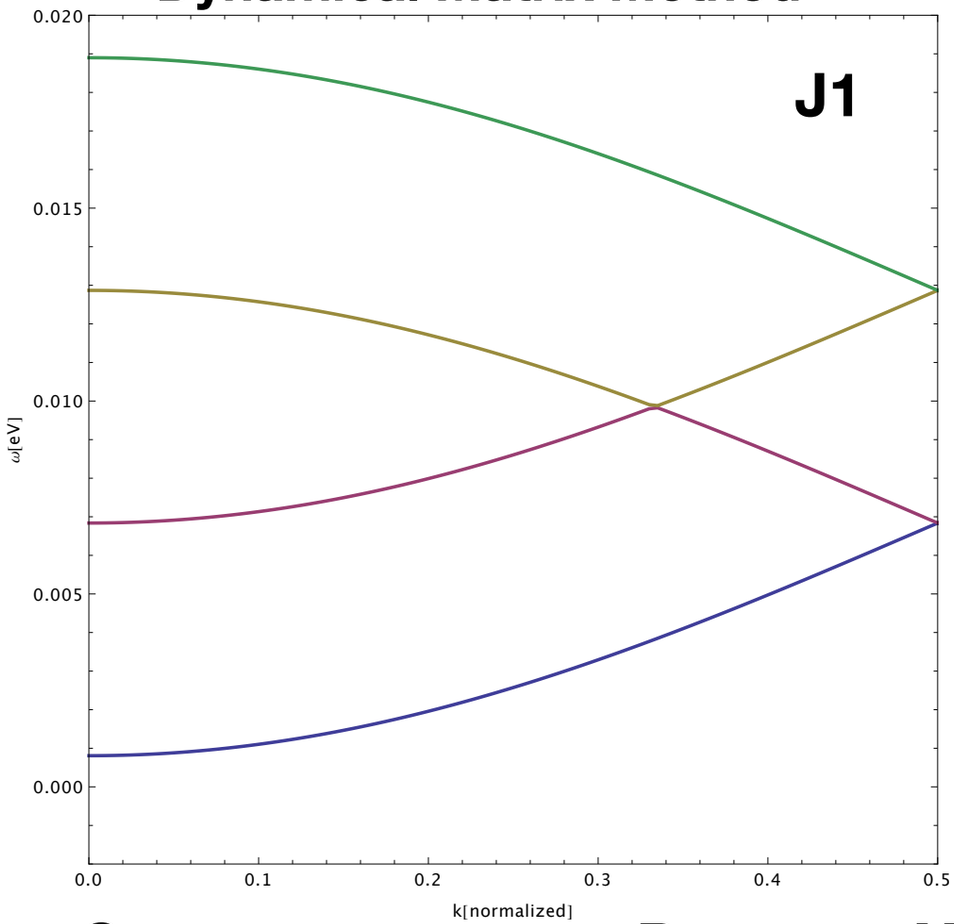
Reciprocal space

$$\vec{b}_{1h} = \frac{2\pi}{a_0}(1,-\frac{1}{\sqrt{3}},0)$$

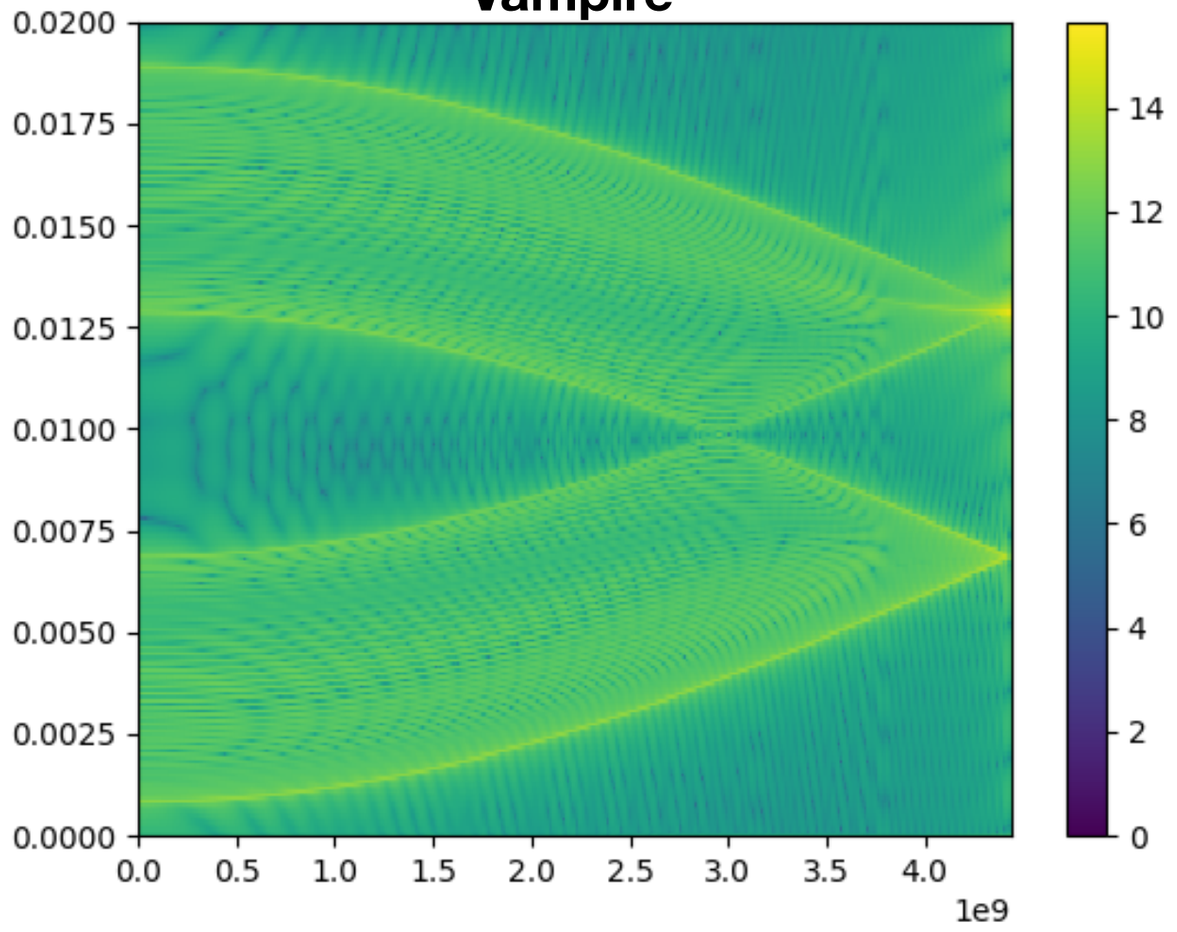
$$\vec{b}_{2h} = \frac{2\pi}{a_0}(1,\frac{2}{\sqrt{3}},0)$$

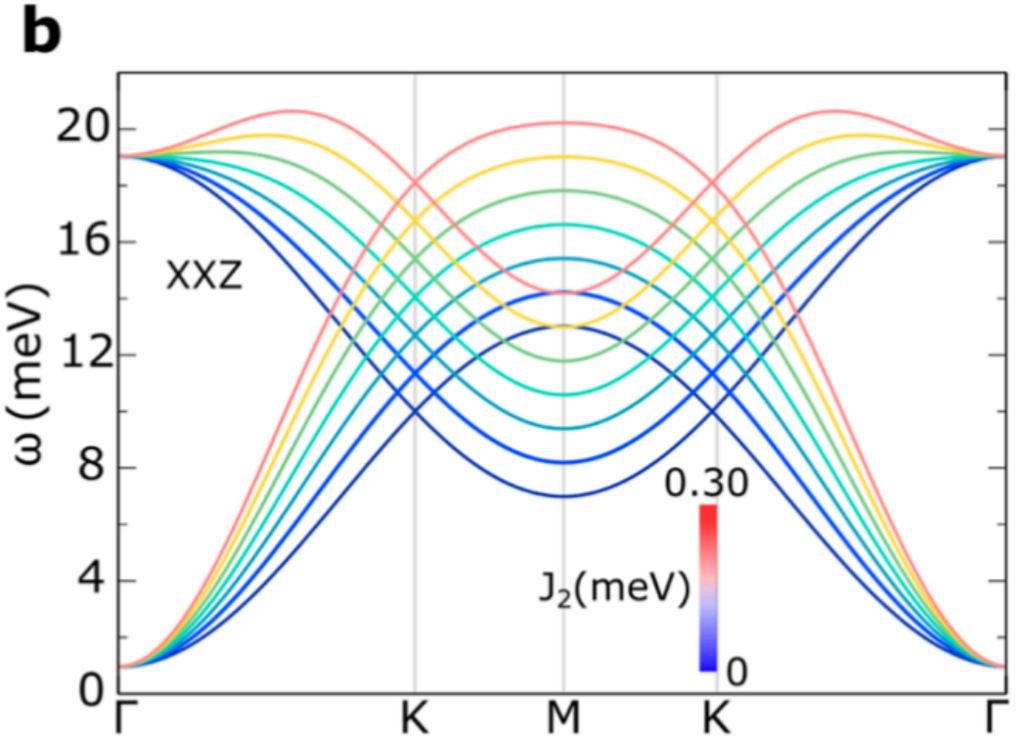
$$\vec{b}_{3h} = \frac{2\pi}{a_0}(0,0,1)$$

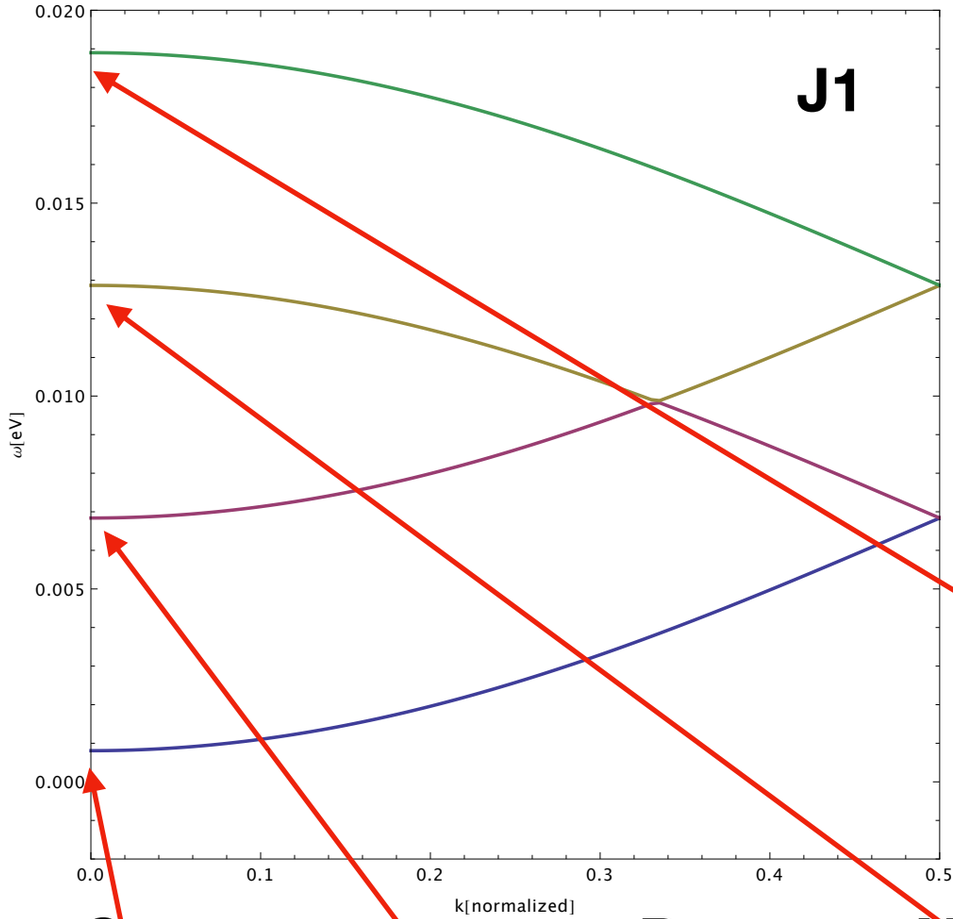
## Dynamical Matrix Method

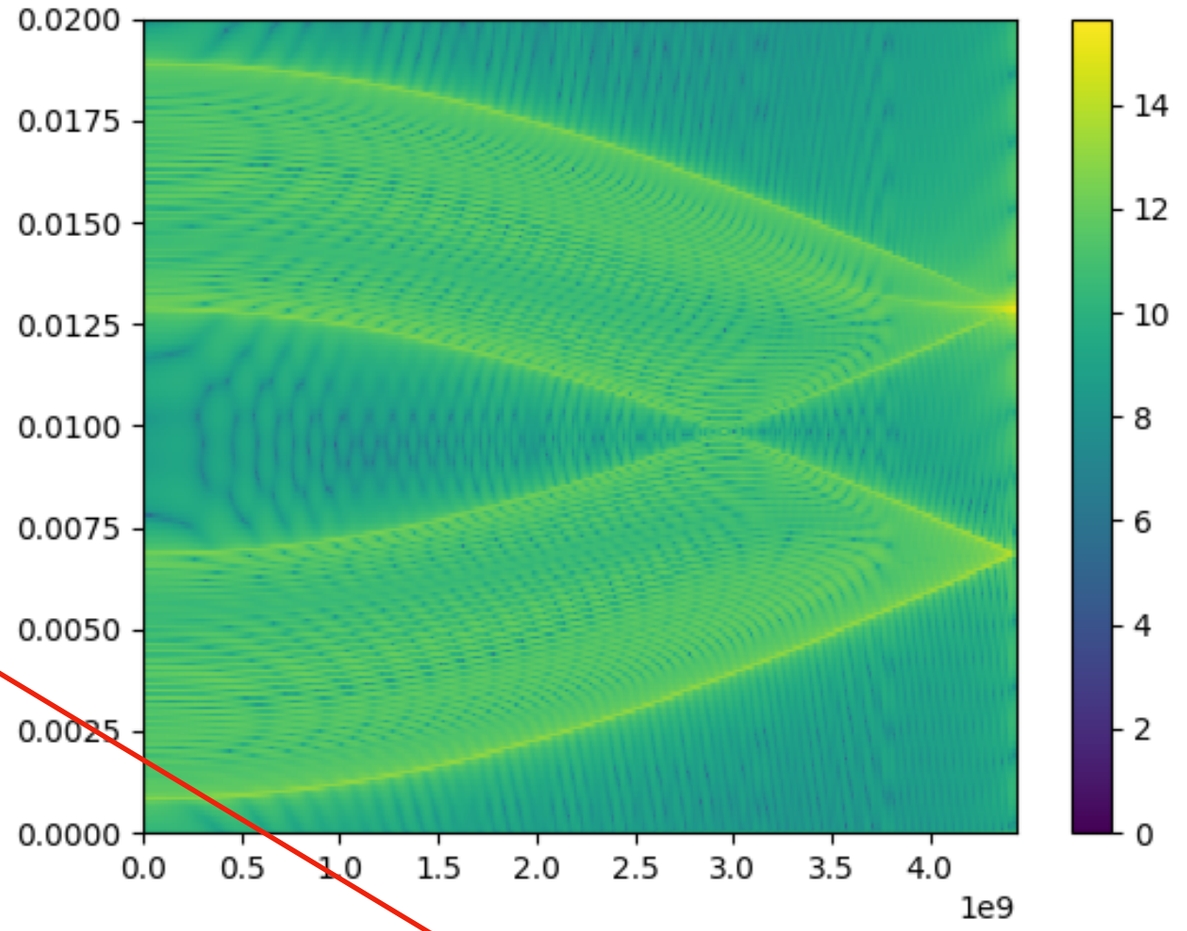



## Vampire



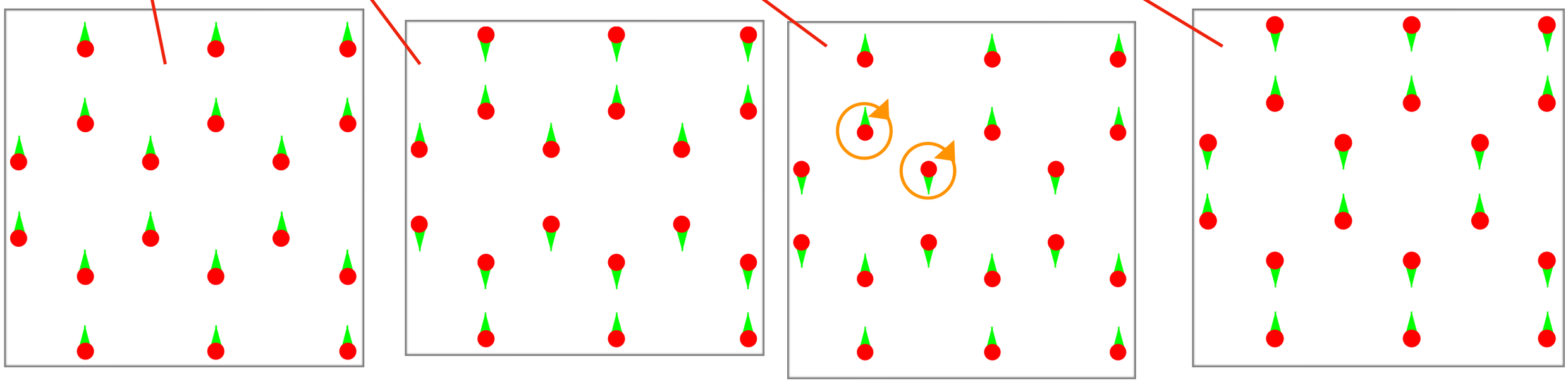


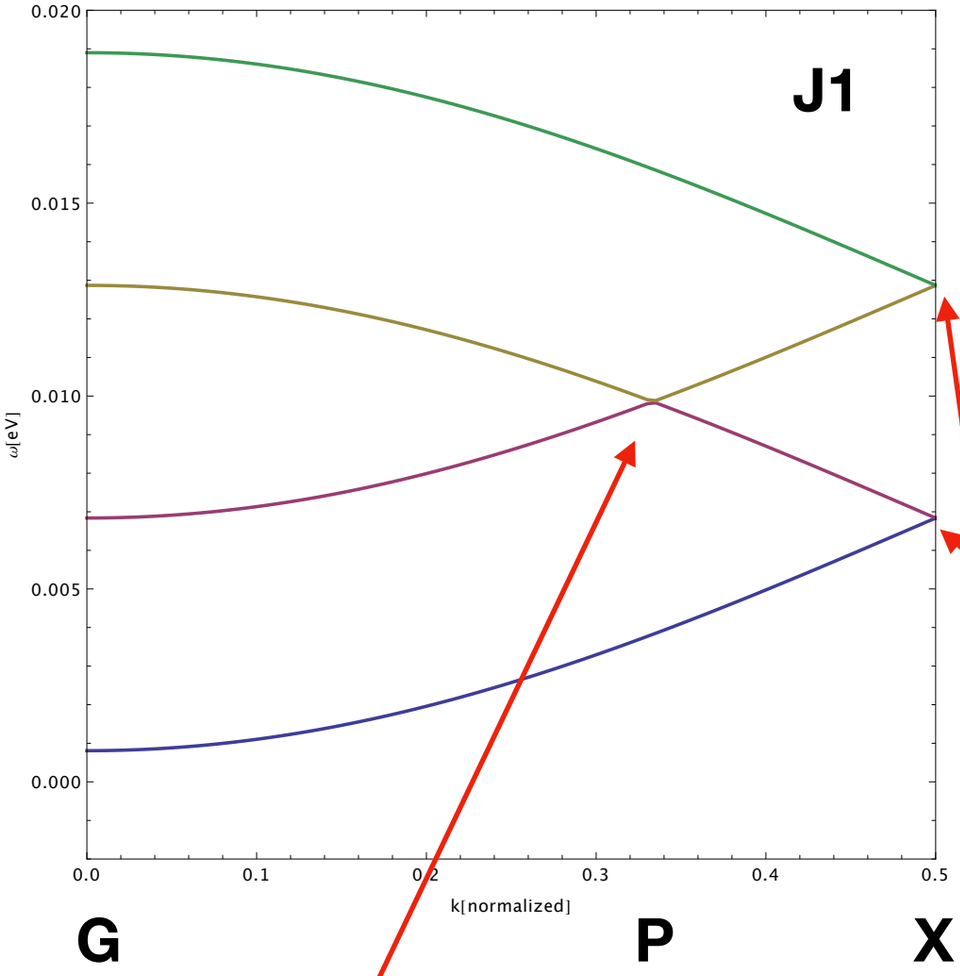

G

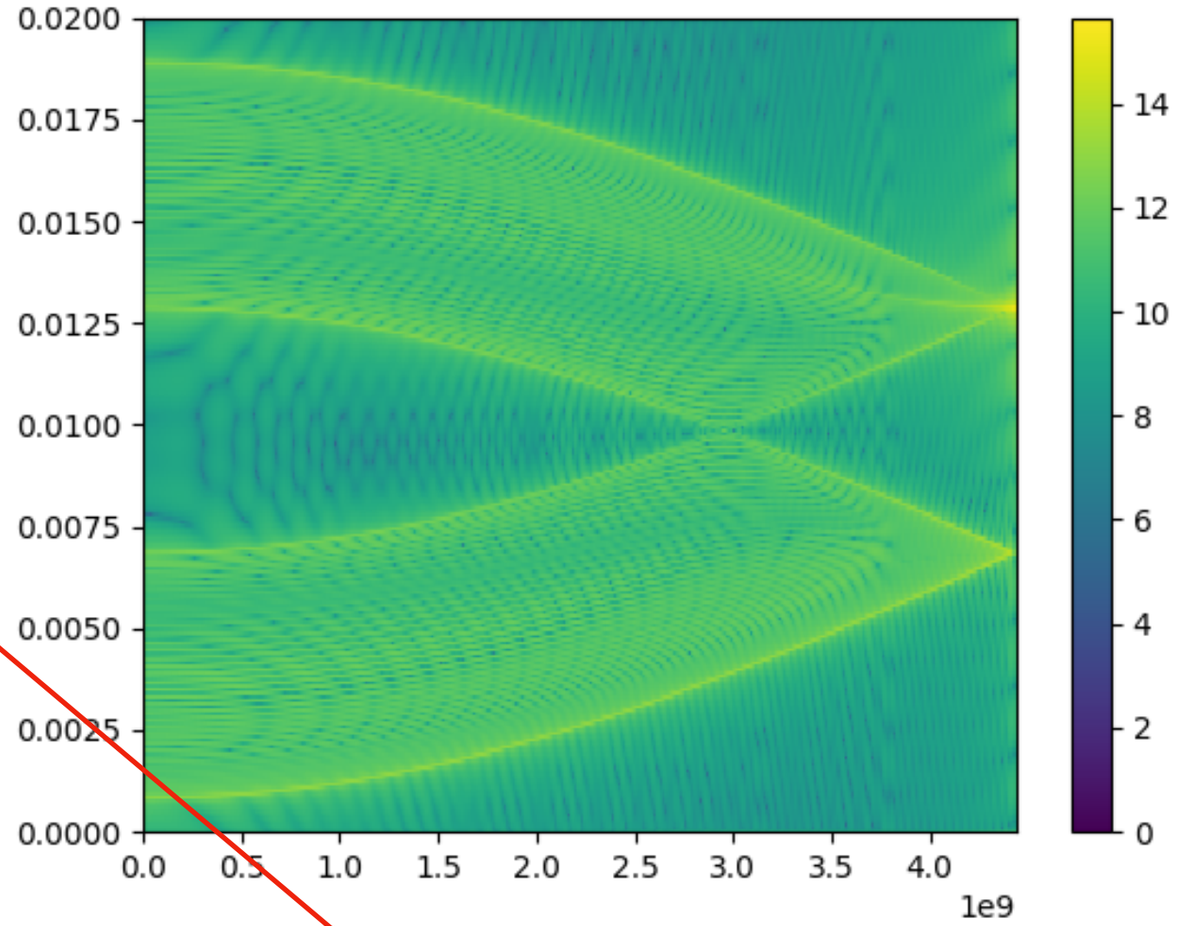
P

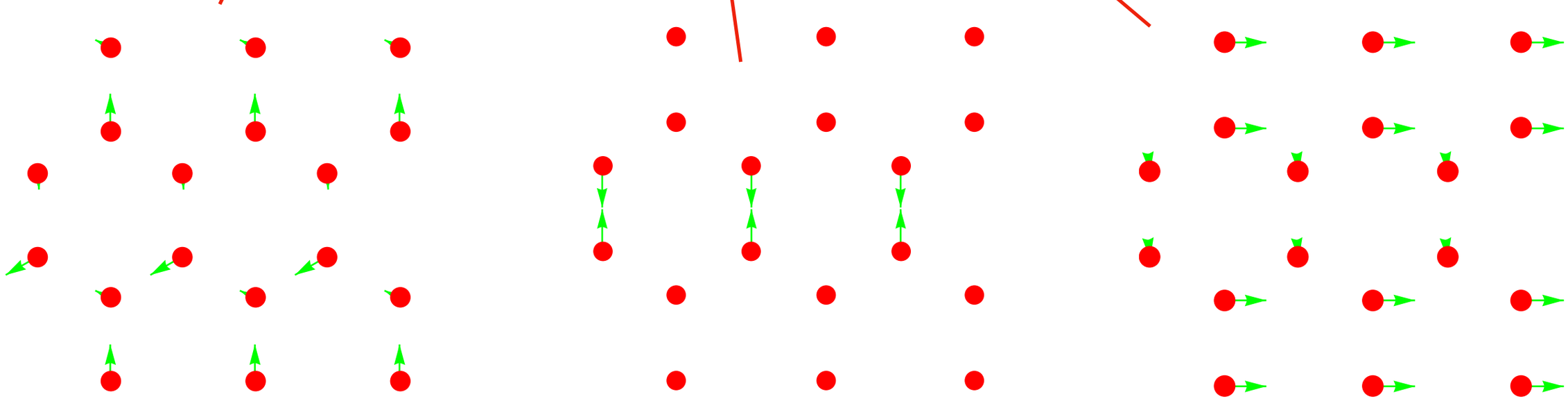
X



**Spin wave polarization**

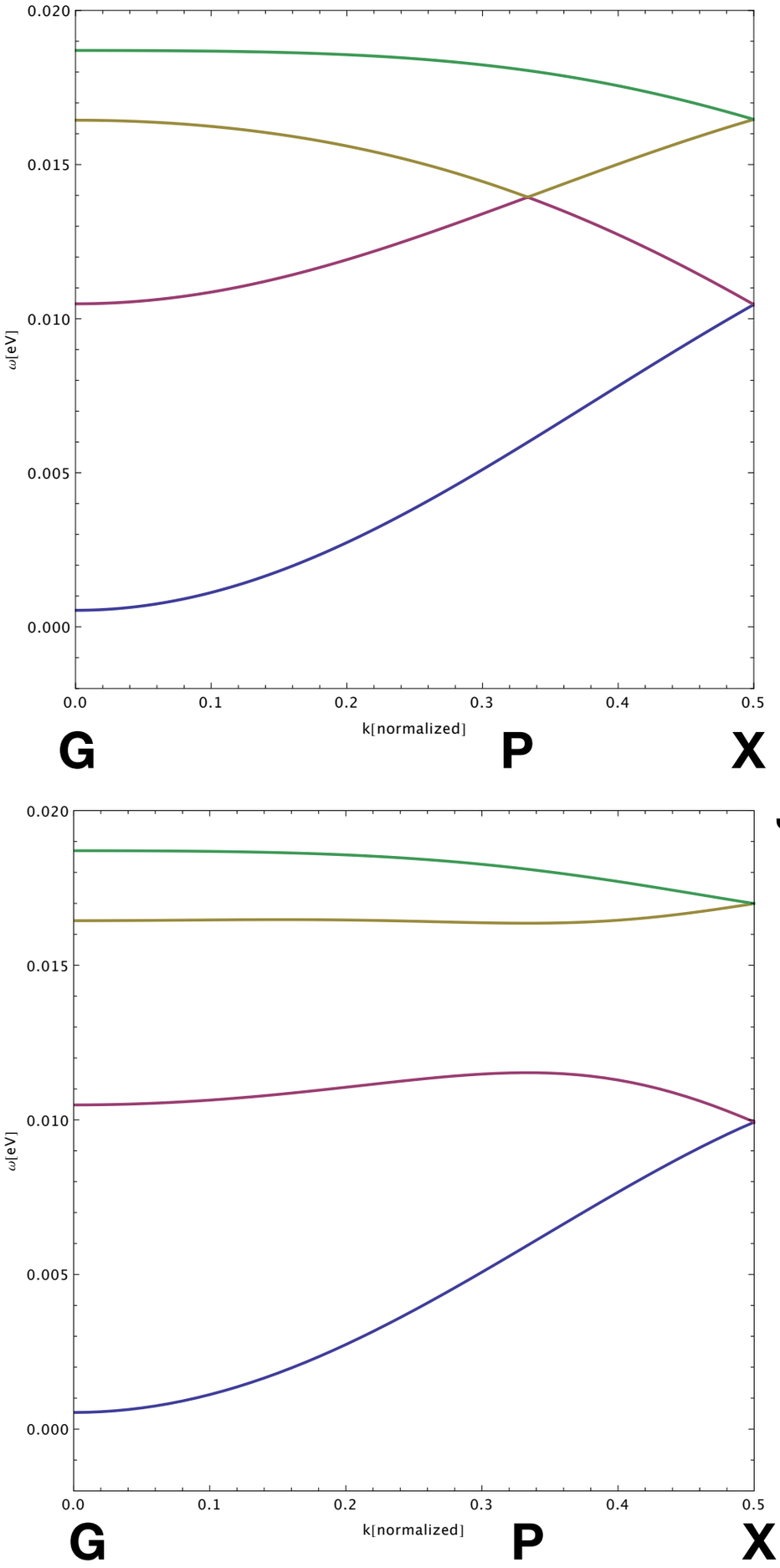


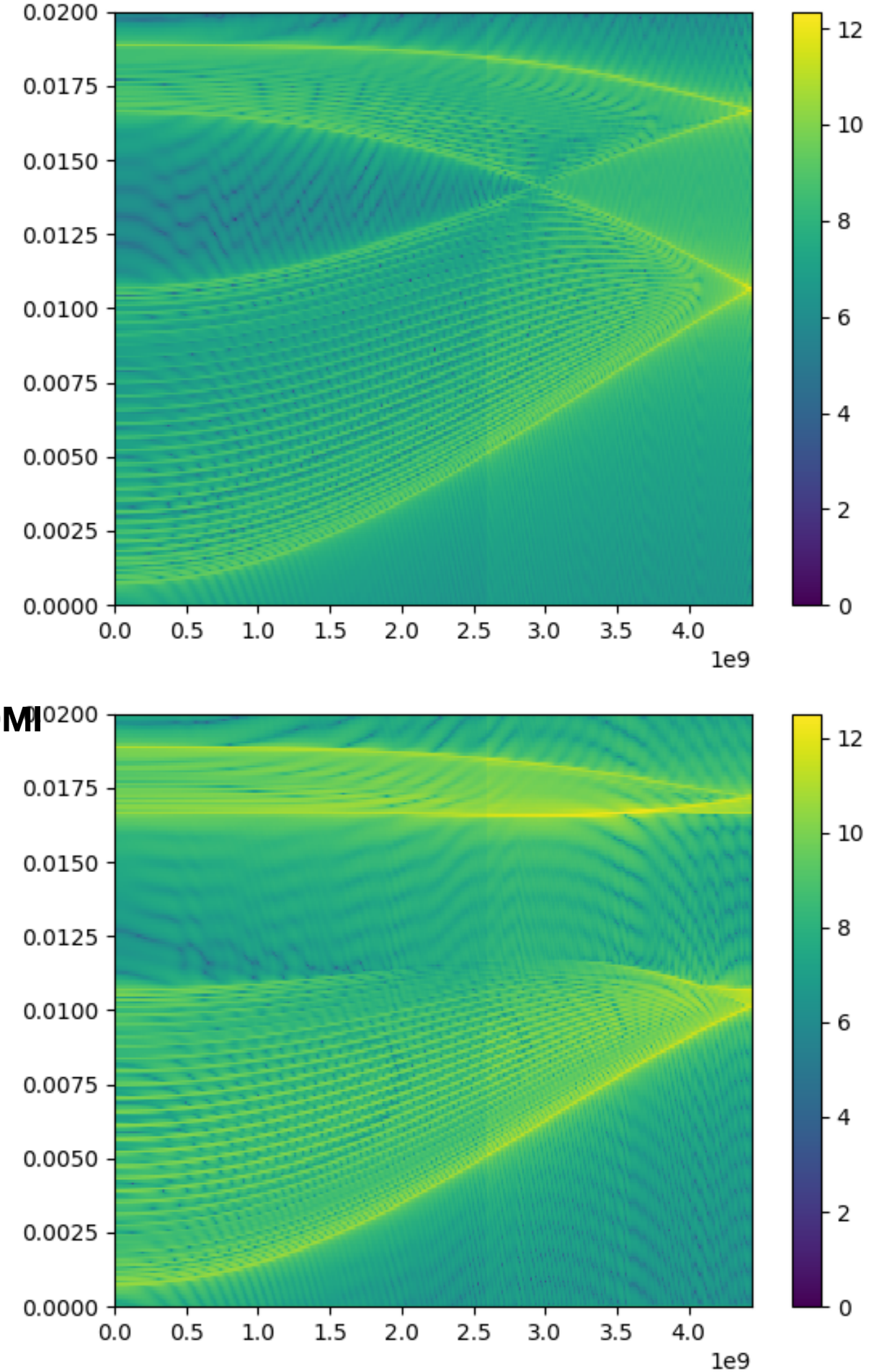



Spin wave polarization

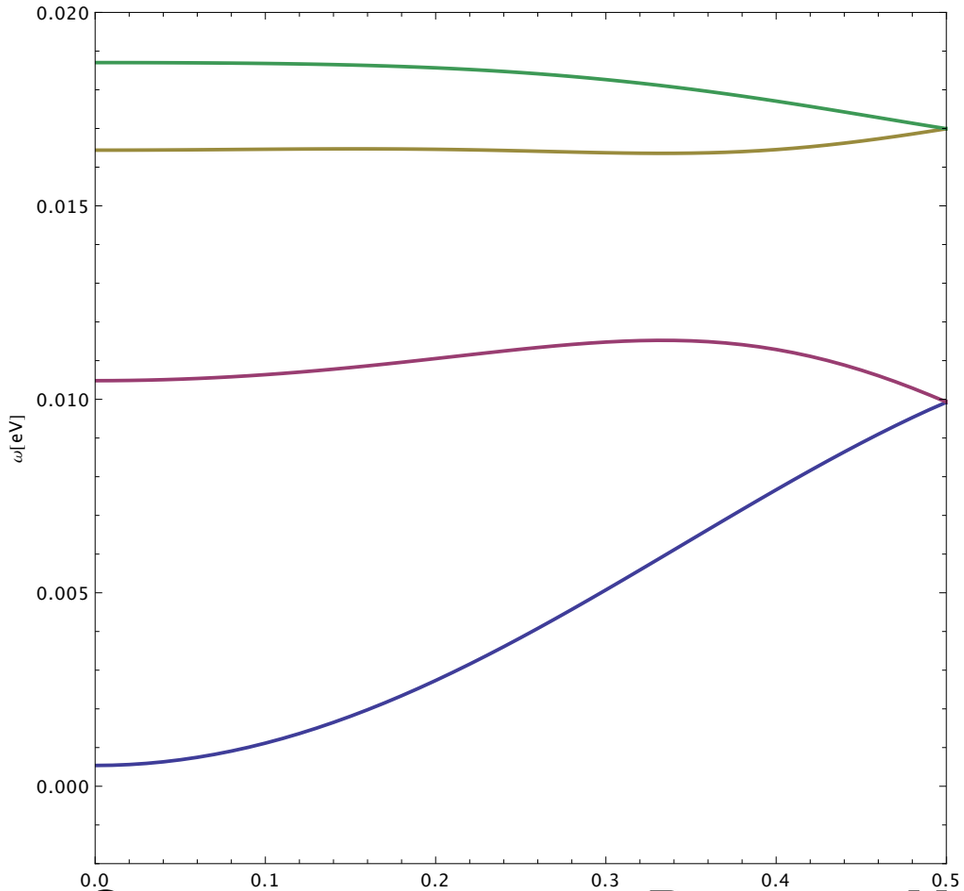
**J1+J2+J3**

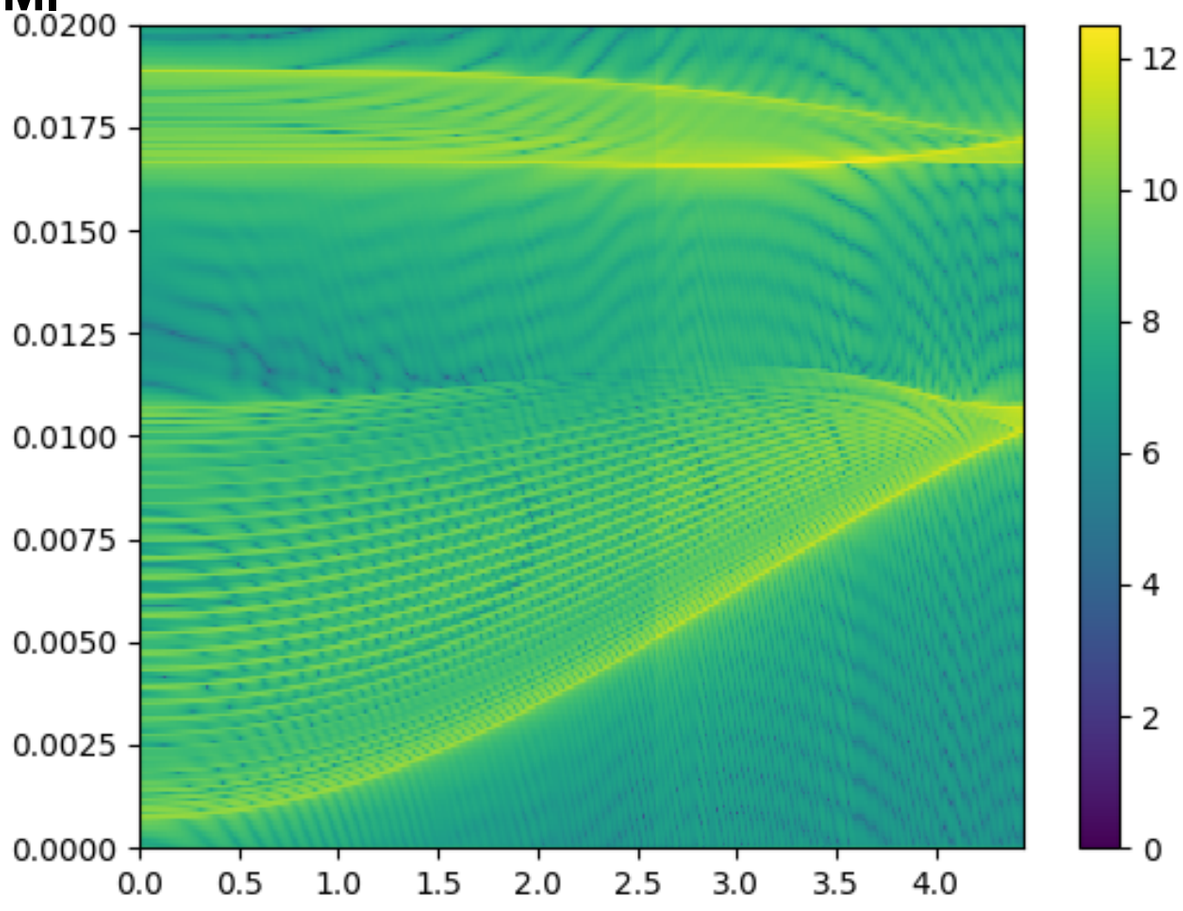



**J1+J2+J3+DMI**

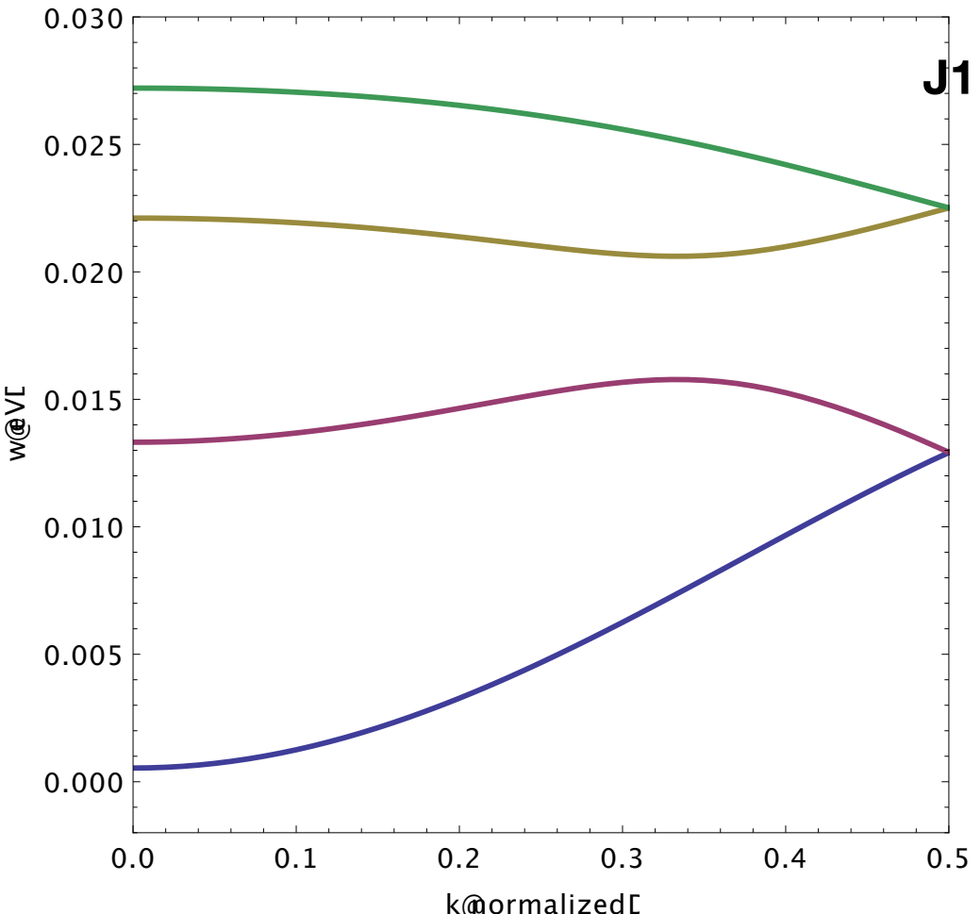
## J1+J2+J3+DMI

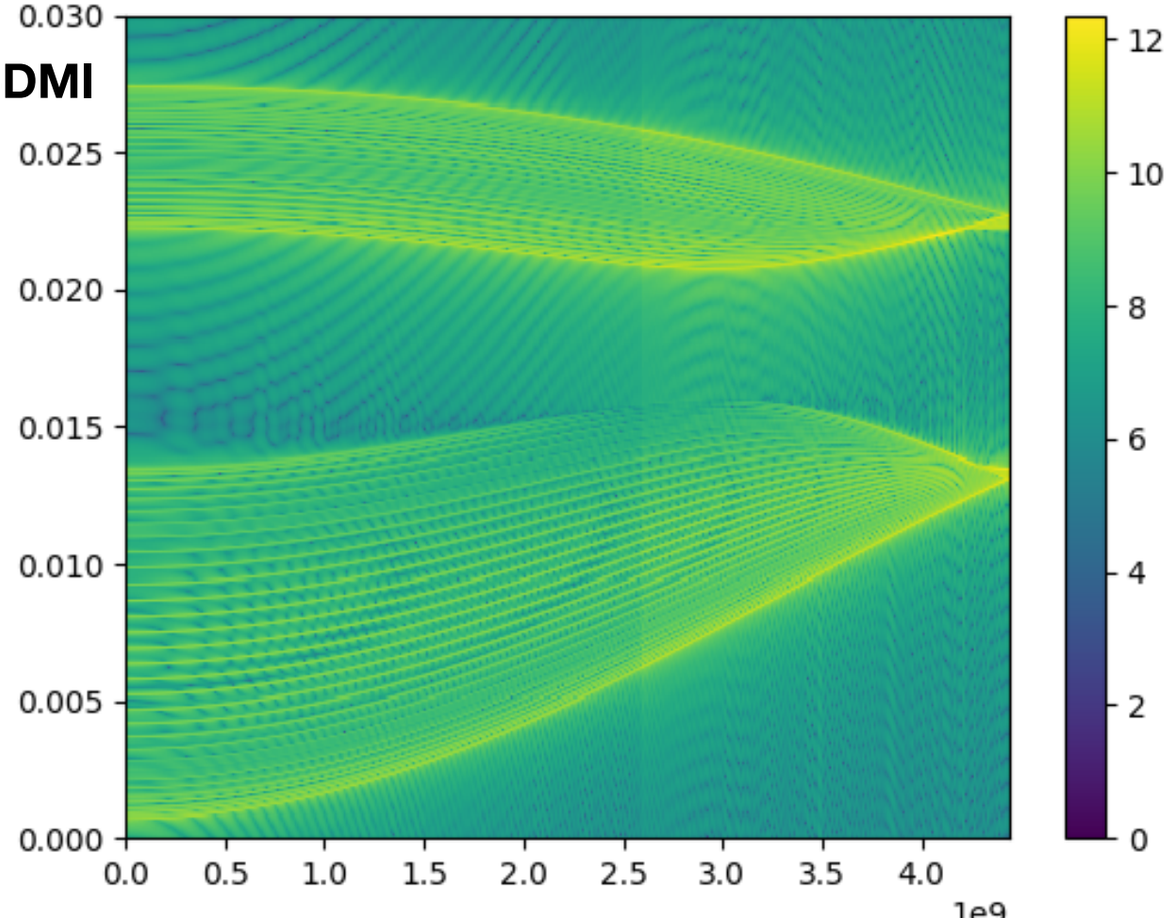



G P X

## J1+J2+J3+BQ+DMI

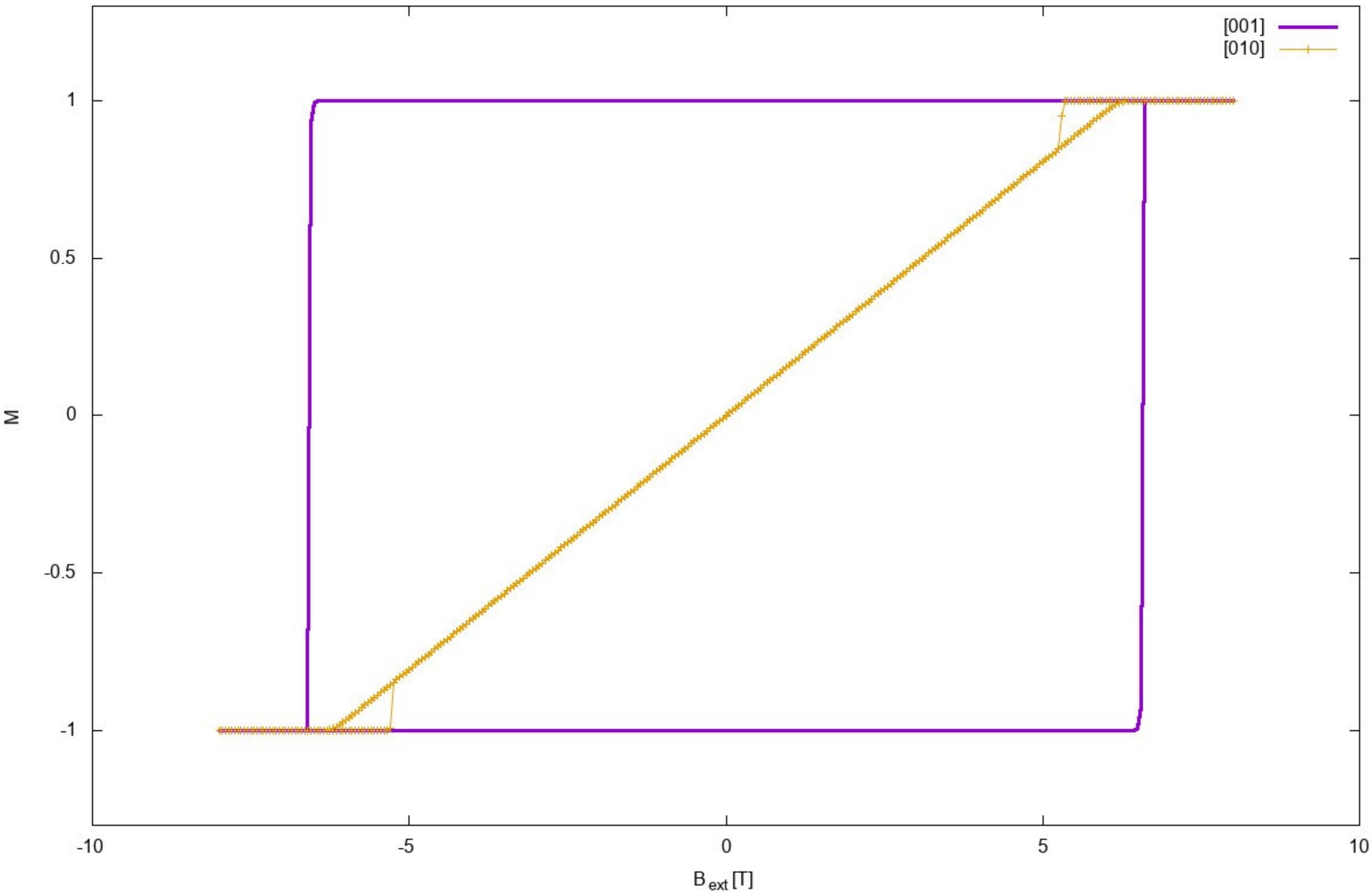


# External field

**J1+J2+J3+BQ+DMI  500K - timestep**

**Hysteresis loops**



# External field

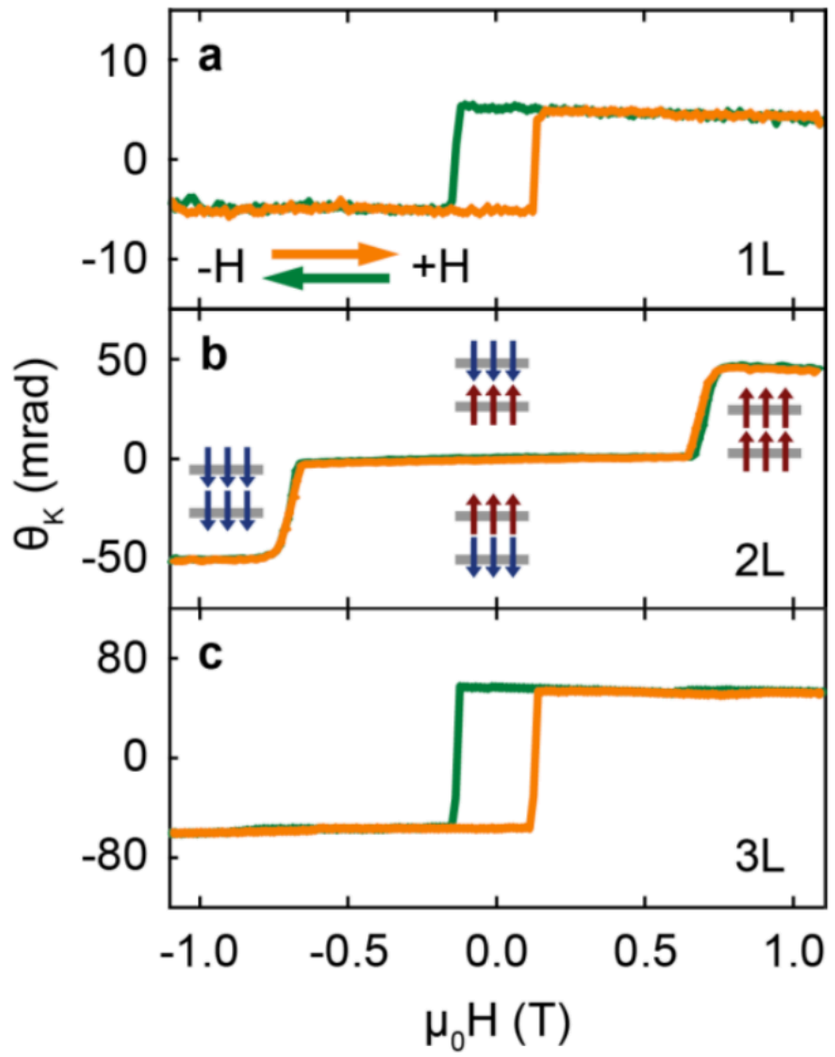


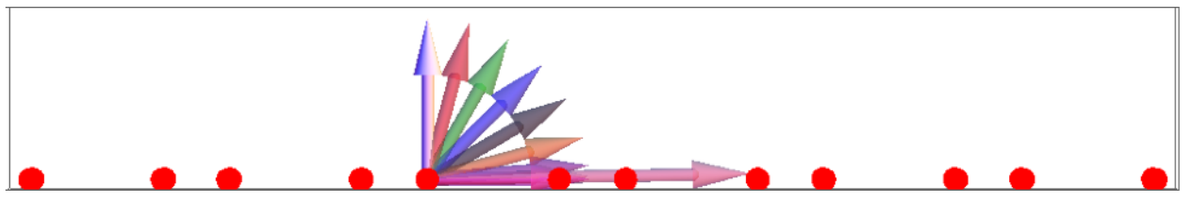

**Figure 3 | Layer-dependent magnetic ordering in atomically-thin $CrI_3$.** (**a**), MOKE signal on a monolayer $CrI_3$ flake, showing hysteresis in the Kerr rotation as a function of applied magnetic field, indicative of ferromagnetic behavior. (**b**), MOKE signal from a bilayer $CrI_3$ showing vanishing Kerr rotation for applied fields between ±0.65 T, suggesting antiferromagnetic behavior. Insets depict bilayer magnetic ground states for different applied fields. (**c**), MOKE signal on a trilayer flake showing a return to ferromagnetic behavior.

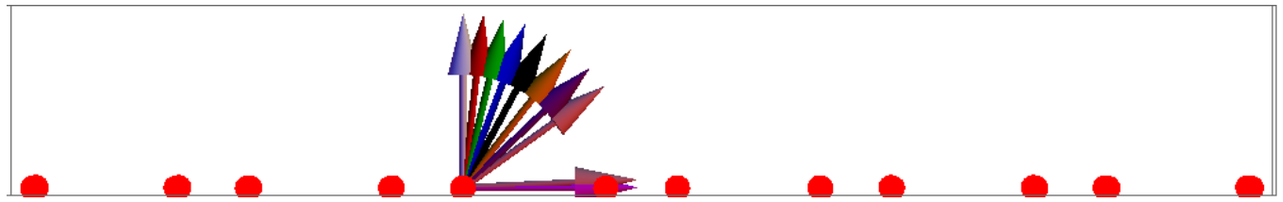
# External field 5T

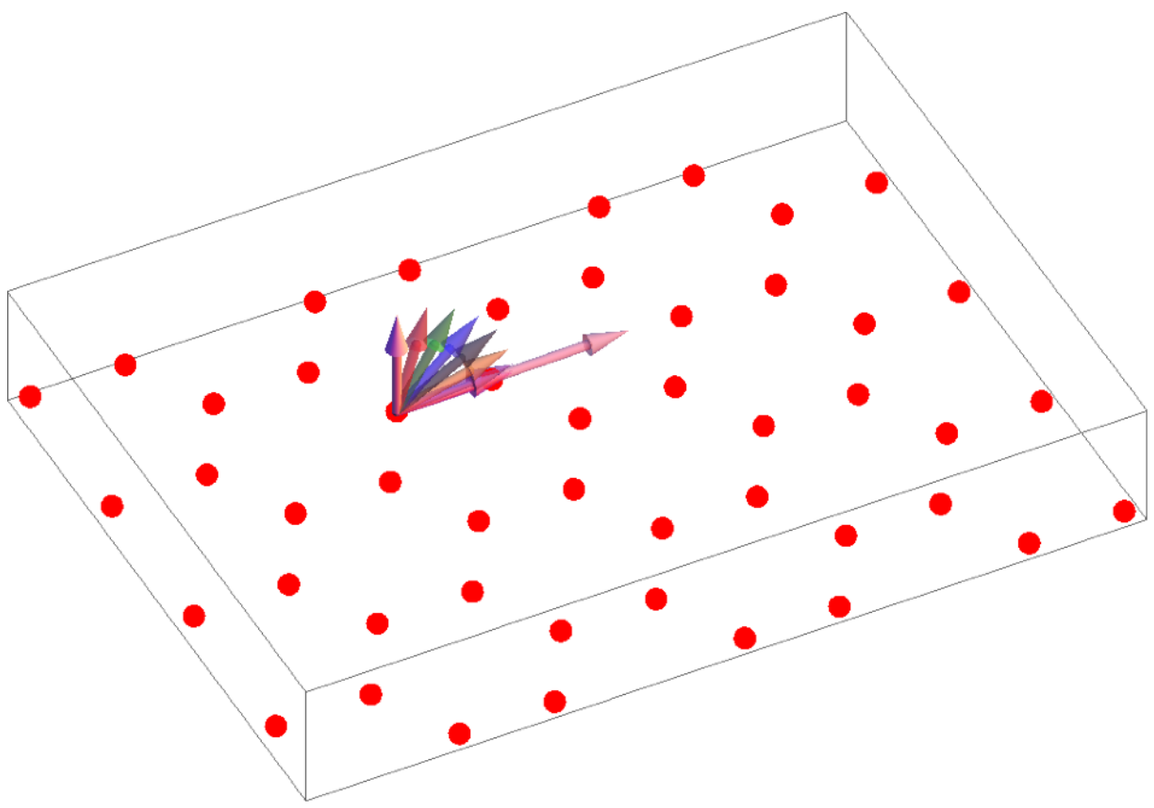
**J1+J2+J3+BQ+DMI**

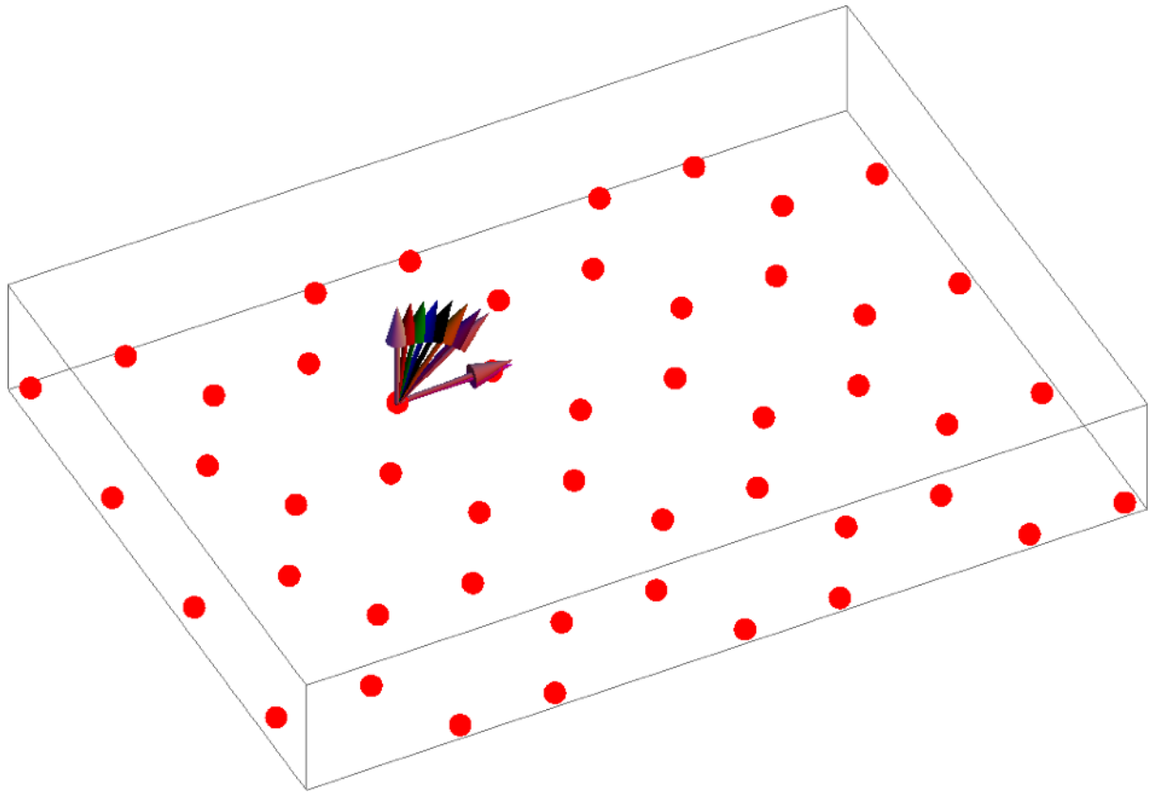
**$B_{ext}$ = 5T**
**Angles= 0, 15, 30,45,60,75,85,89,90 Deg**

**Saturation state**

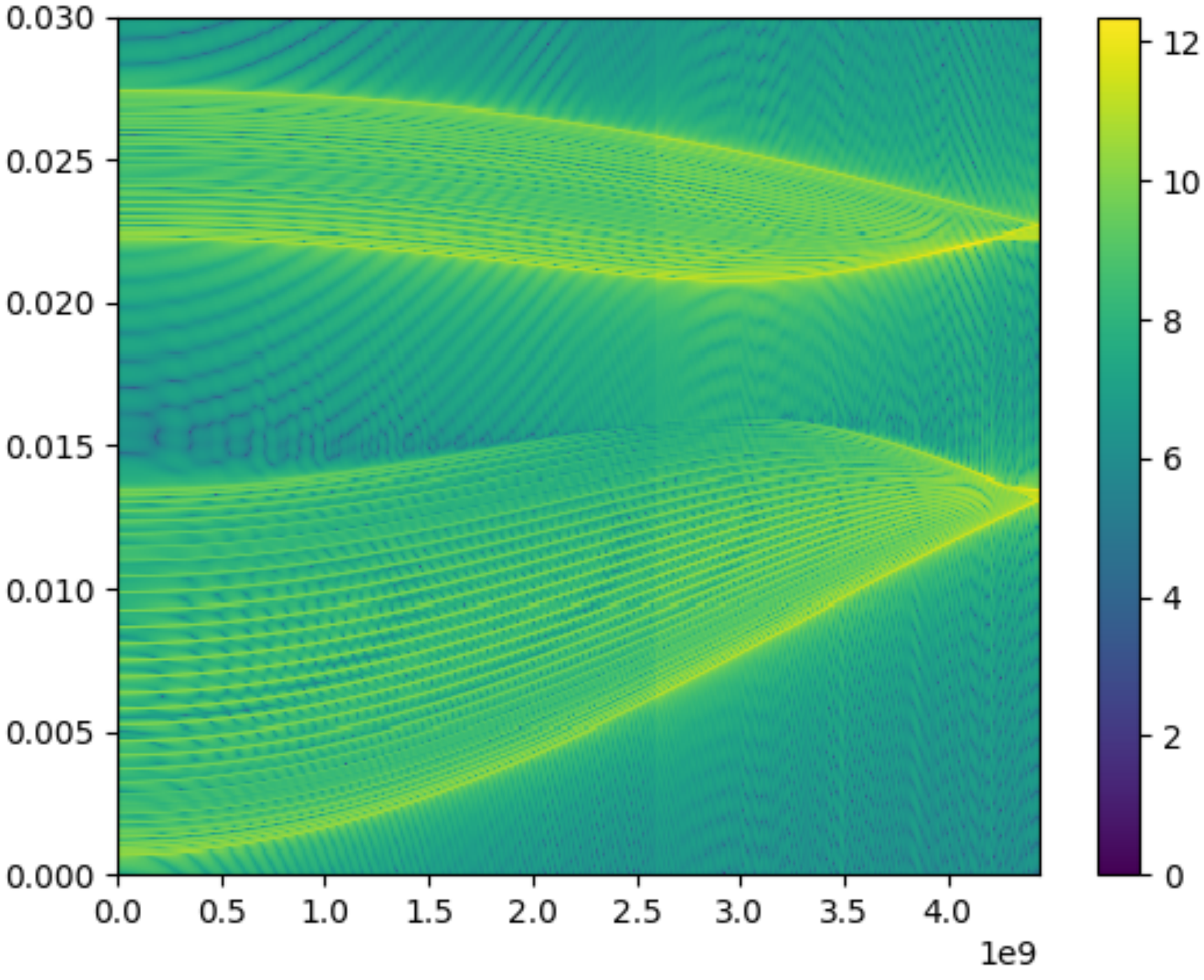




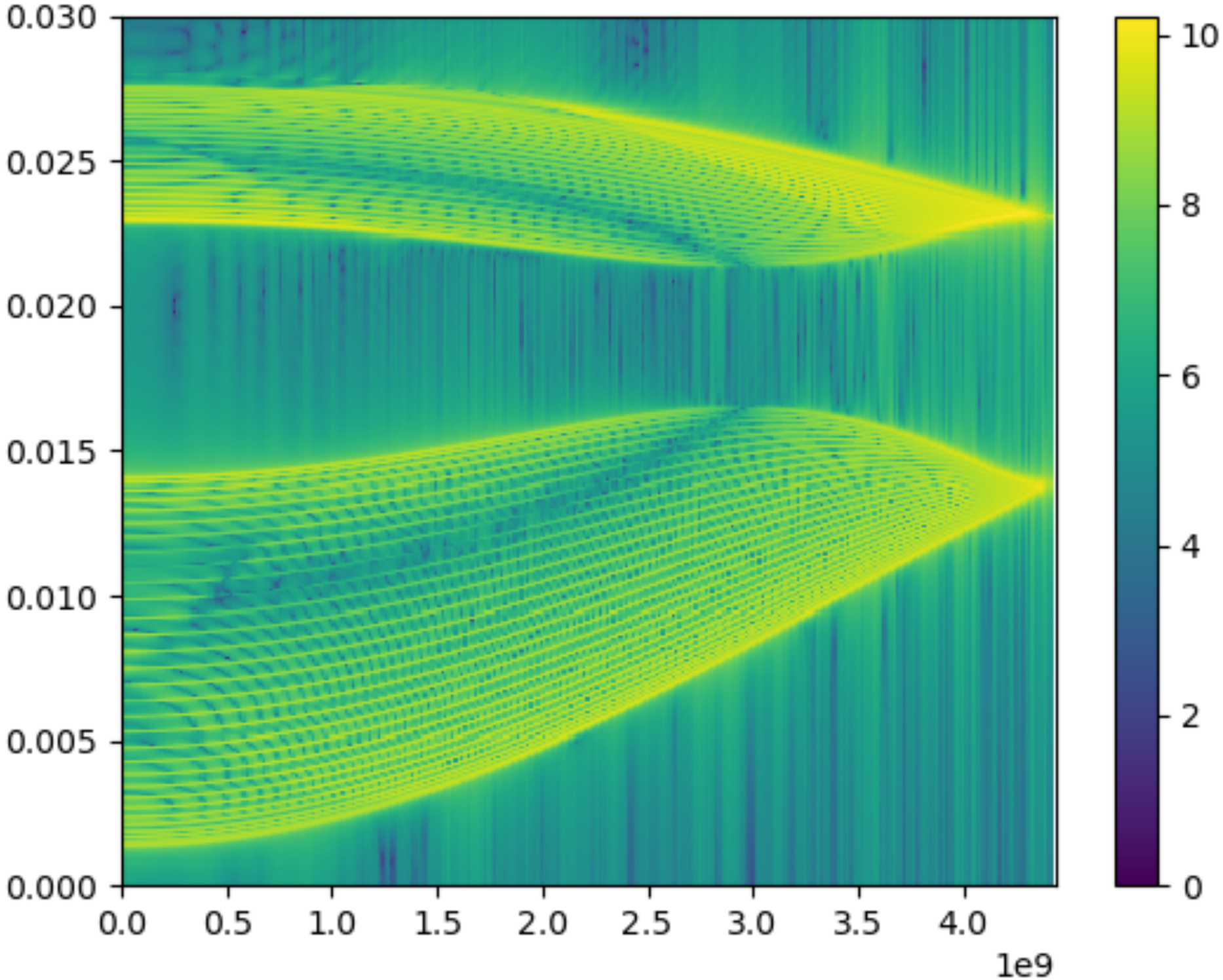




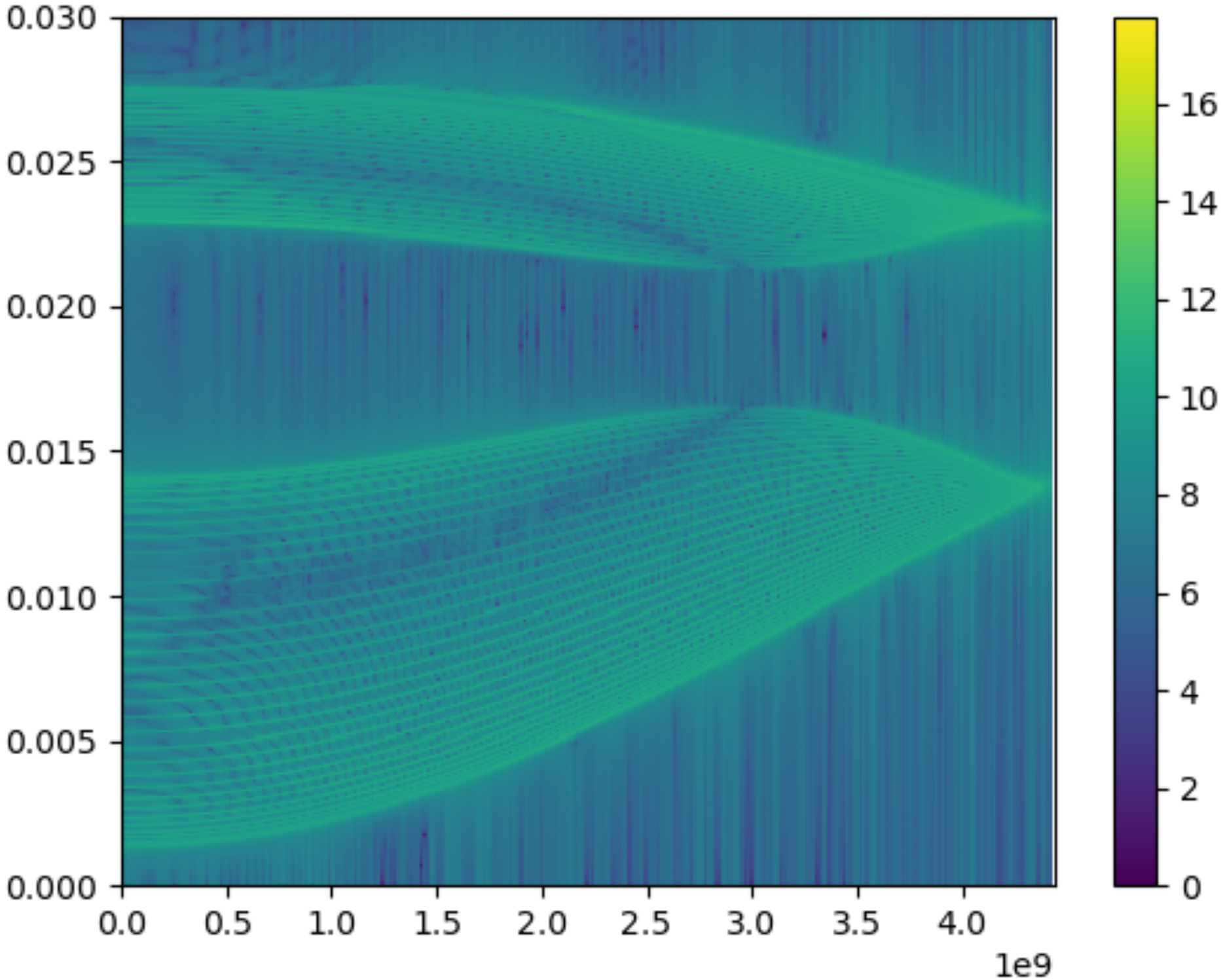
# Bext = 0T - 0 Deg


0.030
0.025
0.020
0.015
0.010
0.005
0.000
0.0
0.5
1.0
1.5
2.0
2.5
3.0
3.5
4.0
1e9
12
10
8
6
4
2
0

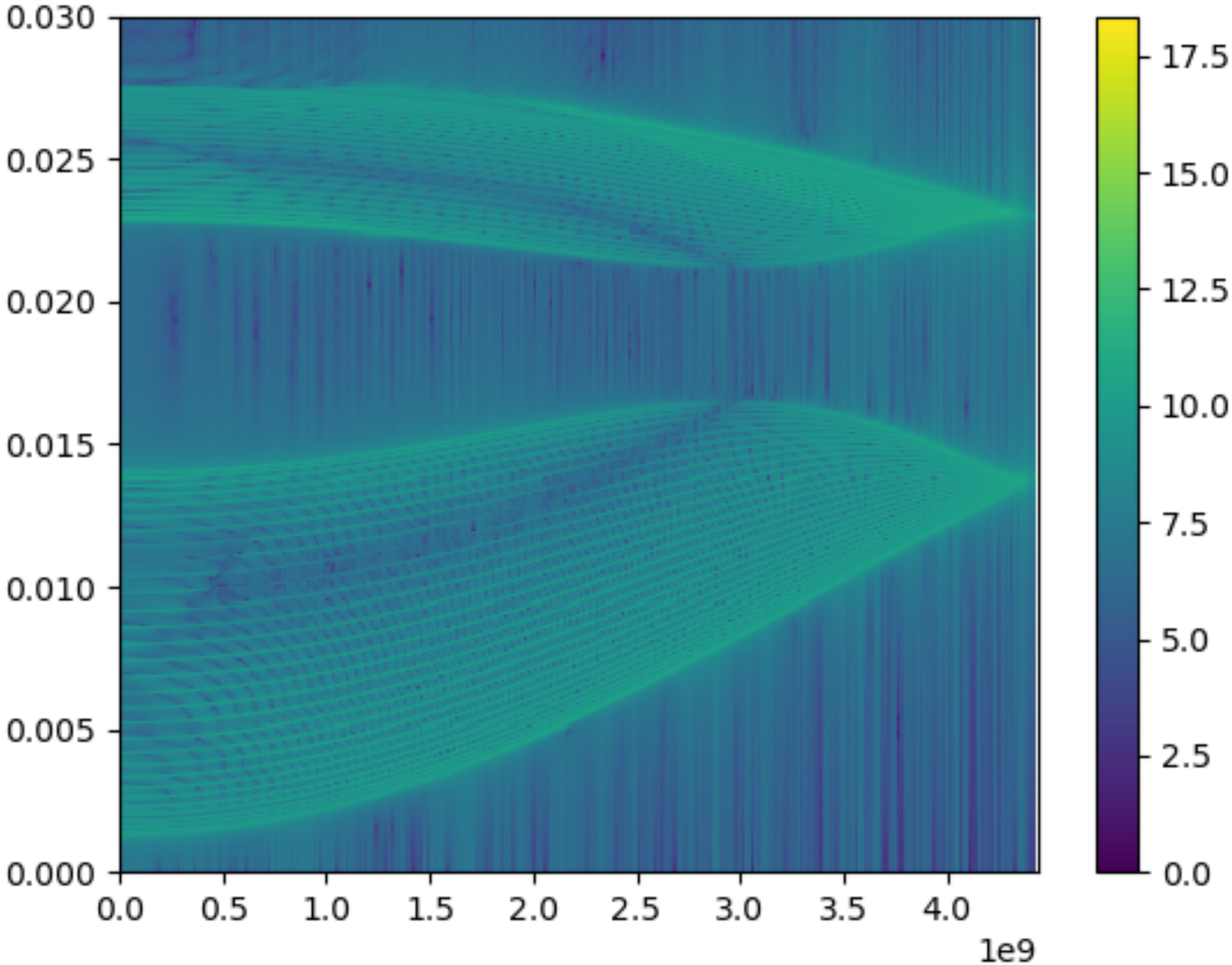
# Bext = 5T - 0 Deg


0.030
0.025
0.020
0.015
0.010
0.005
0.000
0.0
0.5
1.0
1.5
2.0
2.5
3.0
3.5
4.0
1e9
10
8
6
4
2
0

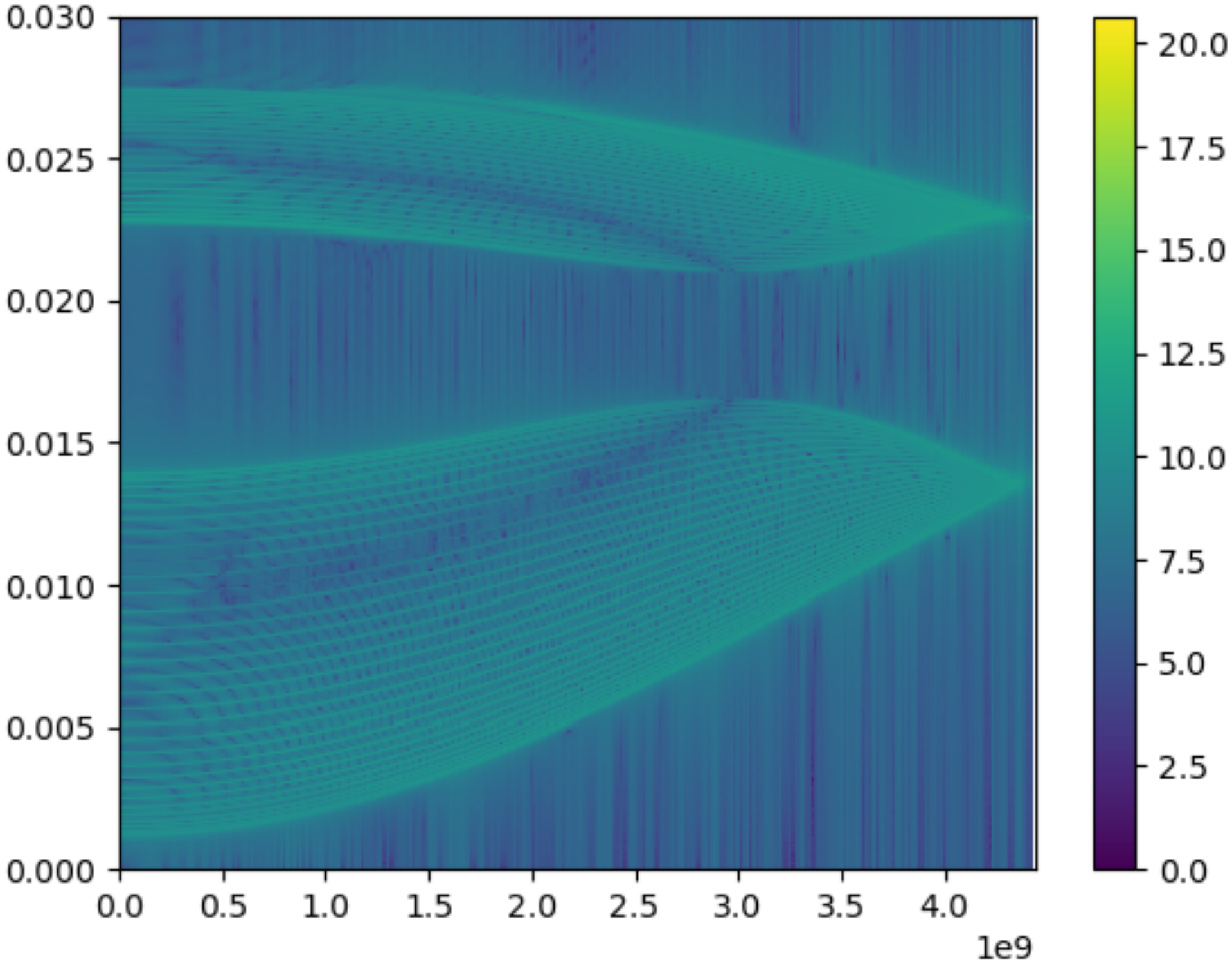
**Bext = 5T - 15 Deg  Ssat = 6.71484 Deg**



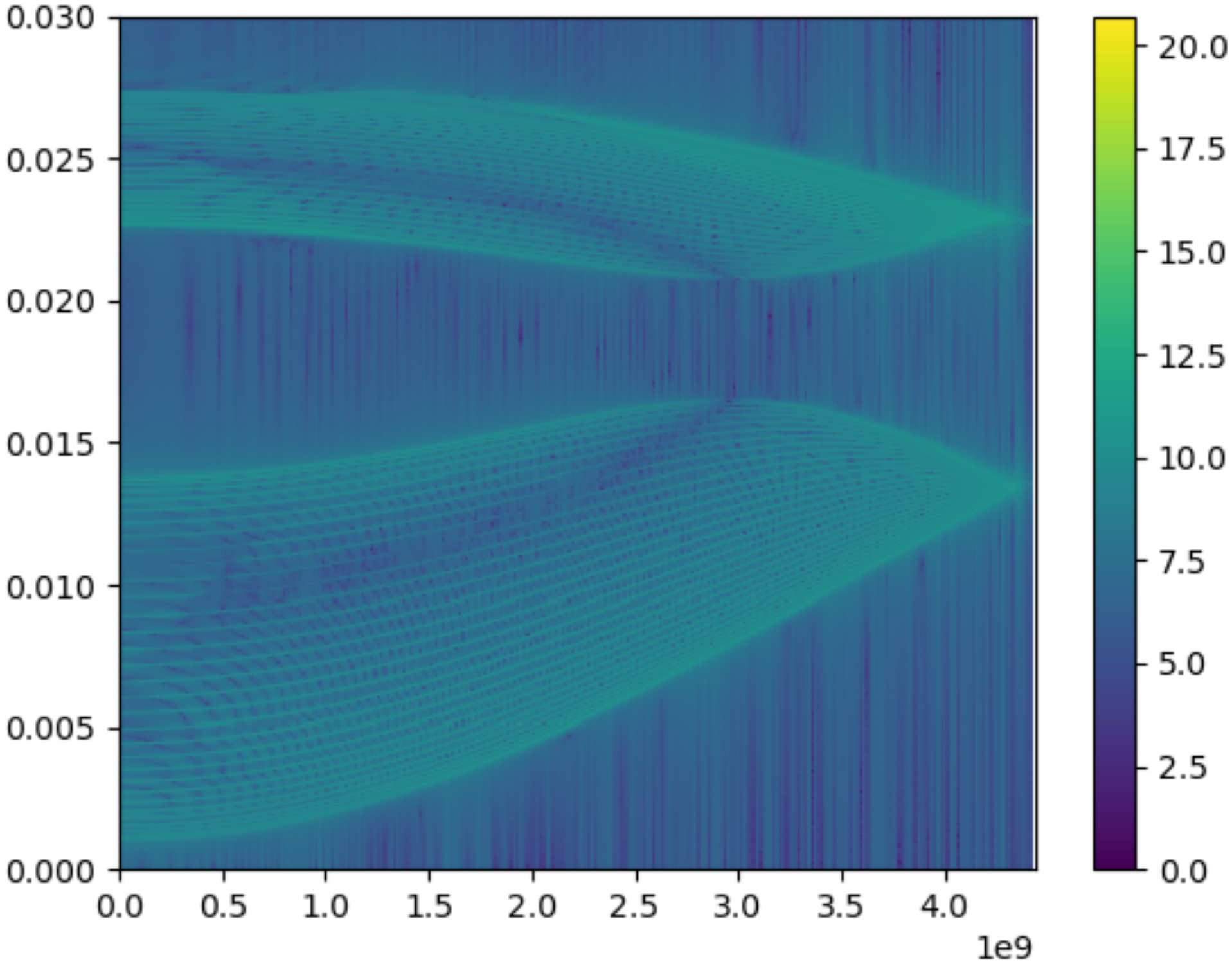
**Bext = 5T - 30 Deg** **Ssat = 13.5649 Deg**



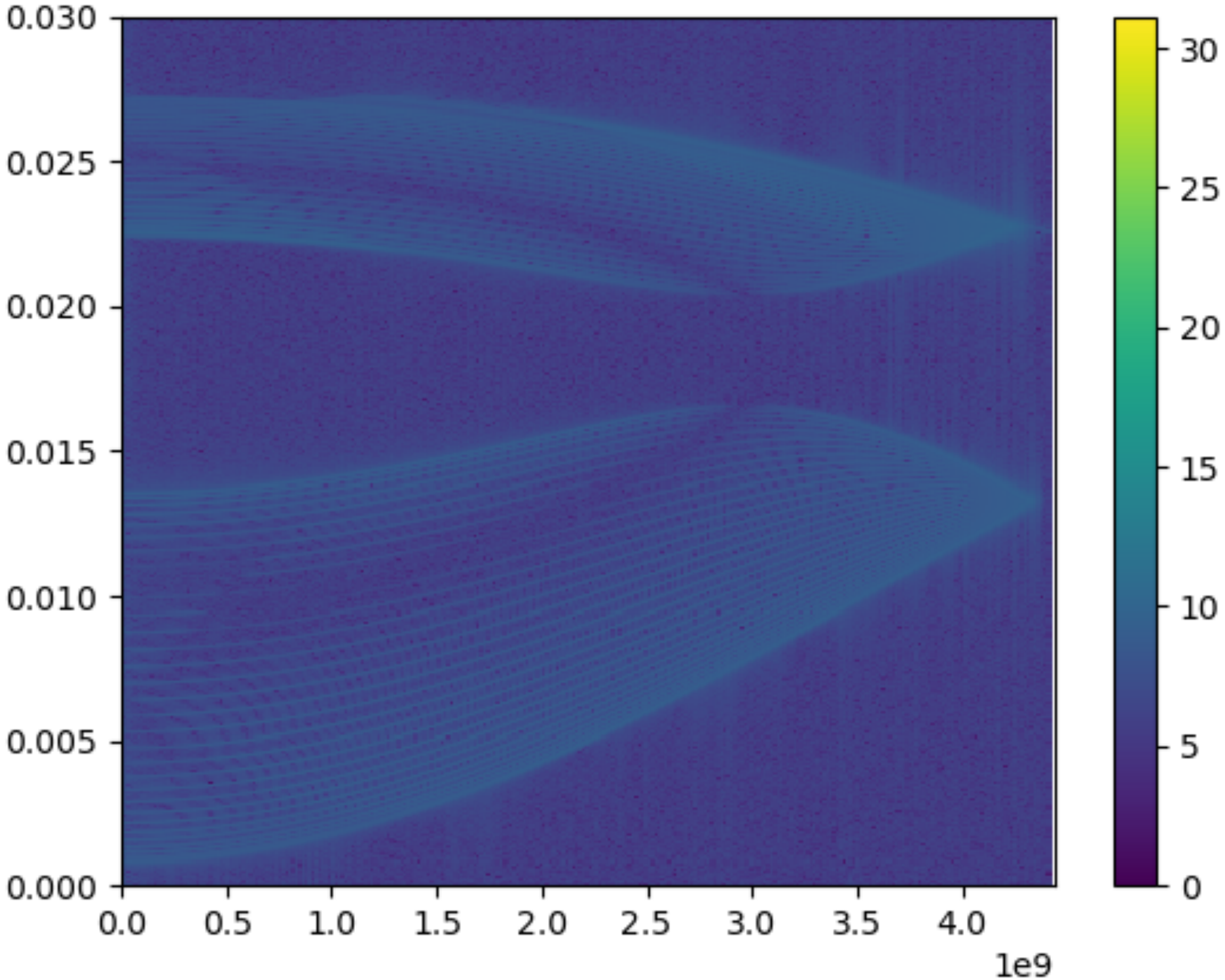
**Bext = 5T - 45 Deg** **Ssat = 20.7376 Deg**



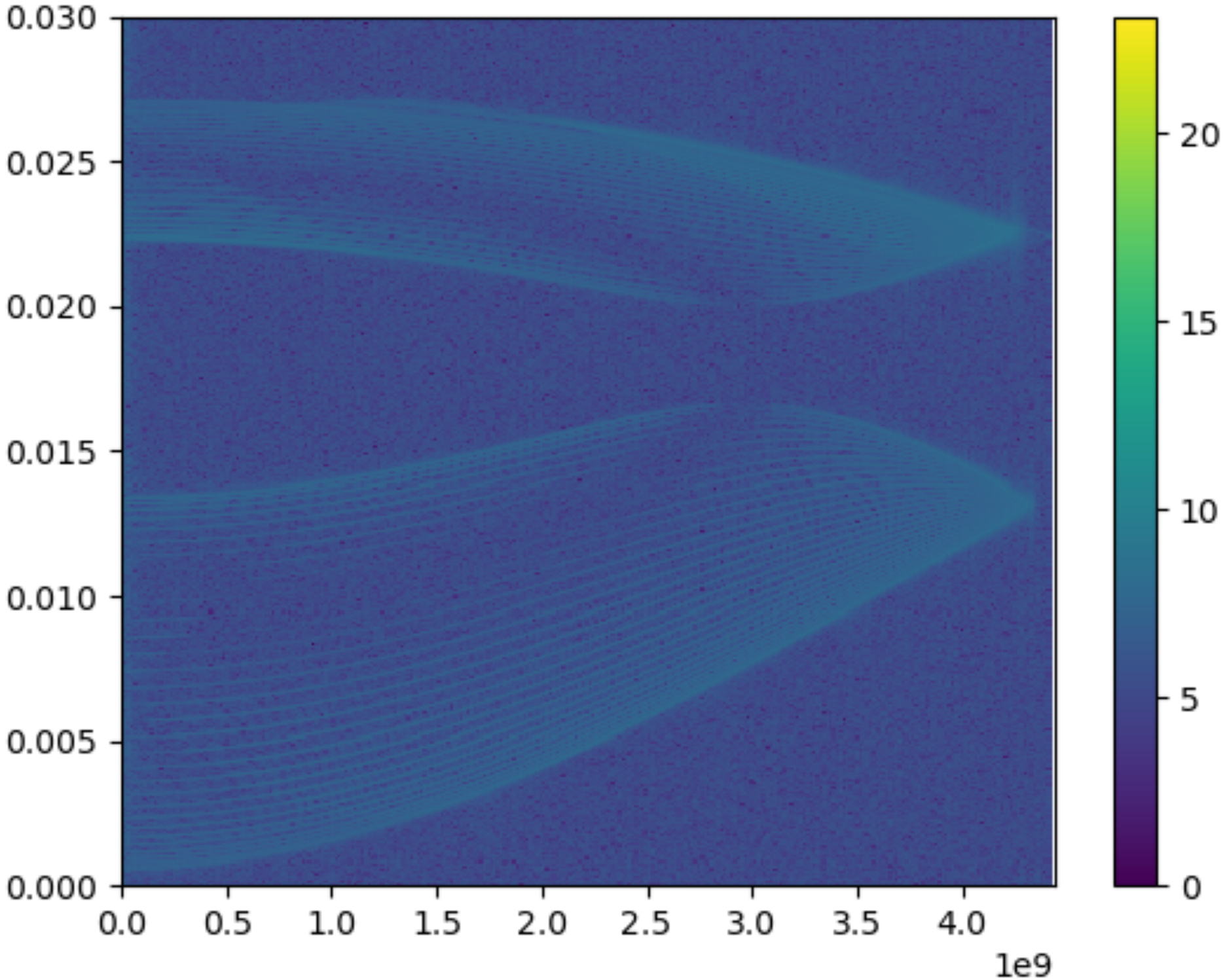
**Bext = 5T - 60 Deg  Ssat = 28.5805 Deg**



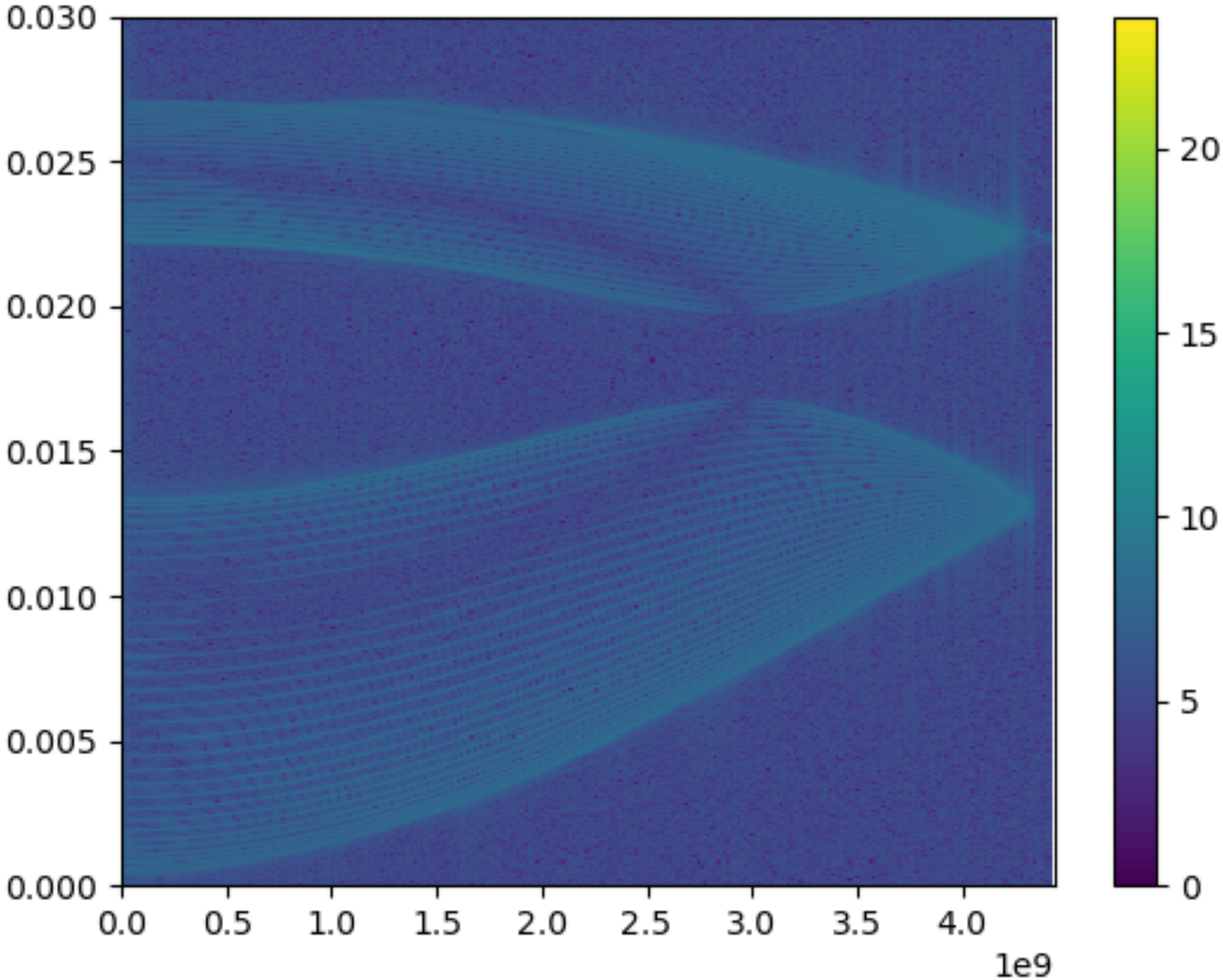
**Bext = 5T - 75 Deg** **Ssat = 37.991 Deg**



**Bext = 5T - 85 Deg  Ssat = 46.6736 Deg**



**Bext = 5T - 89 Deg** **Ssat = 54.4412 Deg**



# External field 10T

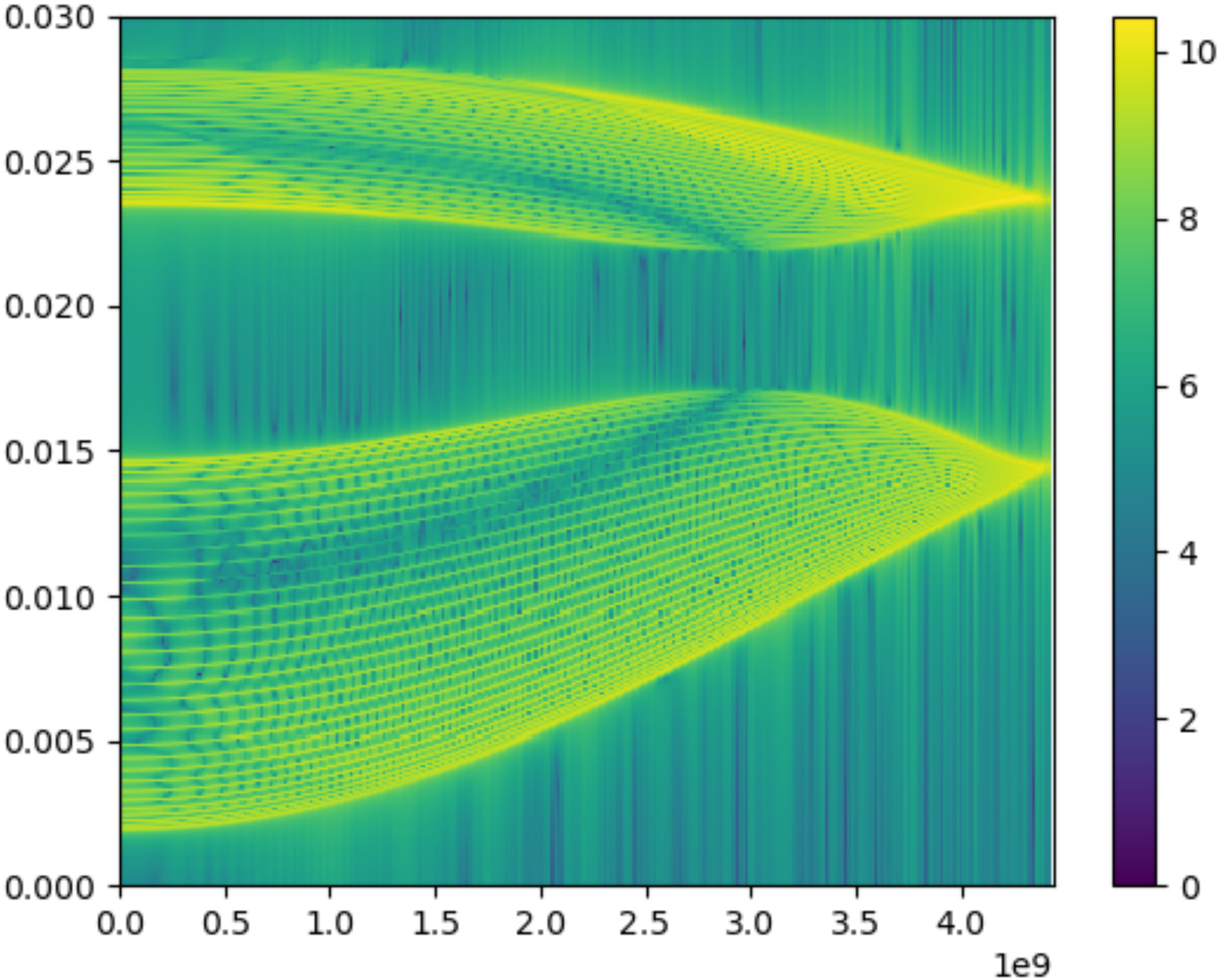
**J1+J2+J3+BQ+DMI**

## External field directions

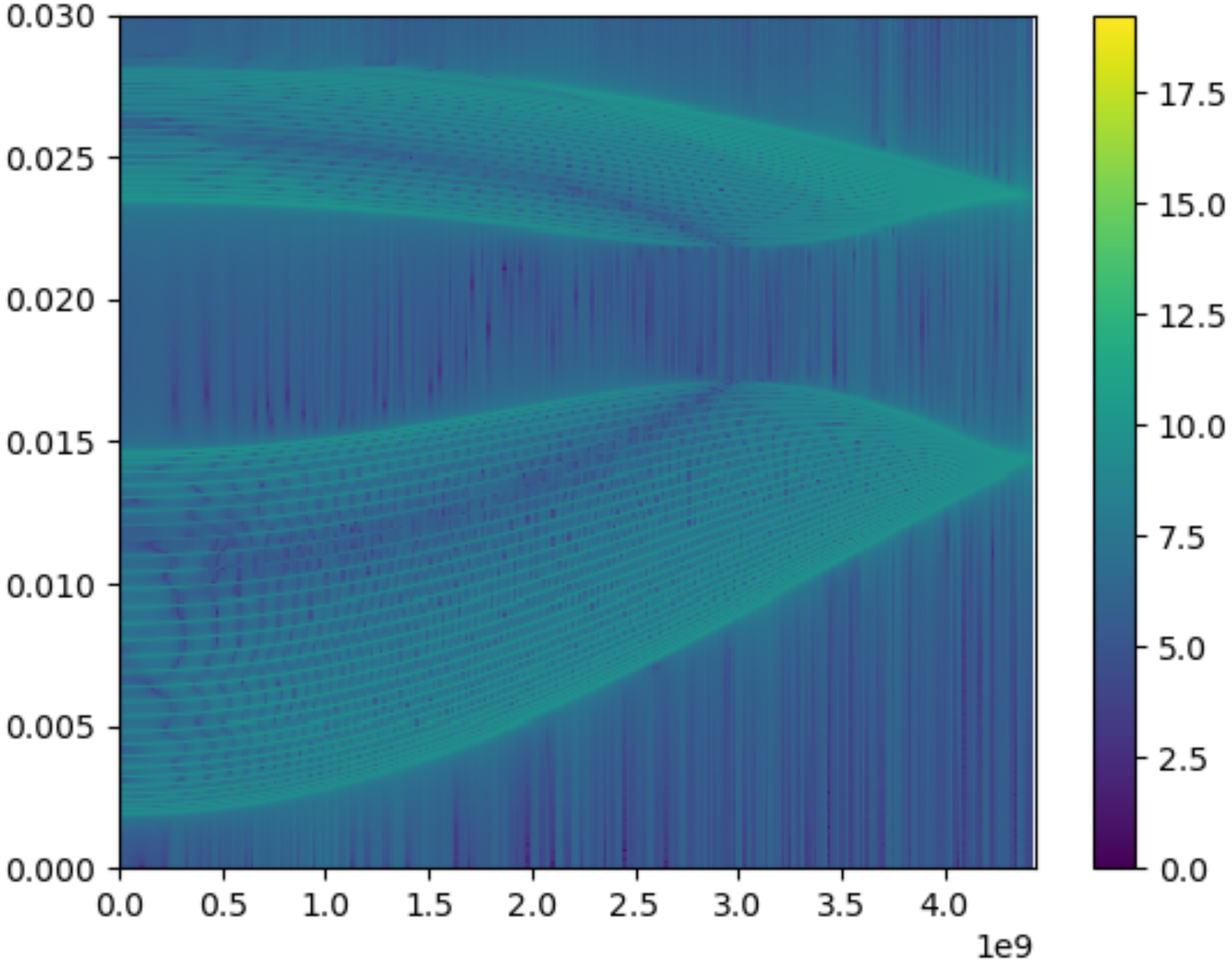
| $B_{ext}$ = 10T | Angles | Saturation state |
|---|---|---|
| | 0 | 0 |
| | 15 | 9.31342 |
| | 30 | 18.9928 |
| | 45 | 29.5592 |
| | 60 | 42.0278 |
| | 75 | 59.1479 |
| | 89 | 87.3708 |

## DMI - 0 Deg - to the normal to the plane

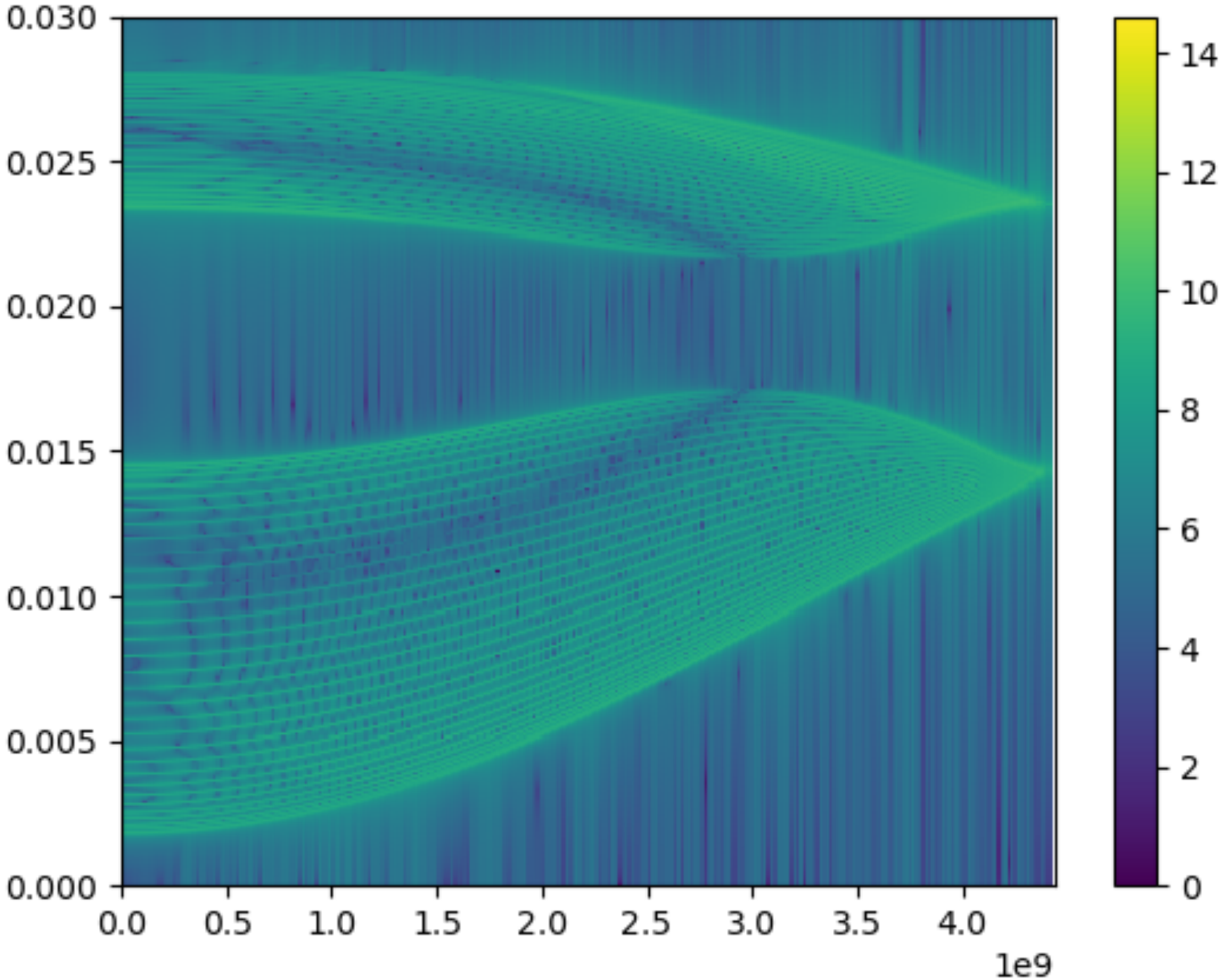
**DMI - 0 Deg** **Bext = 10T - 0 Deg** **Ssat = 0 Deg**



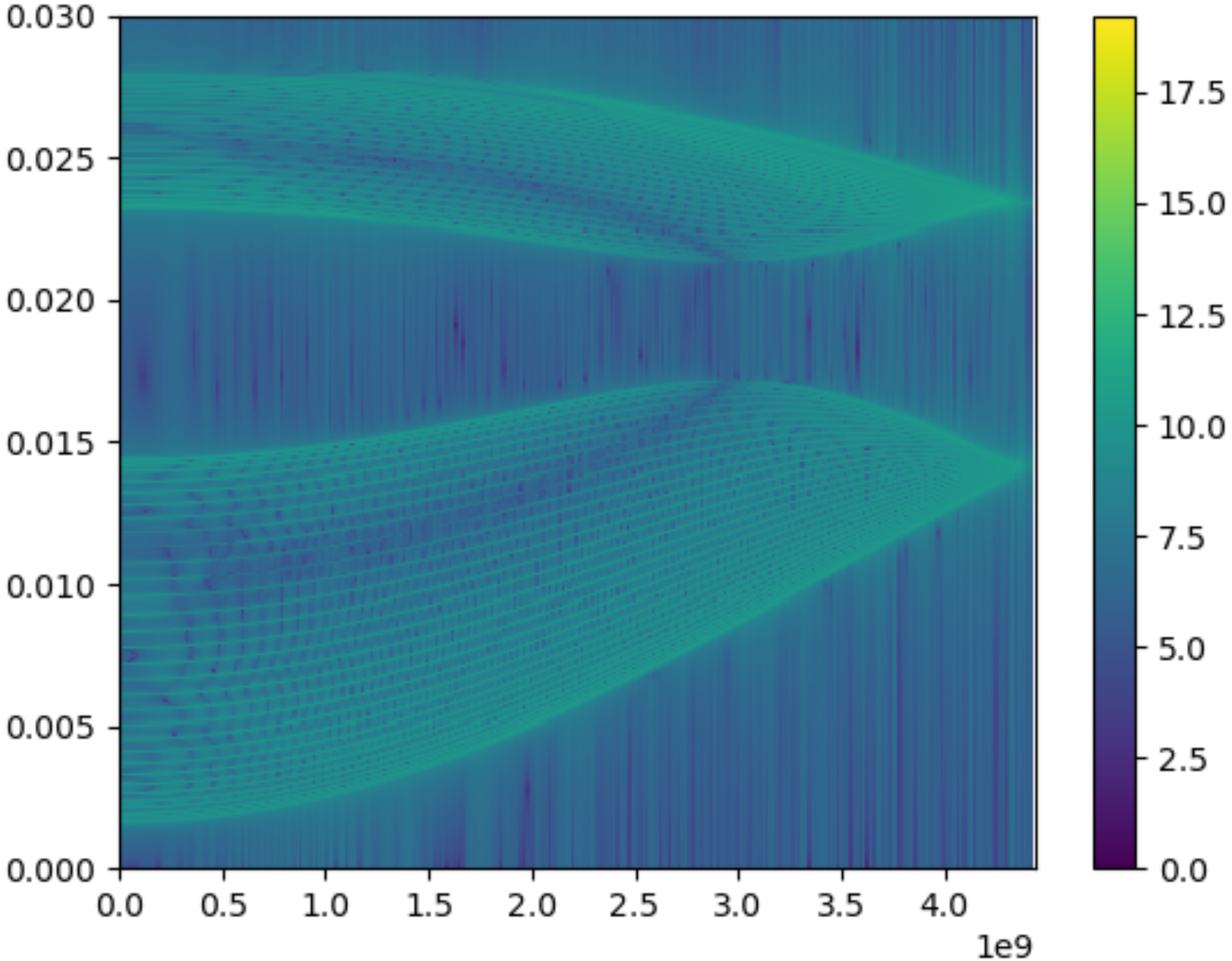
**DMI - 0 Deg** **Bext = 10T - 15 Deg** **Ssat = 9.31342 Deg**



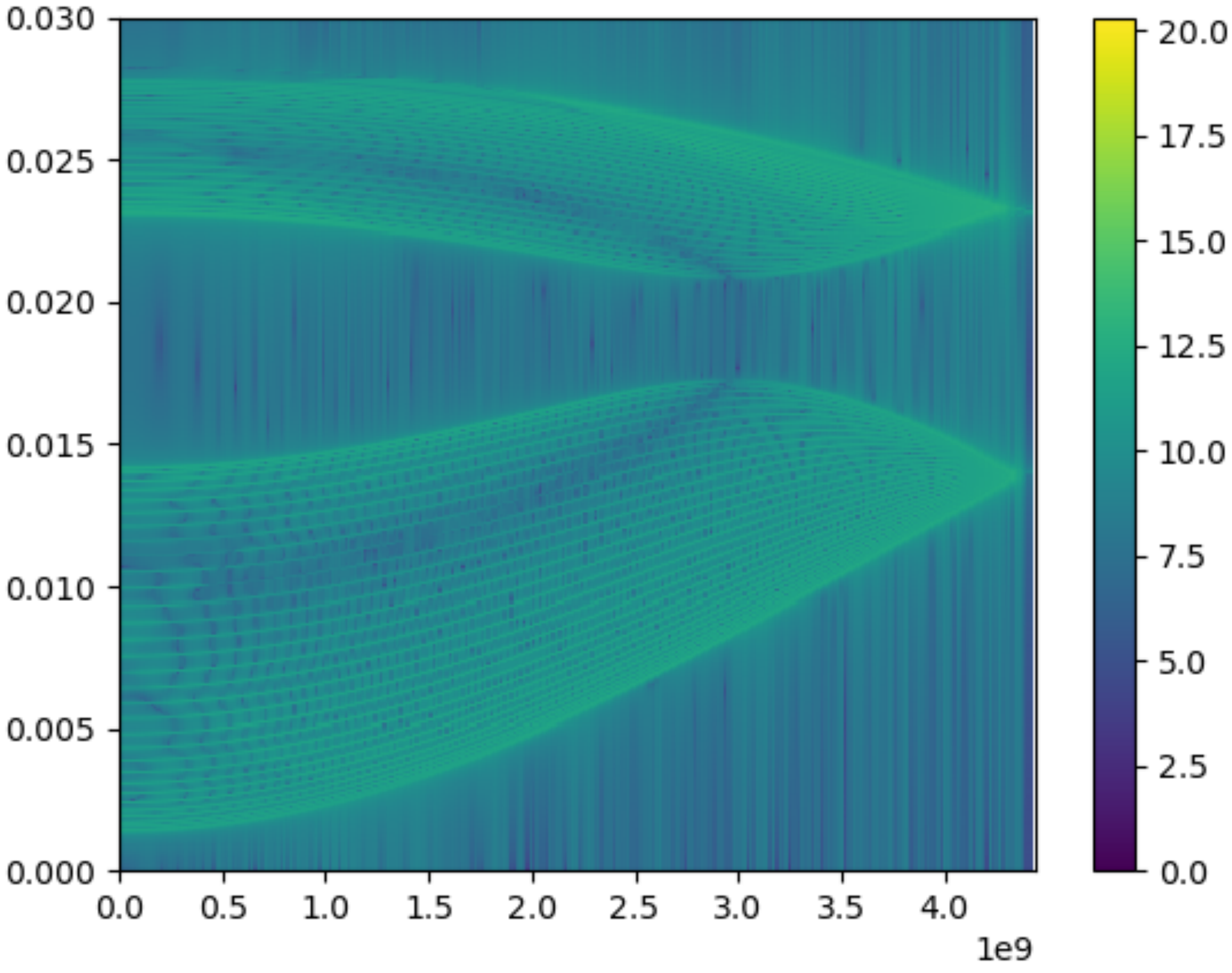
**DMI - 0 Deg** **Bext = 10T - 30 Deg** **Ssat = 18.9928 Deg**



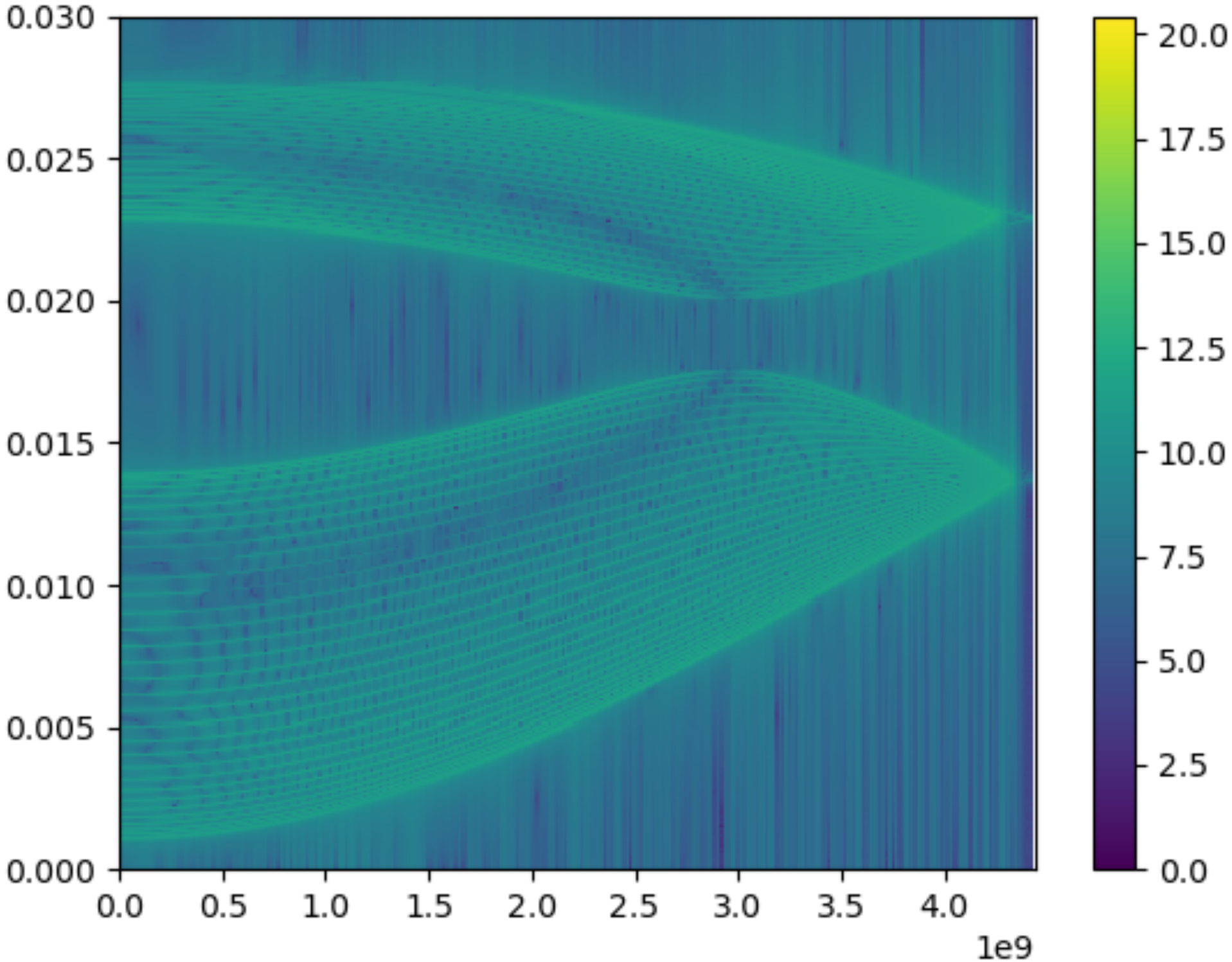
**DMI - 0 Deg** **Bext = 10T - 45 Deg** **Ssat = 29.5592 Deg**



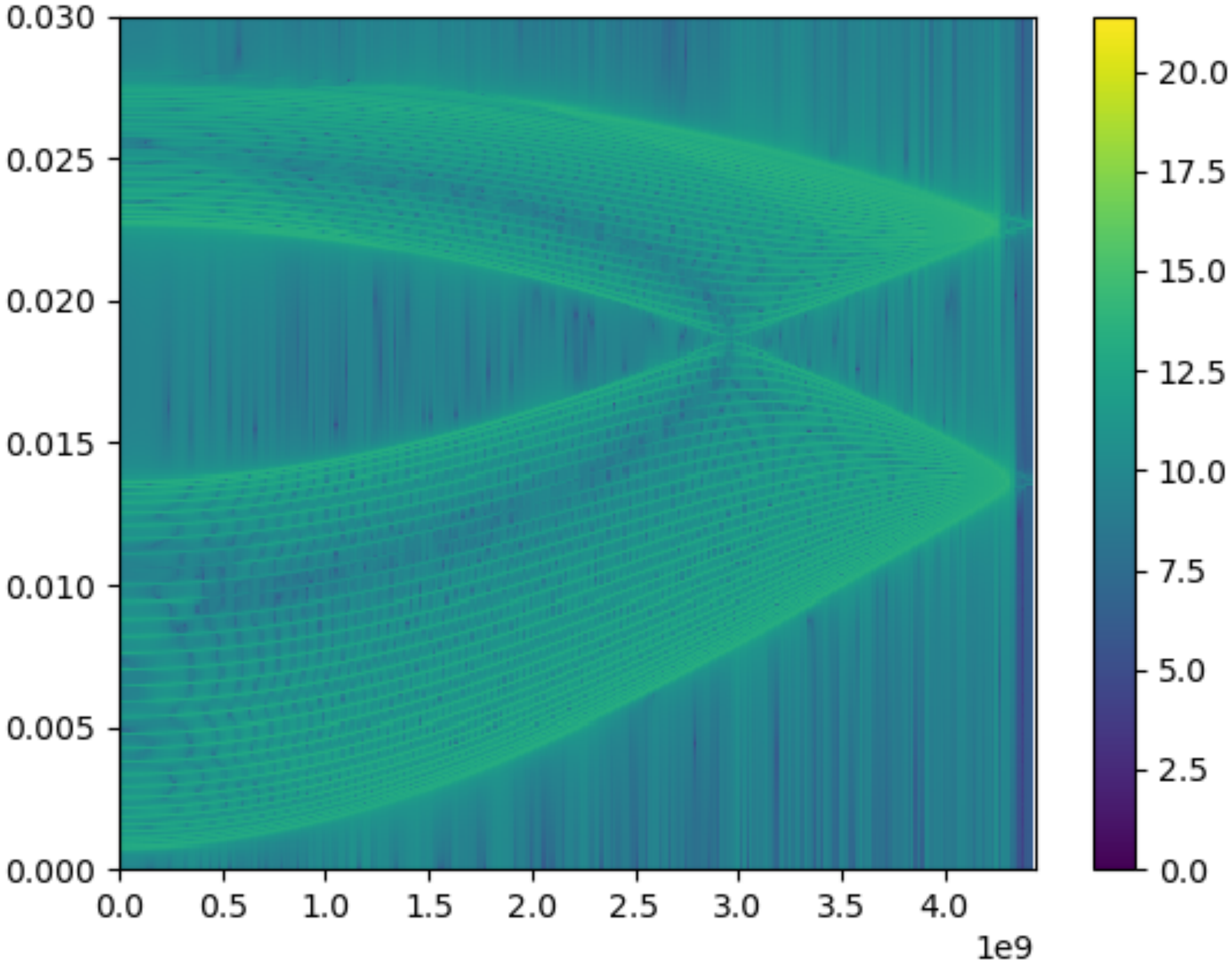
**DMI - 0 Deg** **Bext = 10T - 60 Deg** **Ssat = 42.0278 Deg**



**DMI - 0 Deg** **Bext = 10T - 75 Deg** **Ssat = 59.1479 Deg**



**DMI - 0 Deg** **Bext = 10T - 89 Deg** **Ssat = 87.371 Deg**



# External field 10T  DMI - 15 Deg

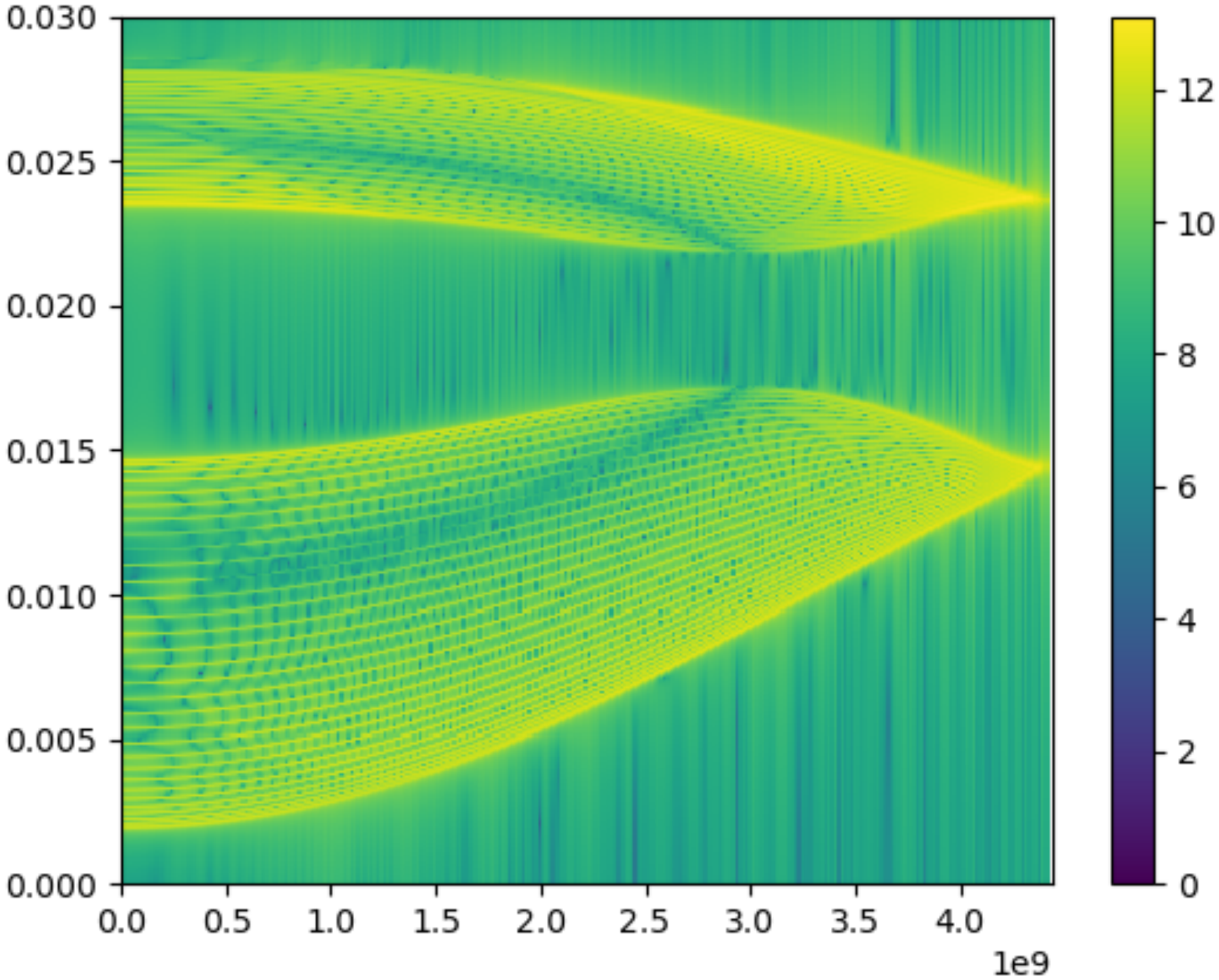
**J1+J2+J3+BQ+DMI**

**External field directions**

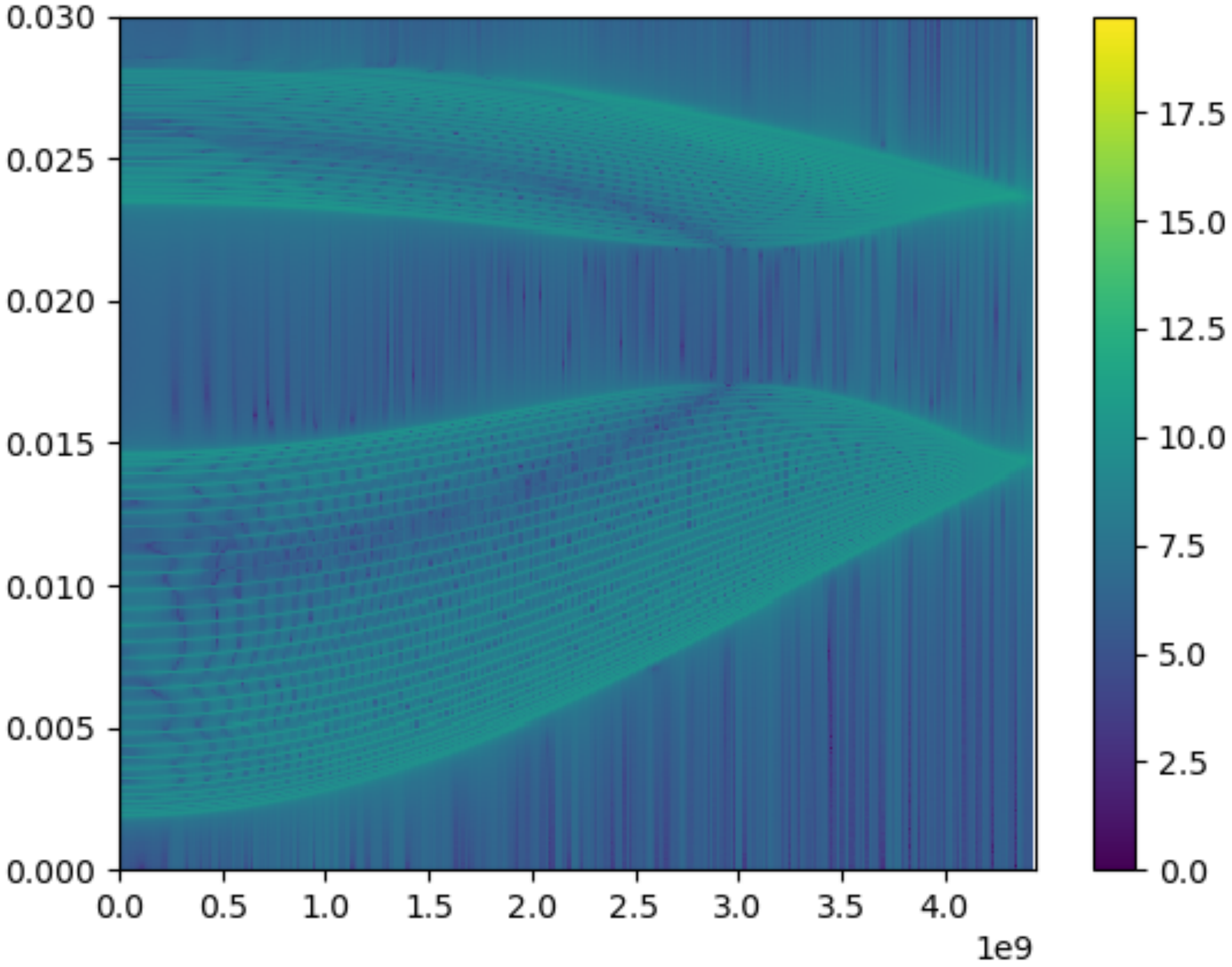
| $B_{ext}$ = 10T Angles | Saturation state |
|---|---|
| 0 | 0 |
| 15 | 9.31342 |
| 30 | 18.9928 |
| 45 | 29.5592 |
| 60 | 42.0278 |
| 75 | 59.1479 |
| 89 | 87.3708 |

## DMI - 15 Deg - to the normal to the plane

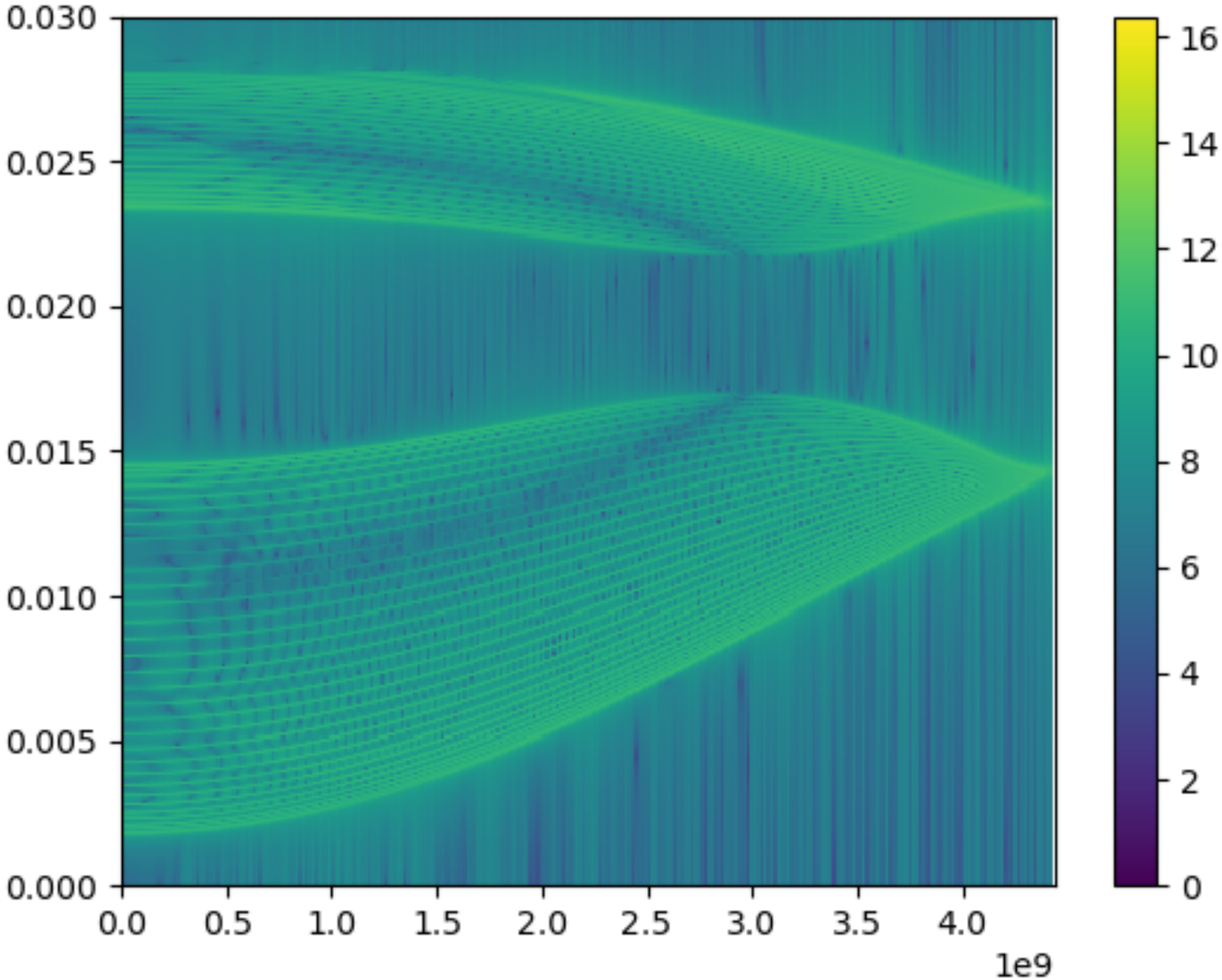
**DMI - 15 Deg** **Bext = 10T - 0 Deg** **Ssat = 9.31342 Deg**



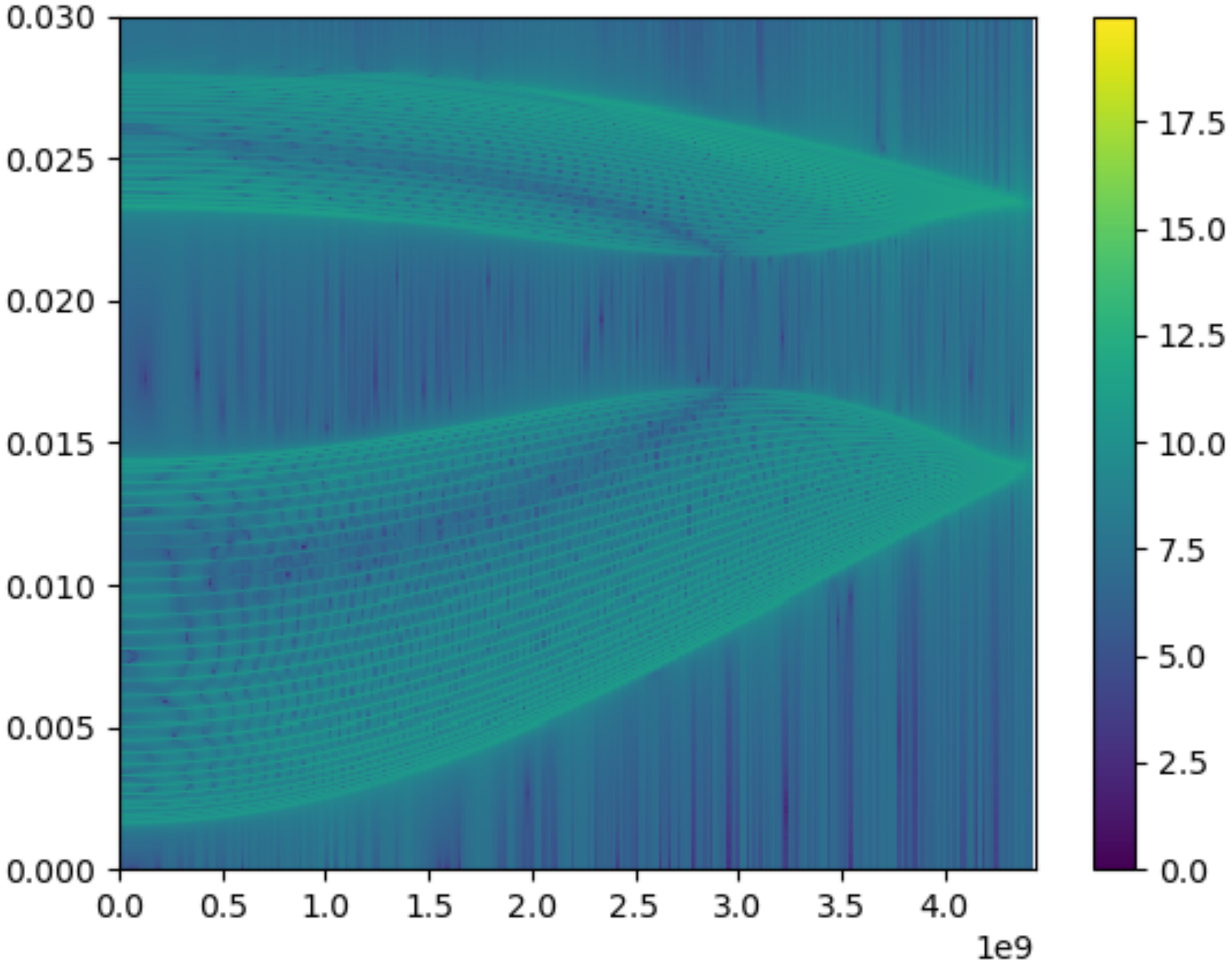
**DMI - 15 Deg** **Bext = 10T - 15 Deg** **Ssat = 9.31342 Deg**



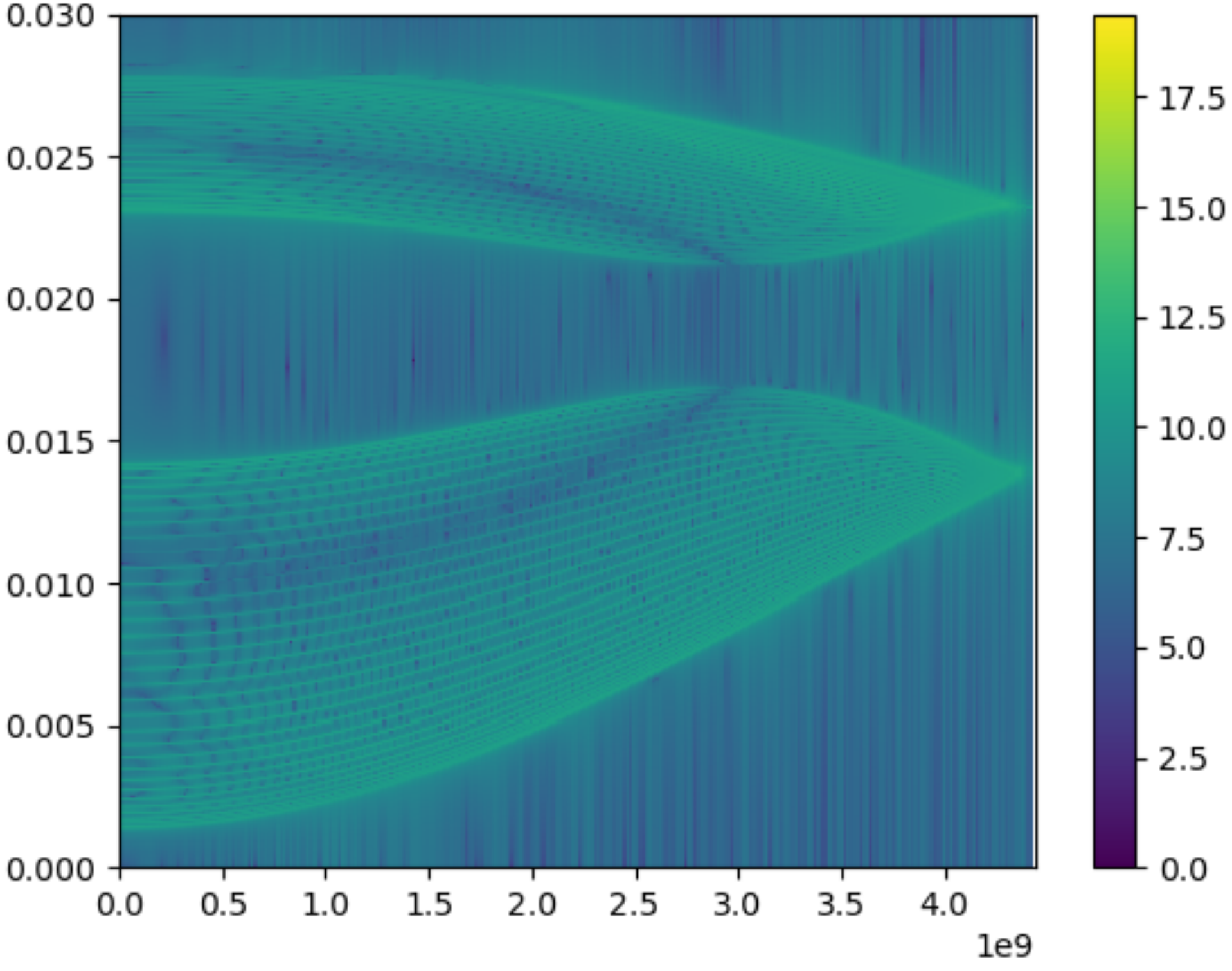
**DMI - 15 Deg** **Bext = 10T - 30 Deg** **Ssat = 18.9928 Deg**



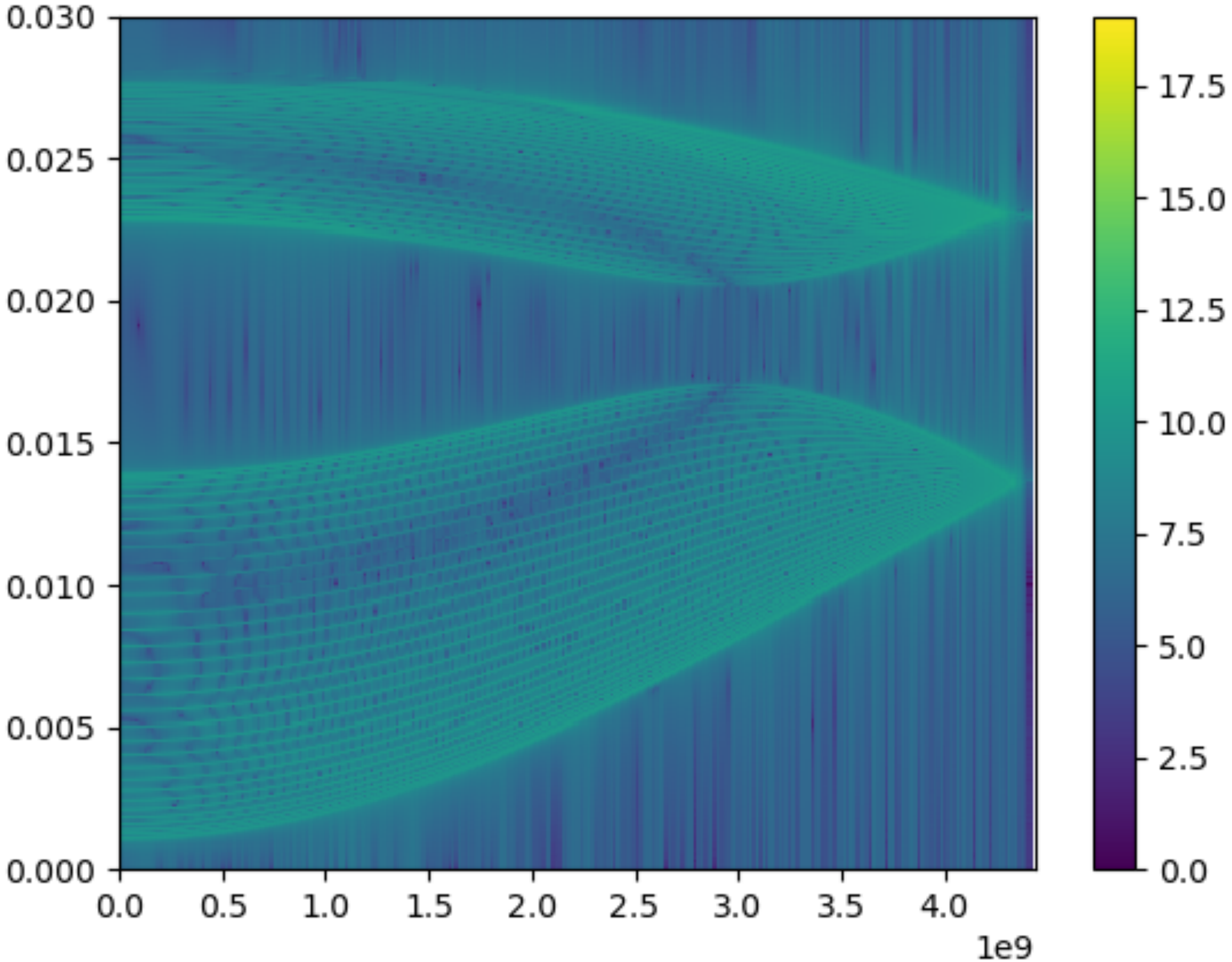
**DMI - 15 Deg** **Bext = 10T - 45 Deg** **Ssat = 29.5592 Deg**



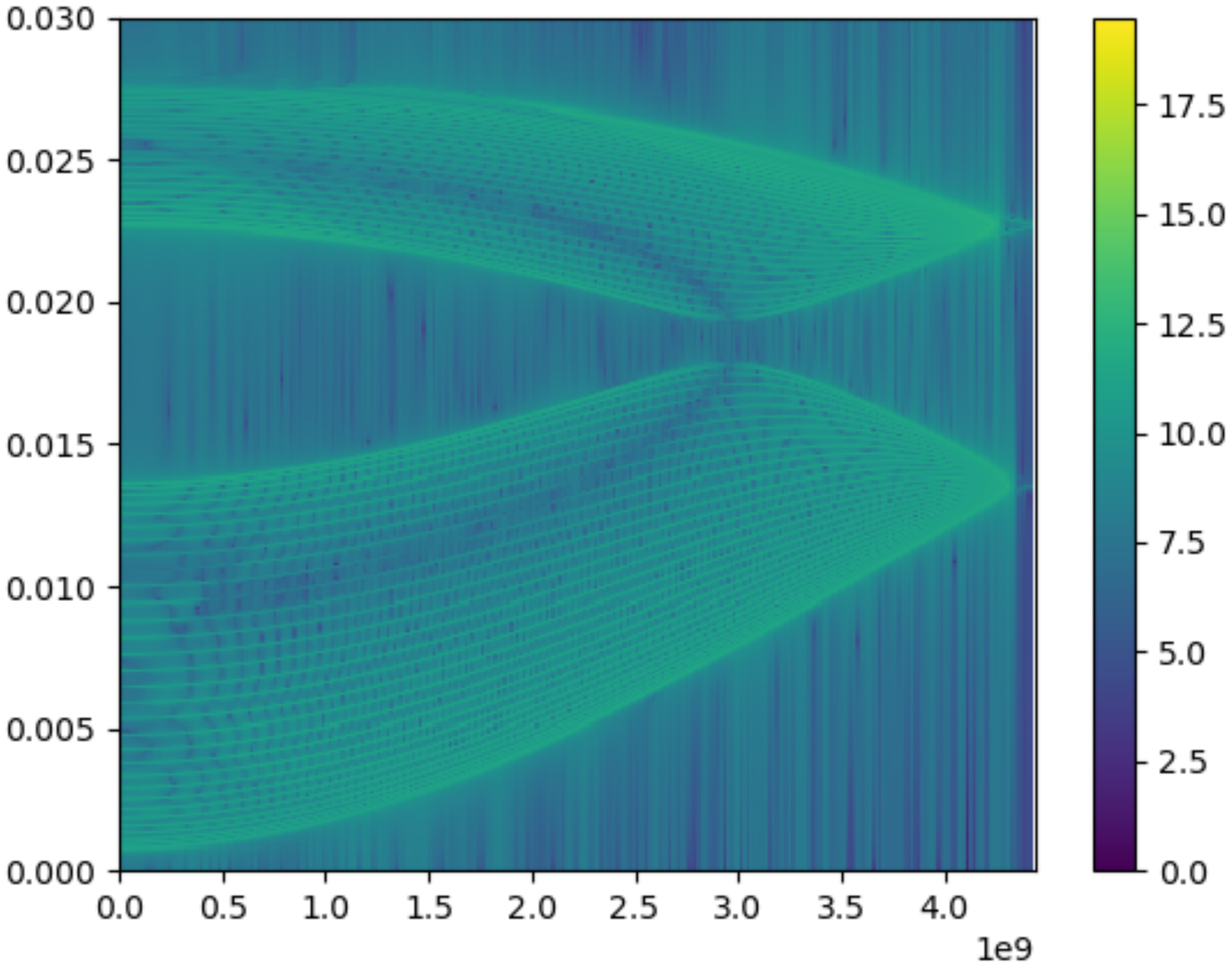
**DMI - 15 Deg** **Bext = 10T - 60 Deg** **Ssat = 42.0278 Deg**



**DMI - 15 Deg** **Bext = 10T - 75 Deg** **Ssat = 59.1479 Deg**



**DMI - 15 Deg** **Bext = 10T - 89 Deg** **Ssat = 87.371 Deg**



# Tilted DMI

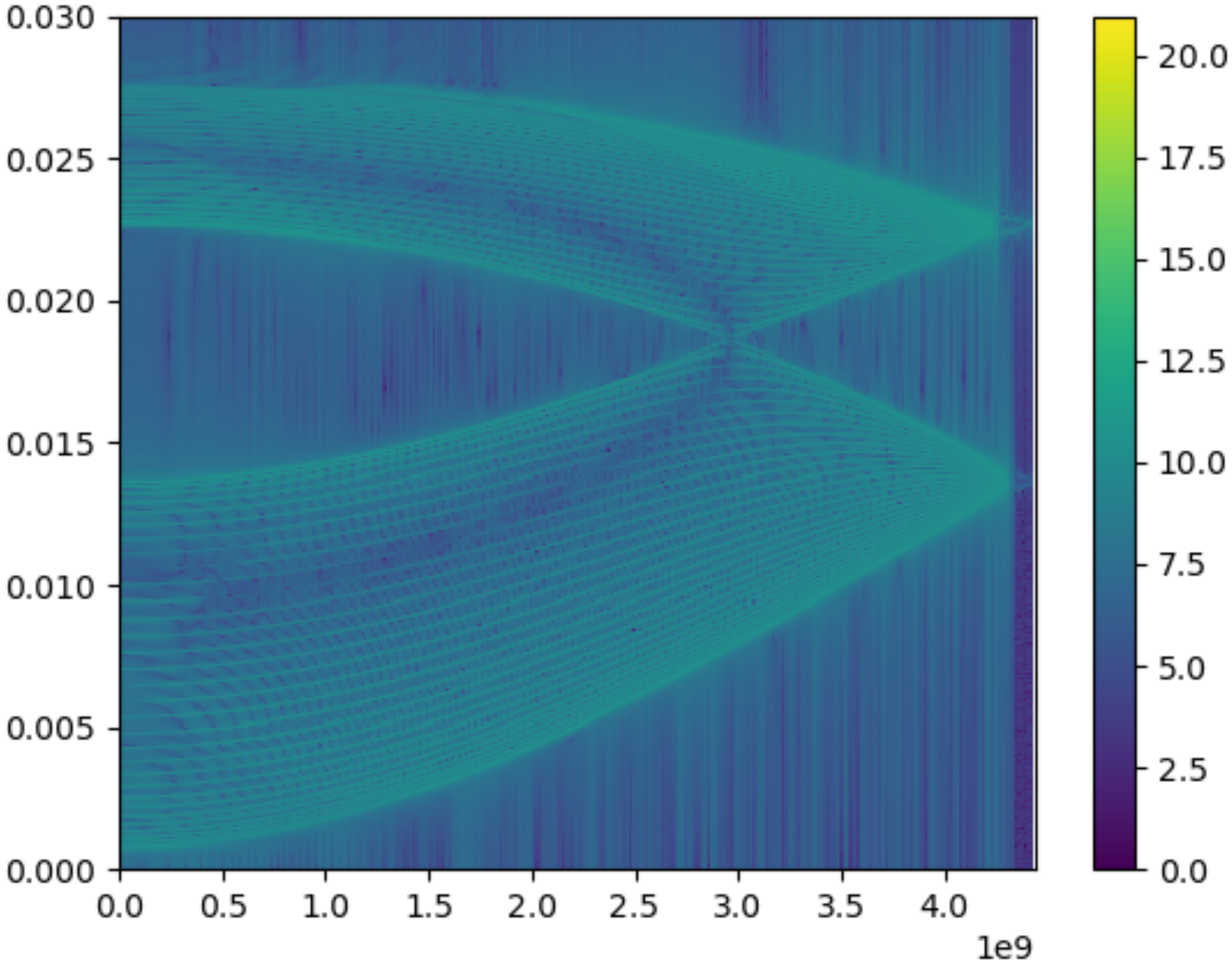
**J1+J2+J3+BQ+DMI**

## External field

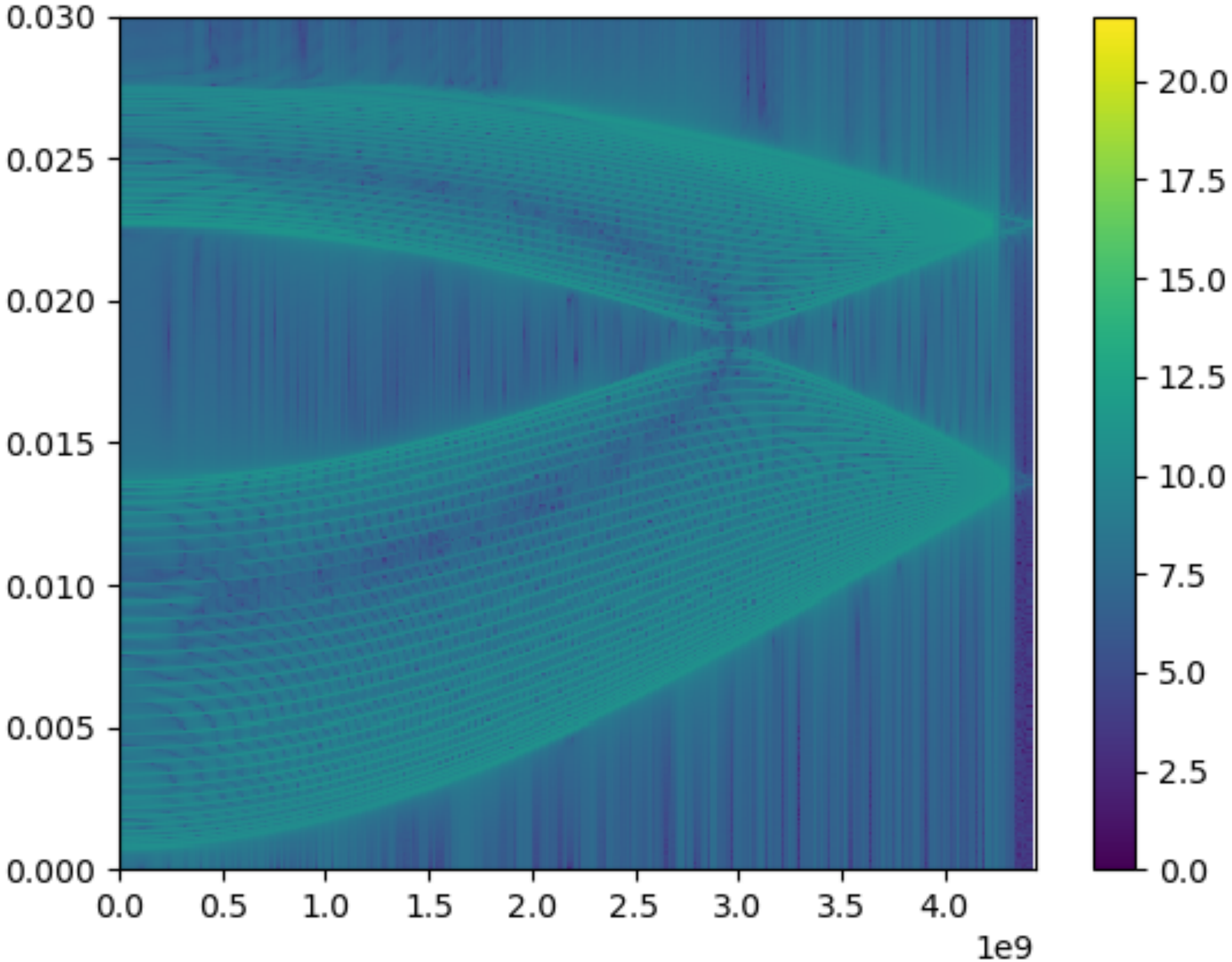
**$B_{ext}$ = 10T  Angle=89 Deg**

**DMI Angles= 0, 5, 10, 15, 30, 45, 60,75,90 Deg  - (X,Z) plane**

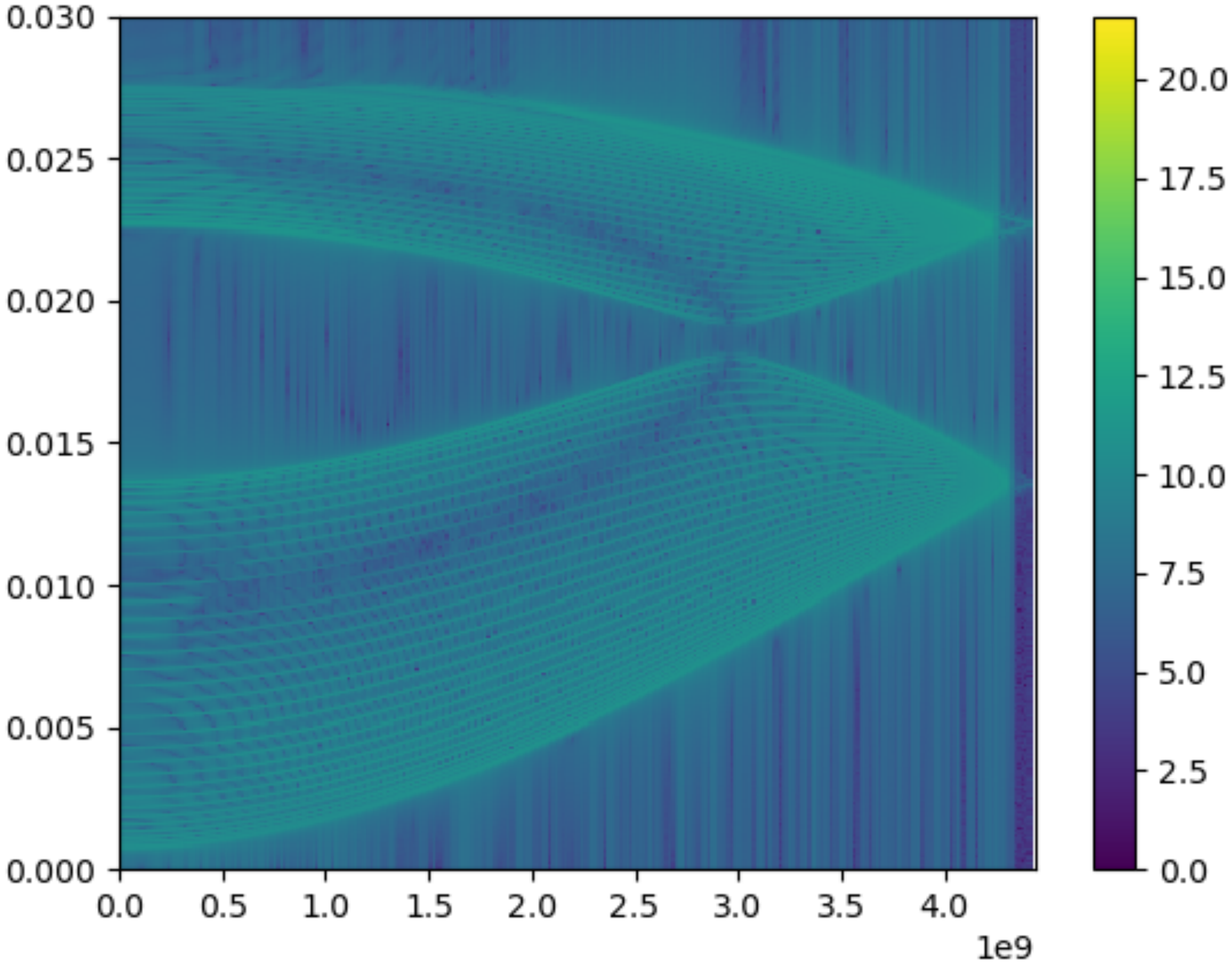
**DMI = 0 Deg** **Bext = 10T - 89 Deg** **Ssat = 87.371 Deg**



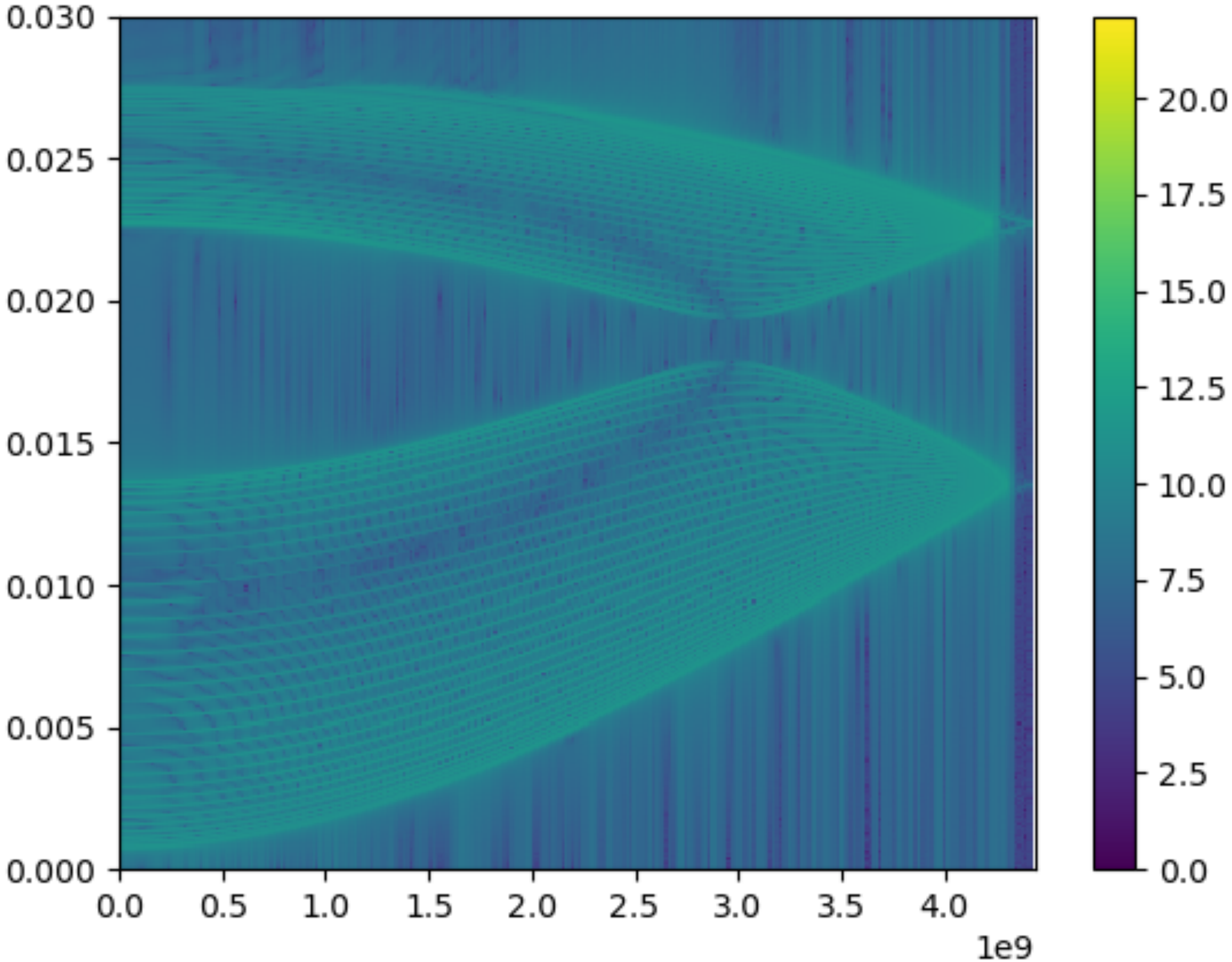
**DMI = 5 Deg** **Bext = 10T - 89 Deg** **Ssat = 87.371 Deg**



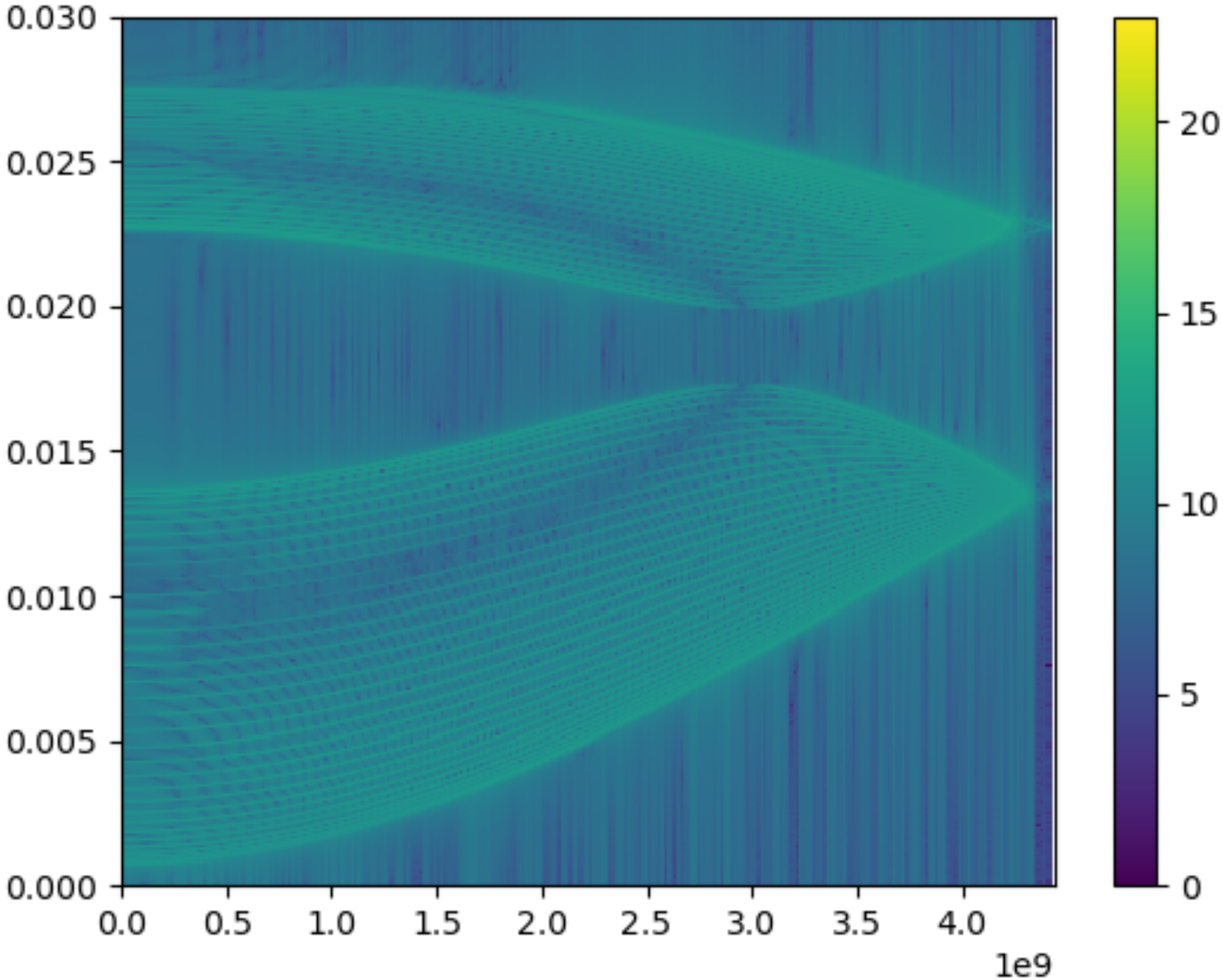
**DMI = 10 Deg** **Bext = 10T - 89 Deg** **Ssat = 87.371 Deg**



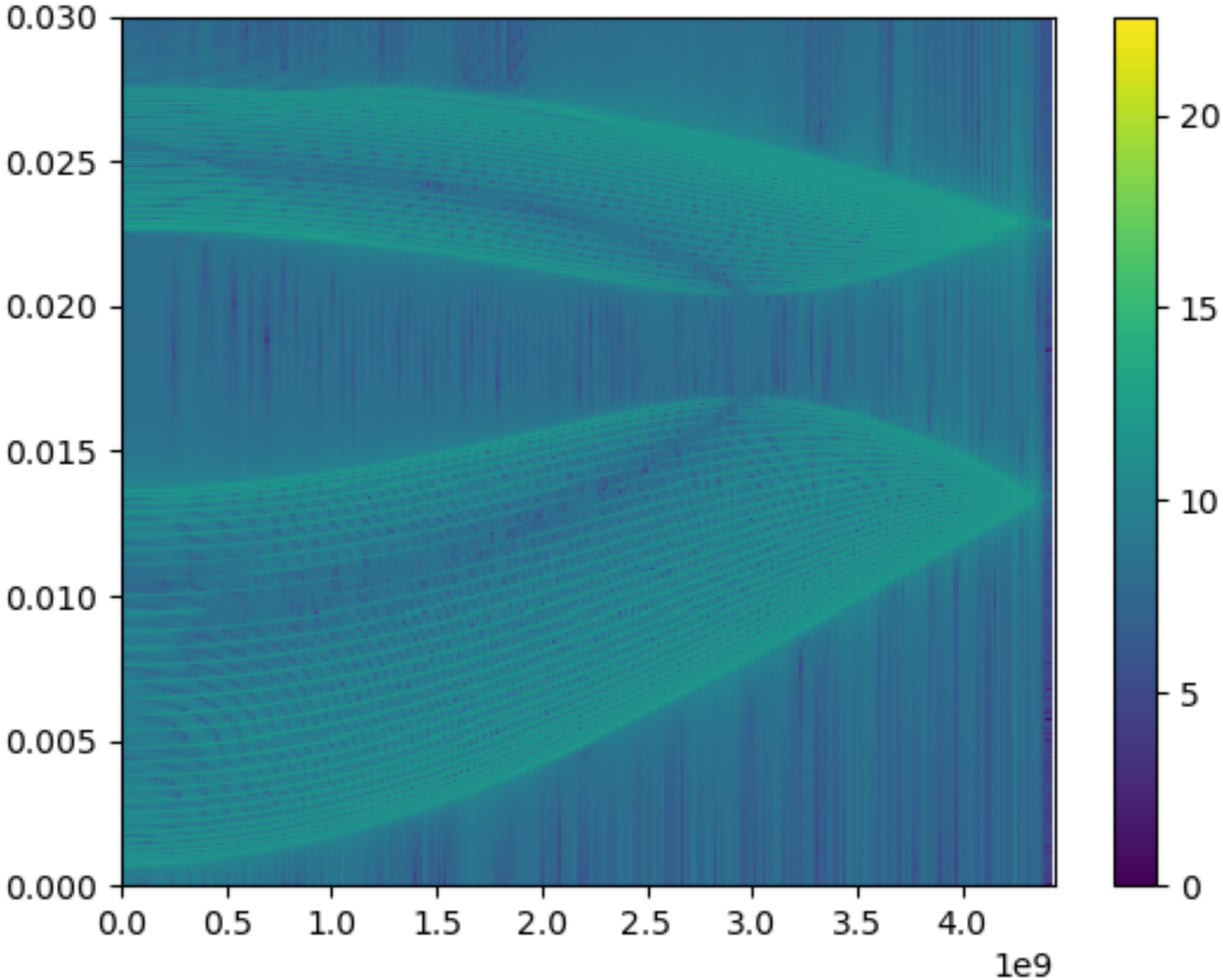
**DMI = 15 Deg** **Bext = 10T - 89 Deg** **Ssat = 87.371 Deg**



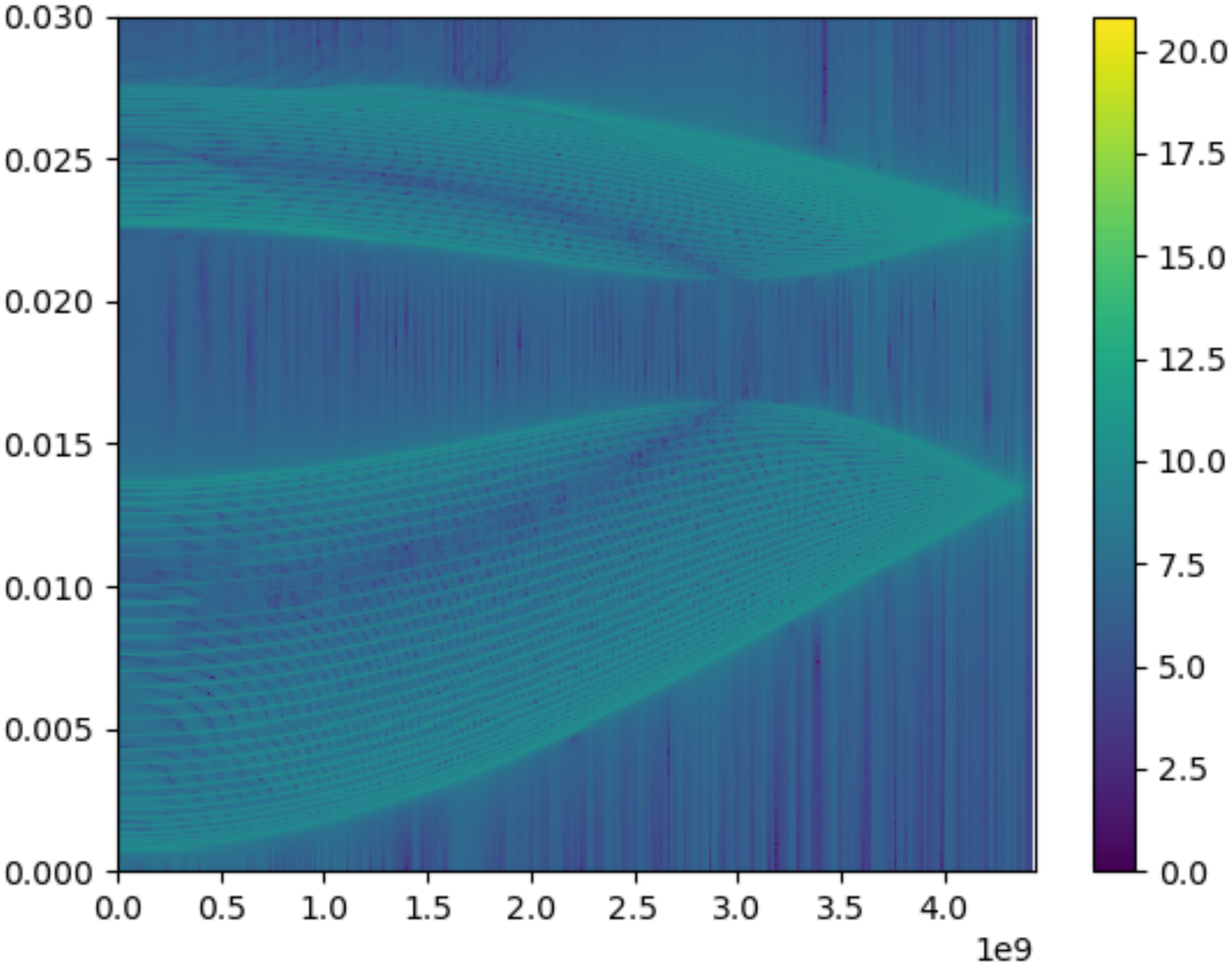
**DMI = 30 Deg** **Bext = 10T - 89 Deg** **Ssat = 87.371 Deg**



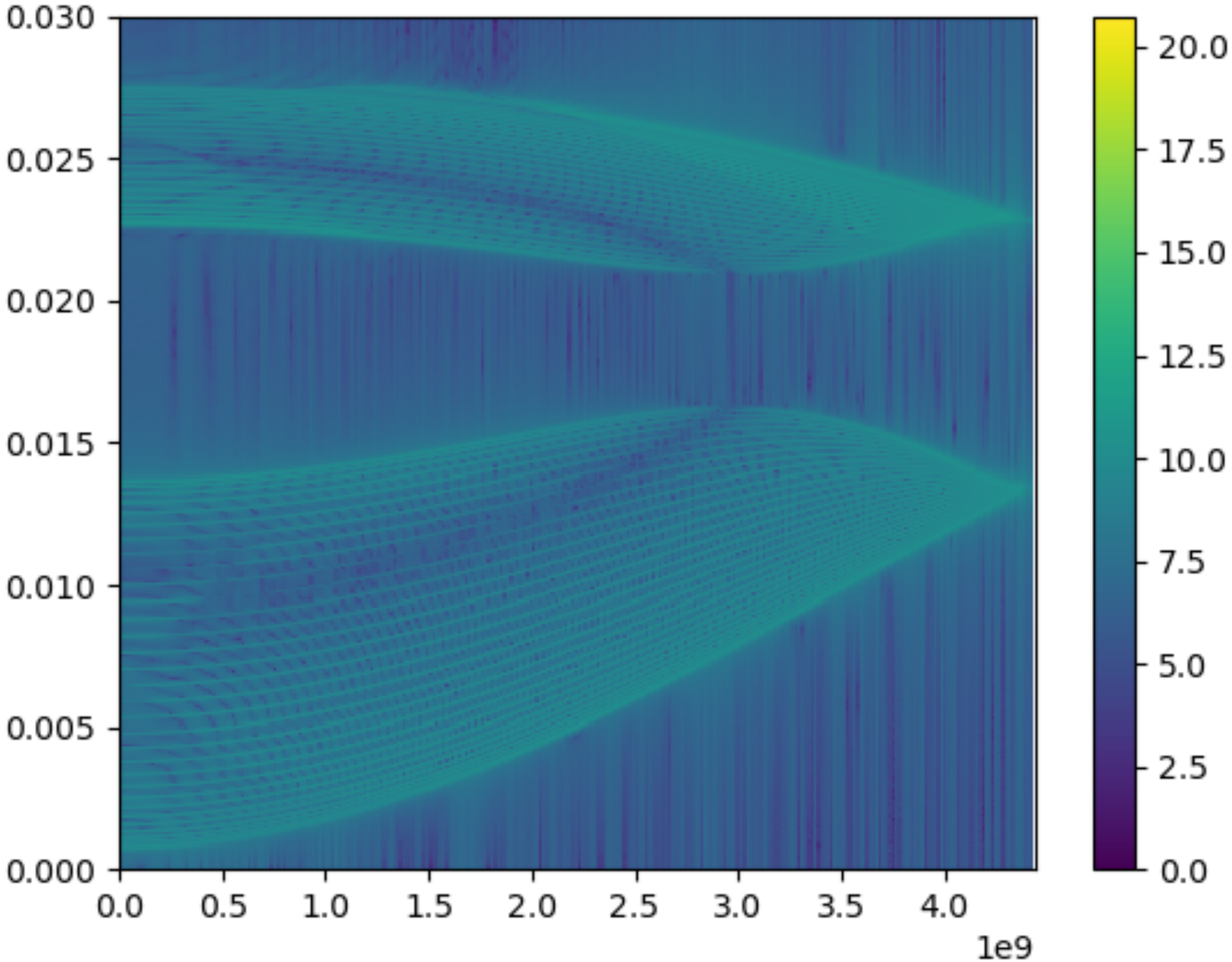
**DMI = 45 Deg** **Bext = 10T - 89 Deg** **Ssat = 87.371 Deg**



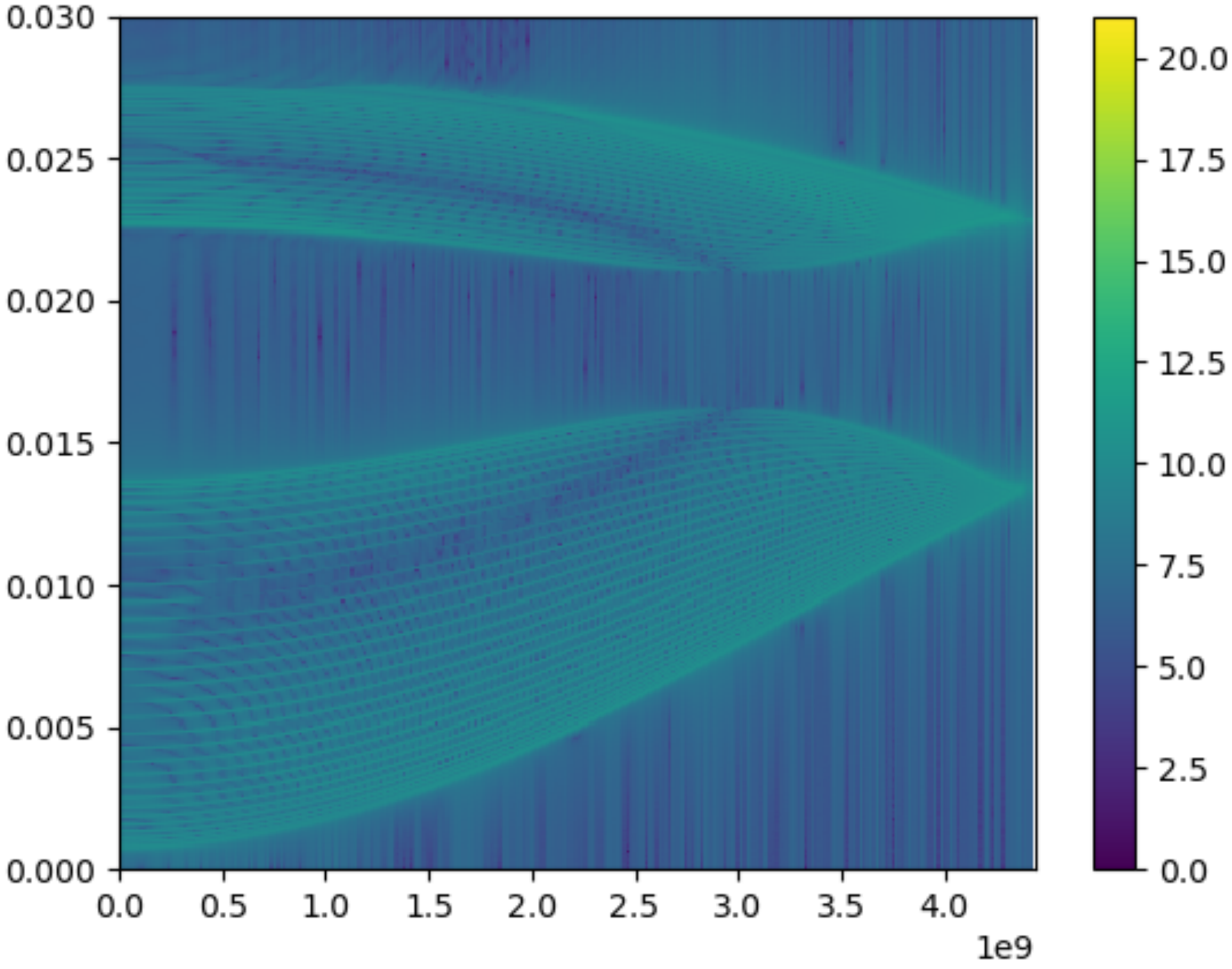
**DMI = 60 Deg** **Bext = 10T - 89 Deg** **Ssat = 87.371 Deg**



**DMI = 75 Deg** **Bext = 10T - 89 Deg** **Ssat = 87.371 Deg**



**DMI = 90 Deg** **Bext = 10T - 89 Deg** **Ssat = 87.371 Deg**



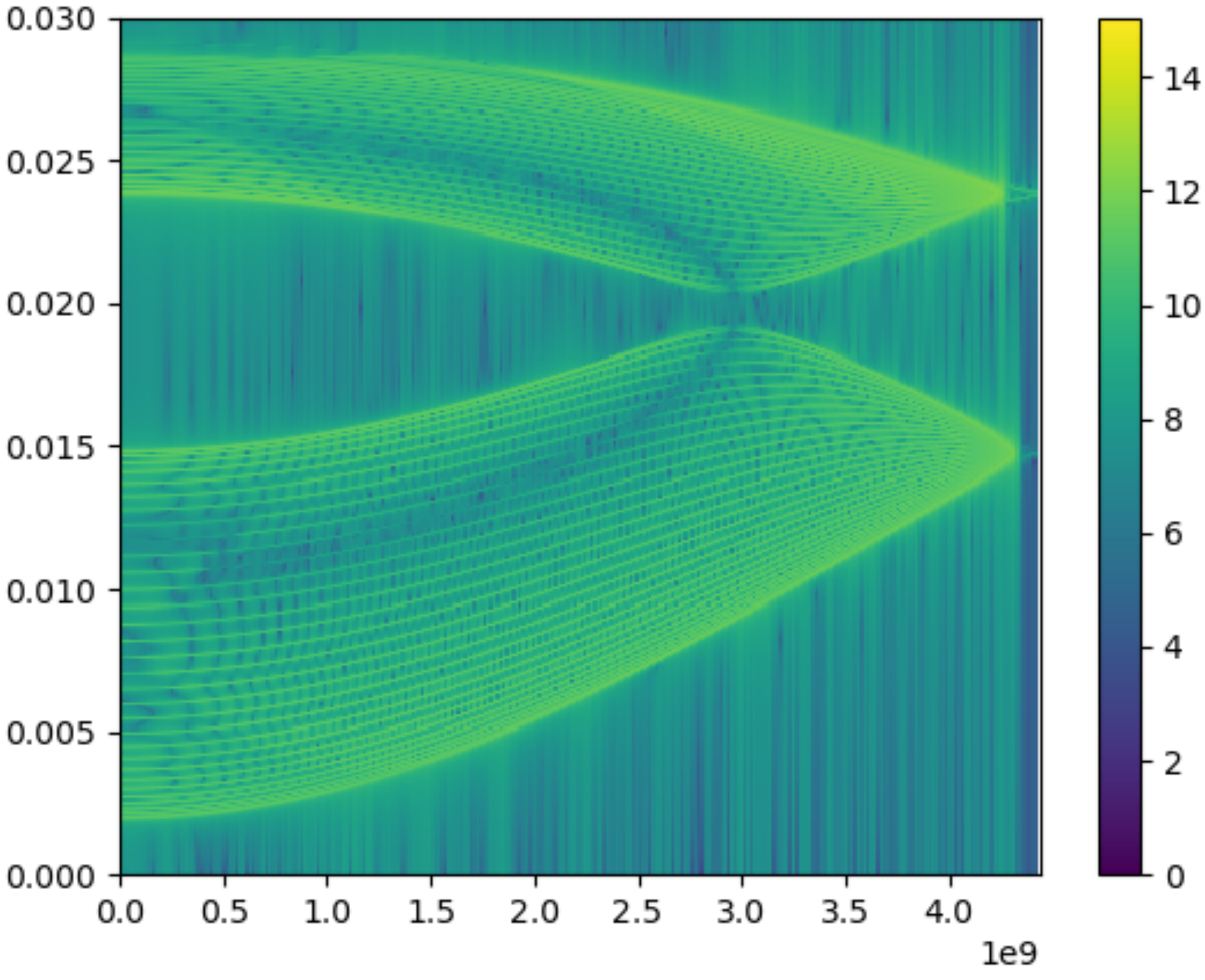
# Tilted DMI

**J1+J2+J3+BQ+DMI**

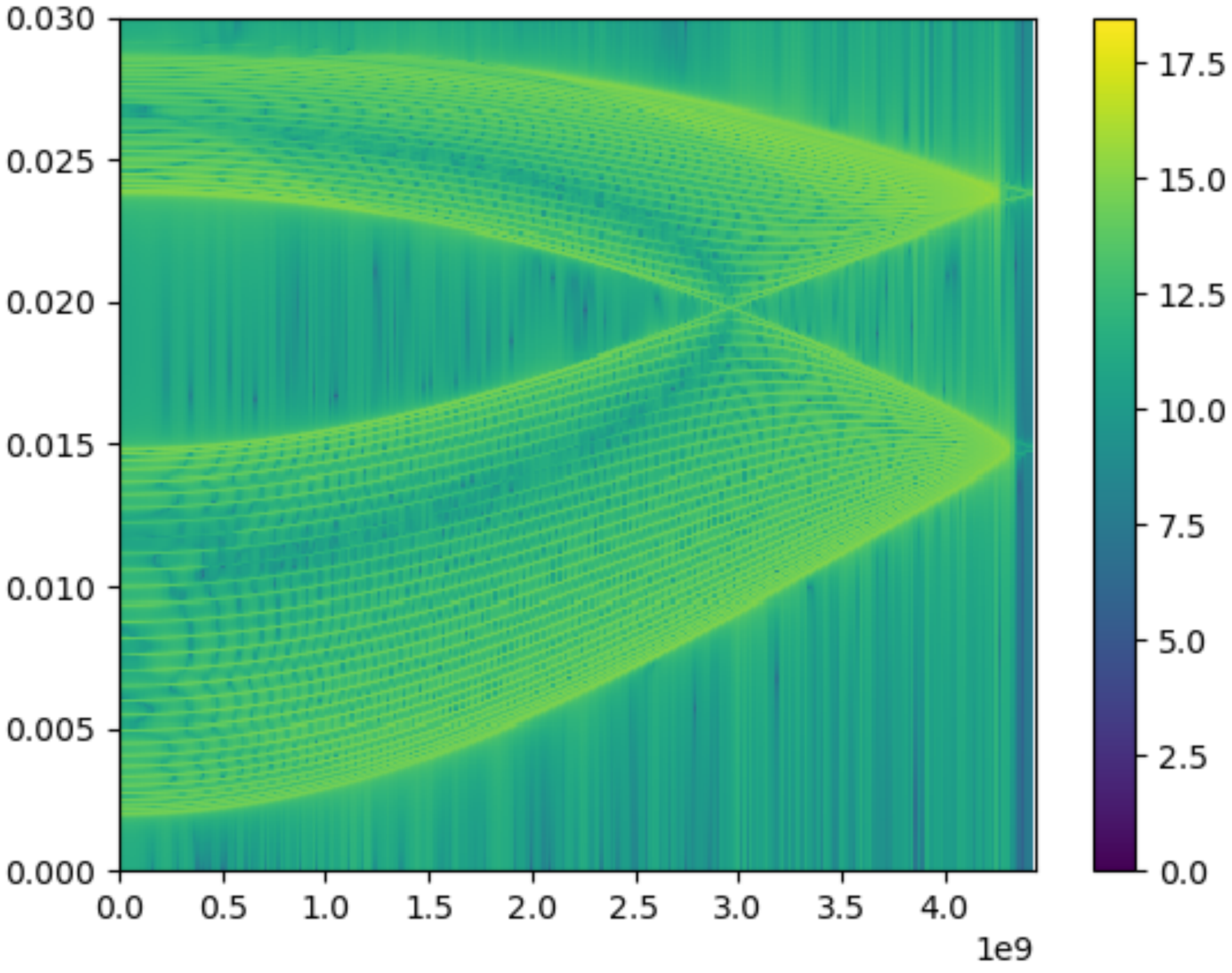
## Short conclusions:

- **tilting of DMI direction changes the gap value at P (K)- point**
- **branches at Gamma-point does not change**

**DMI = 15 Deg (Y,Z)- plane** **Bext = 20T - 89.9 Deg (Y,Z)- plane** **Ssat = 89.855 Deg**

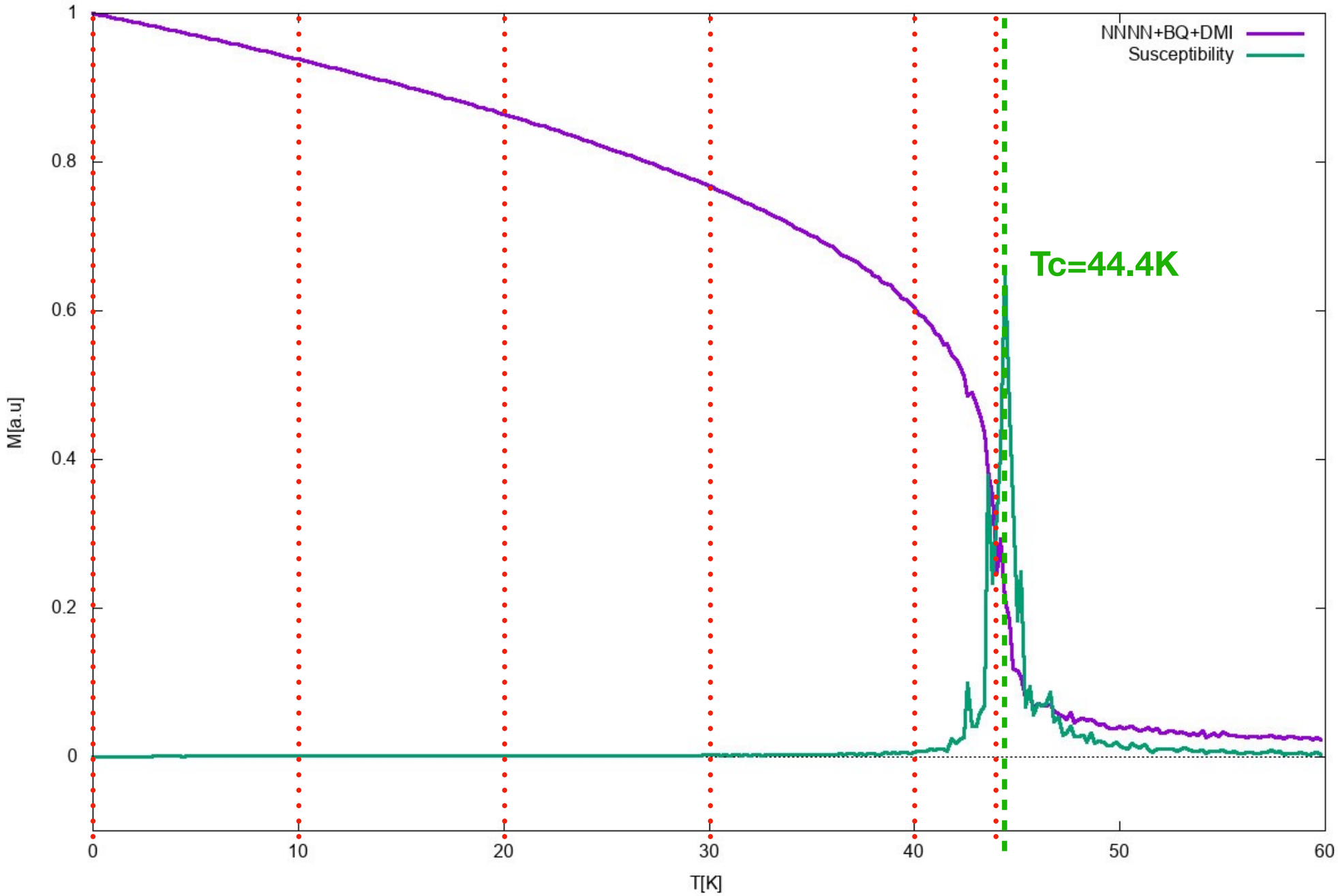


**DMI = 15 Deg (X,Z)- plane** **Bext = 20T - 89.9 Deg (Y,Z)- plane** **Ssat = 89.855 Deg**



# Temperature

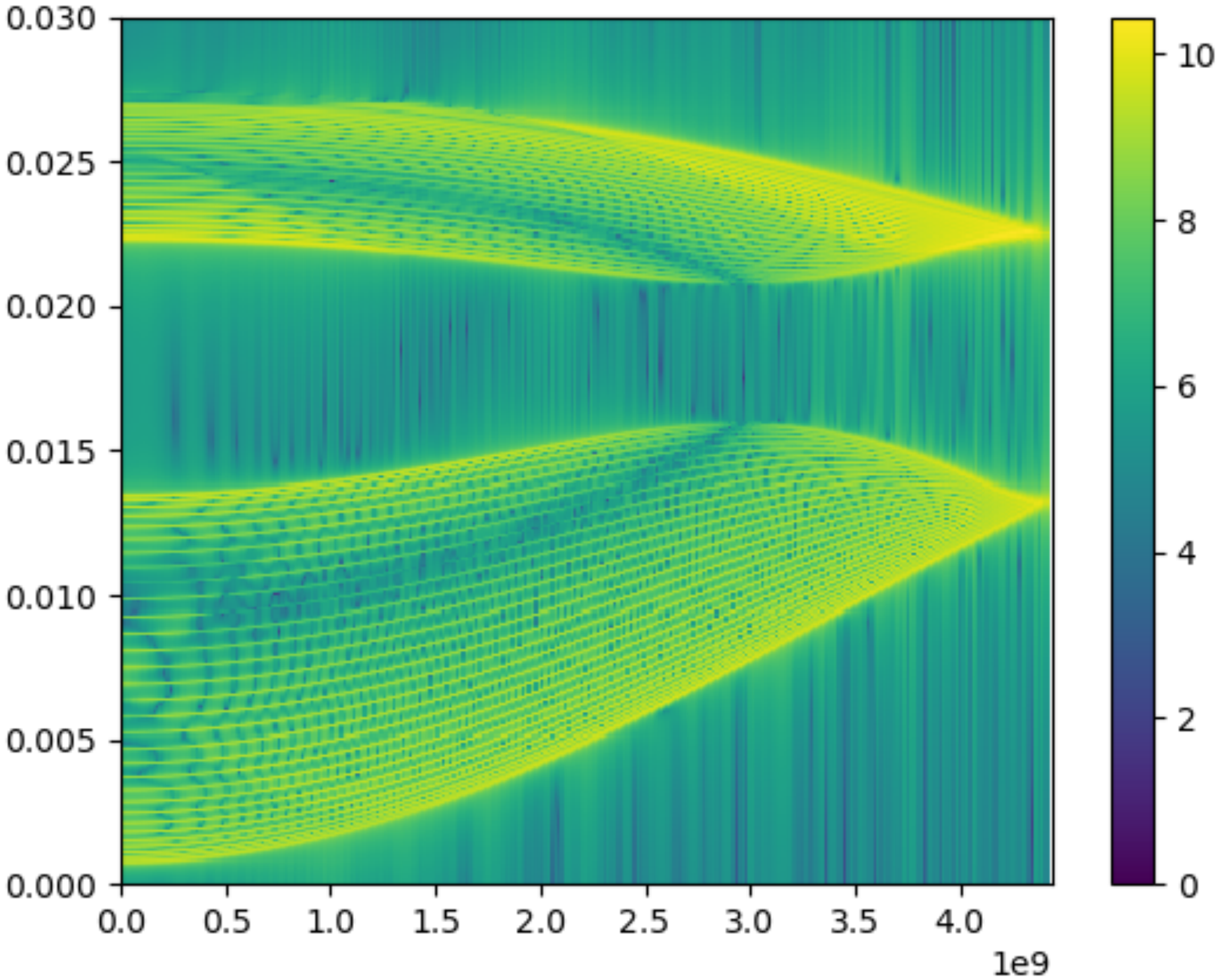
## J1+J2+J3+BQ+DMI



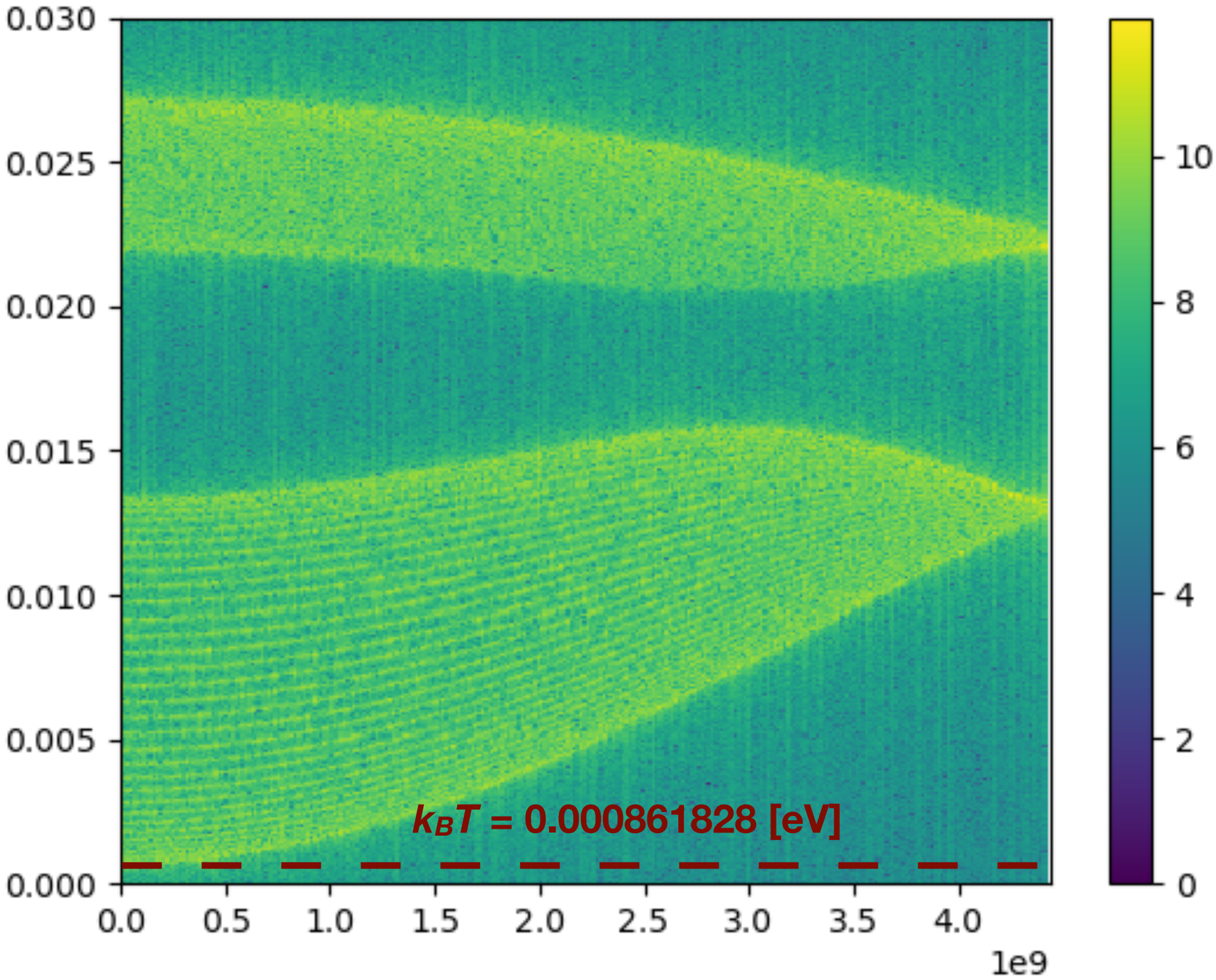

**T= 0K, 10K, 20K, 30K, 40K, 44K**

**Tc=44.4K**

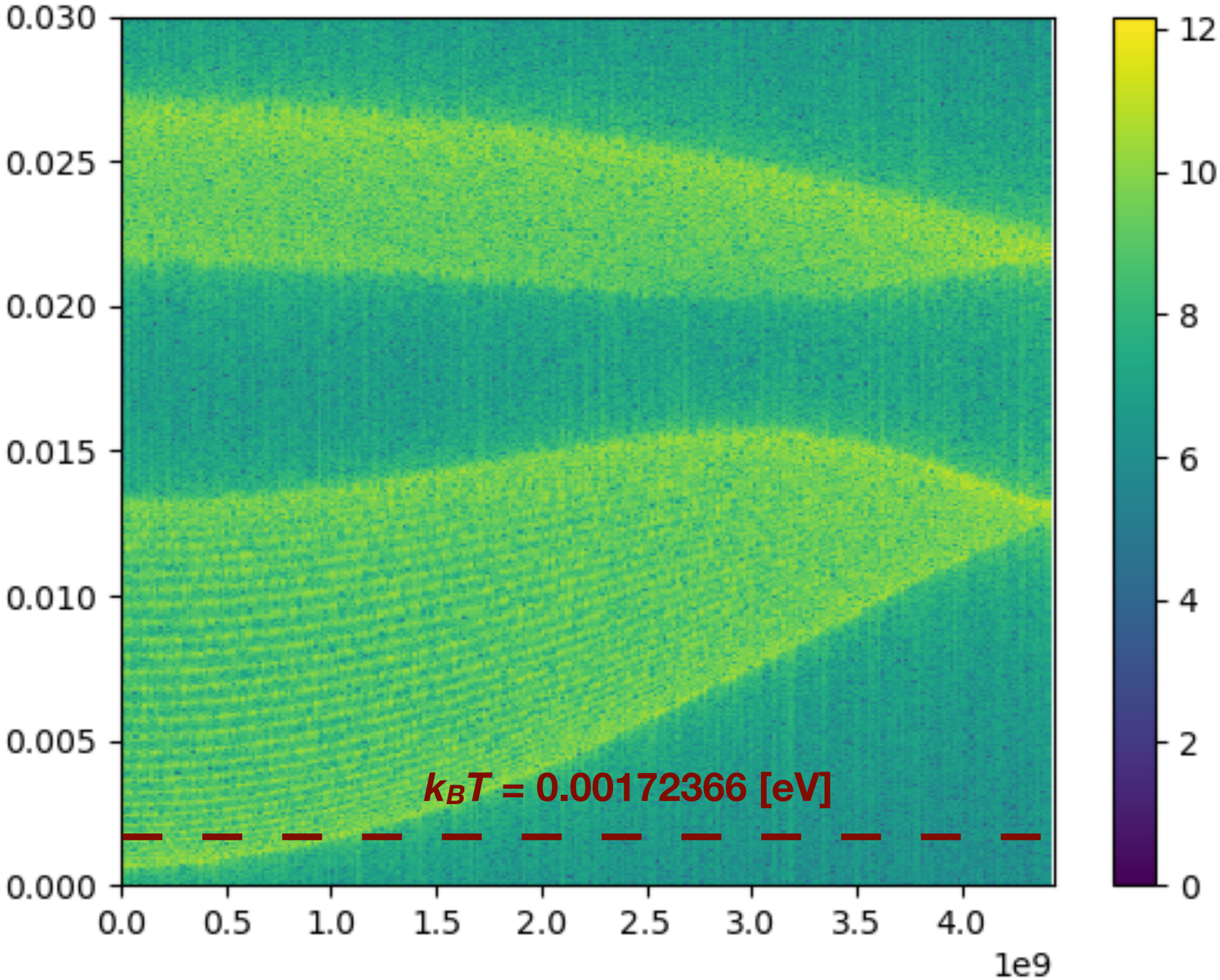
# Temperature 0K



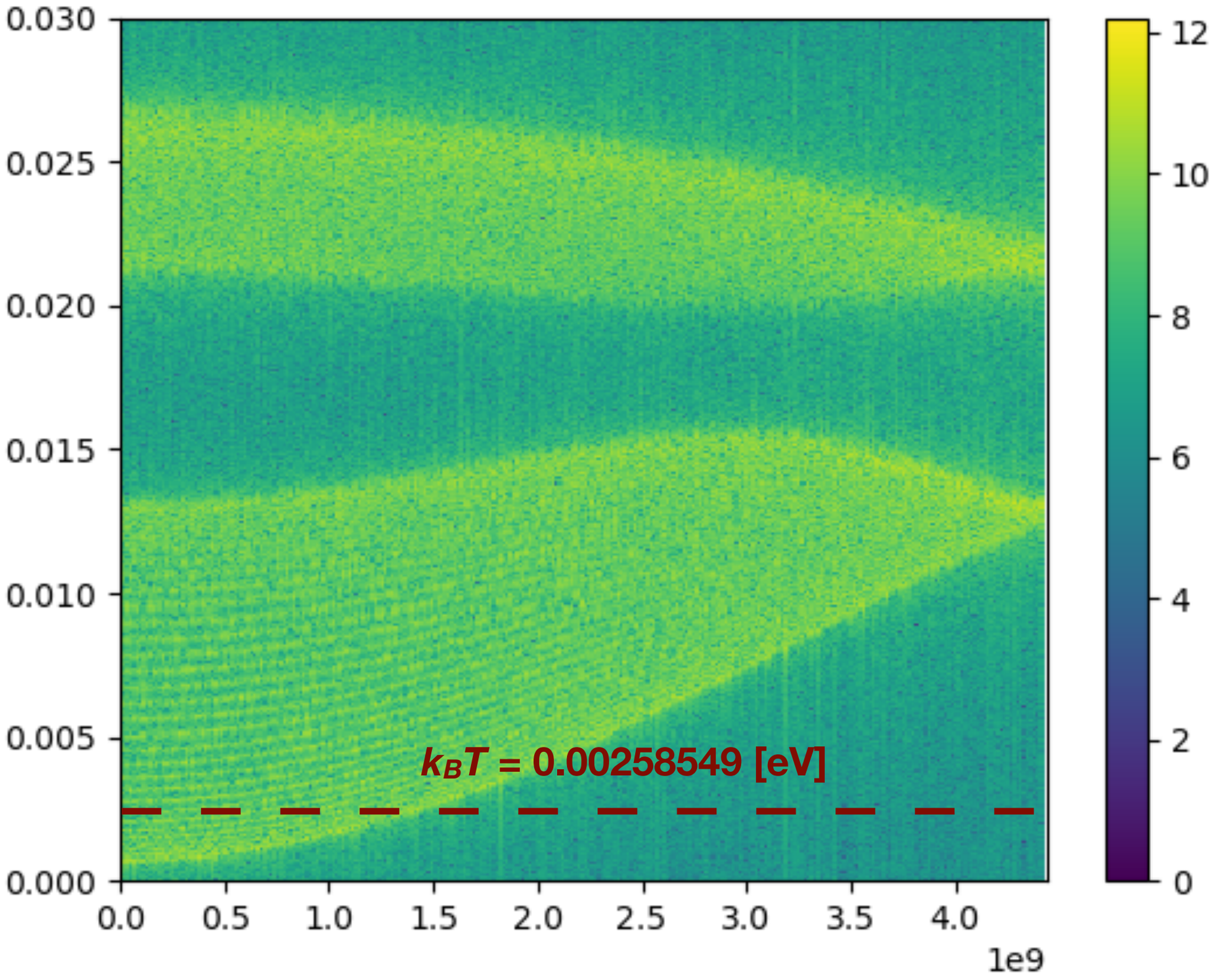
# Temperature 10K



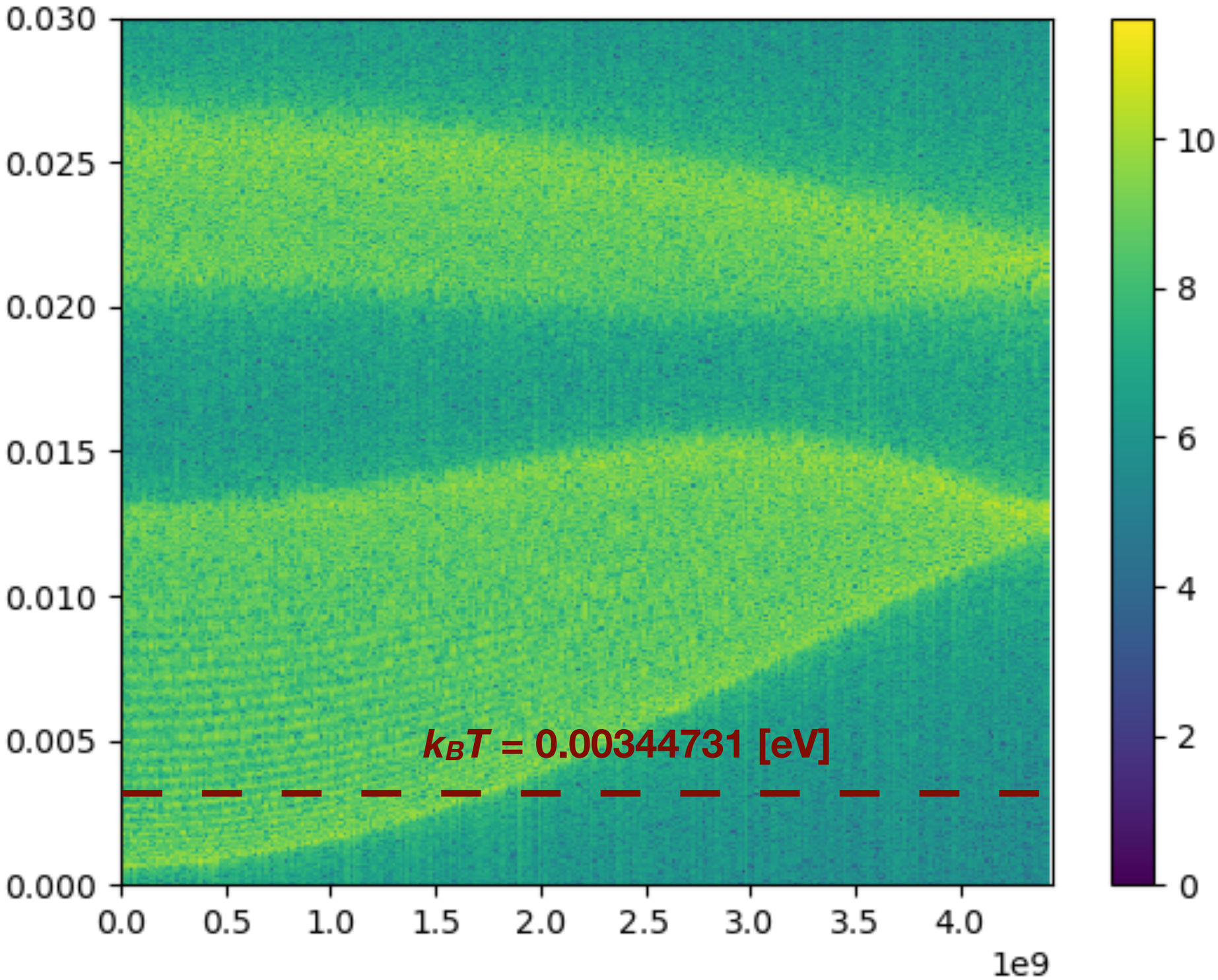
# Temperature 20K



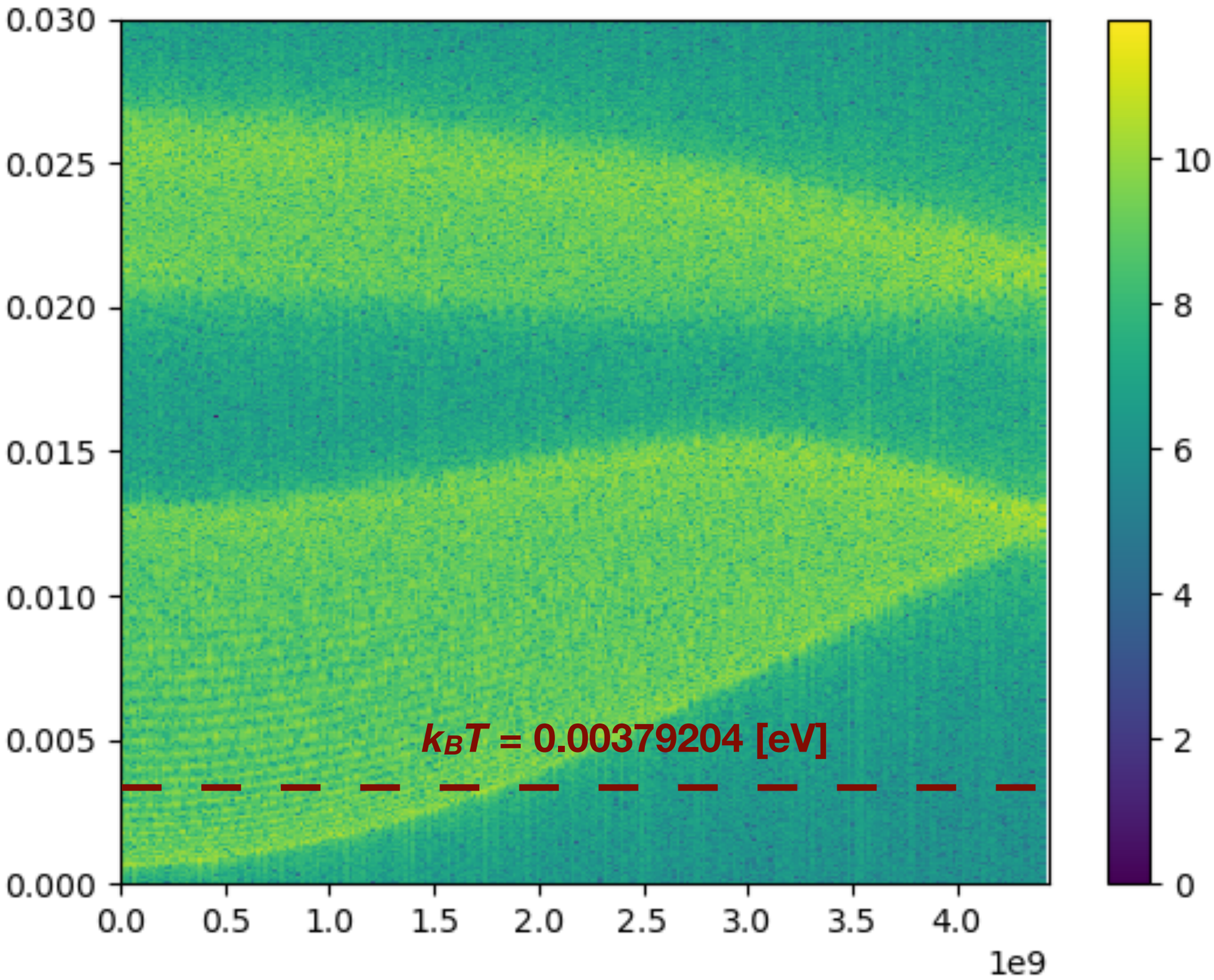
# Temperature 30K



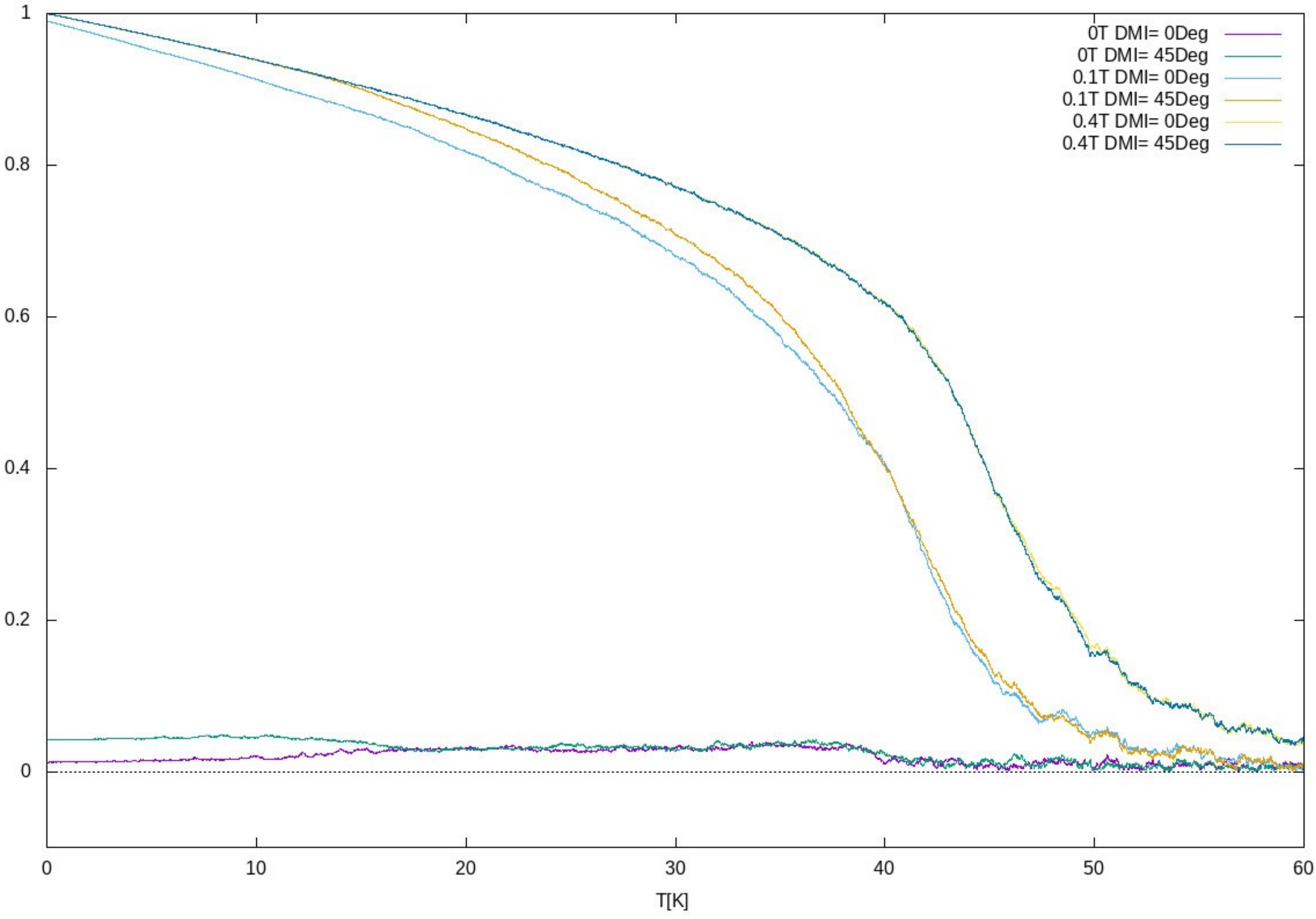
# Temperature 40K



# Temperature 44K = 0,99099099 Tc



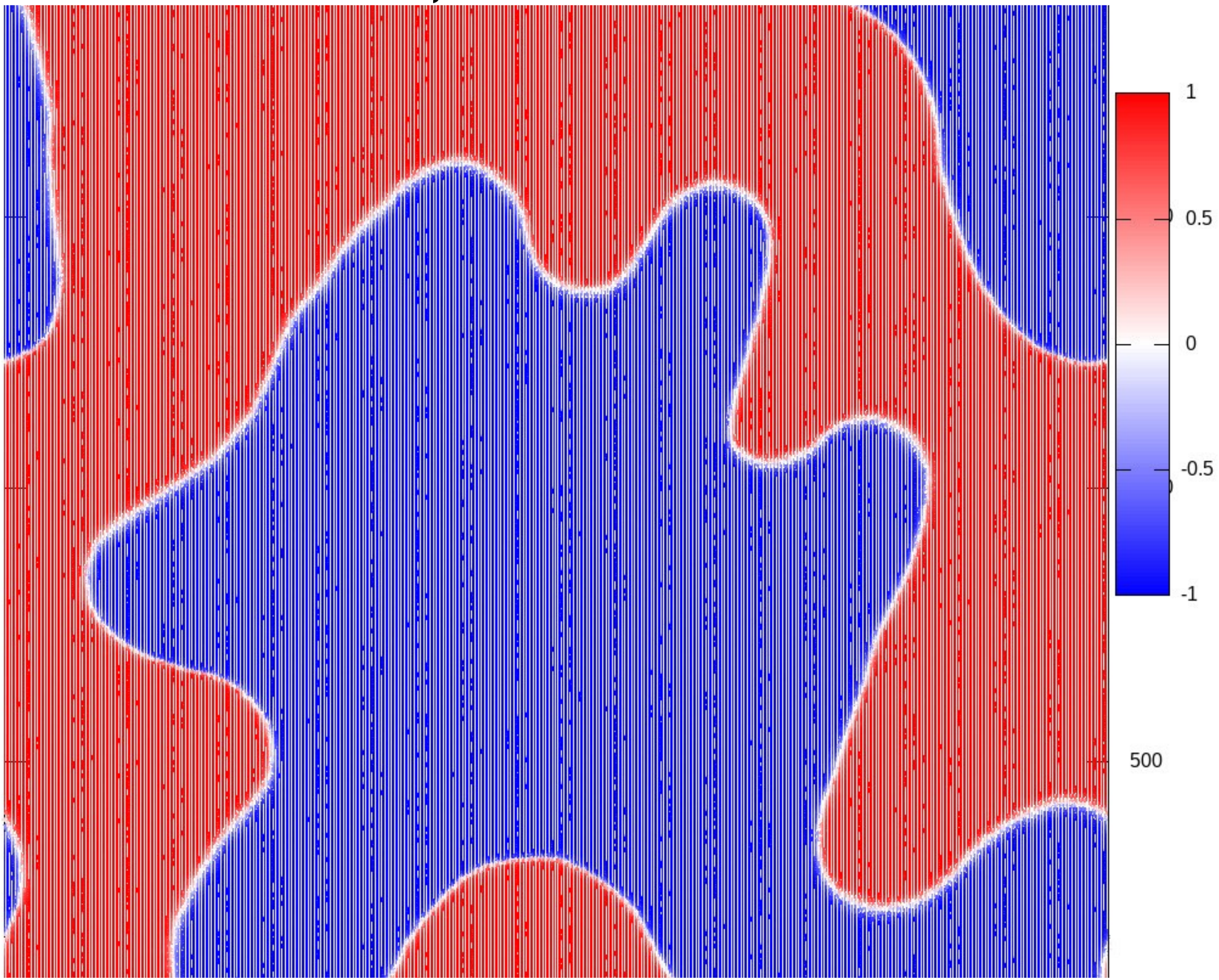
# FC, Remanent curves



**Bext = 0 T**

**DMI = 0 Deg (Y,Z)- plane**

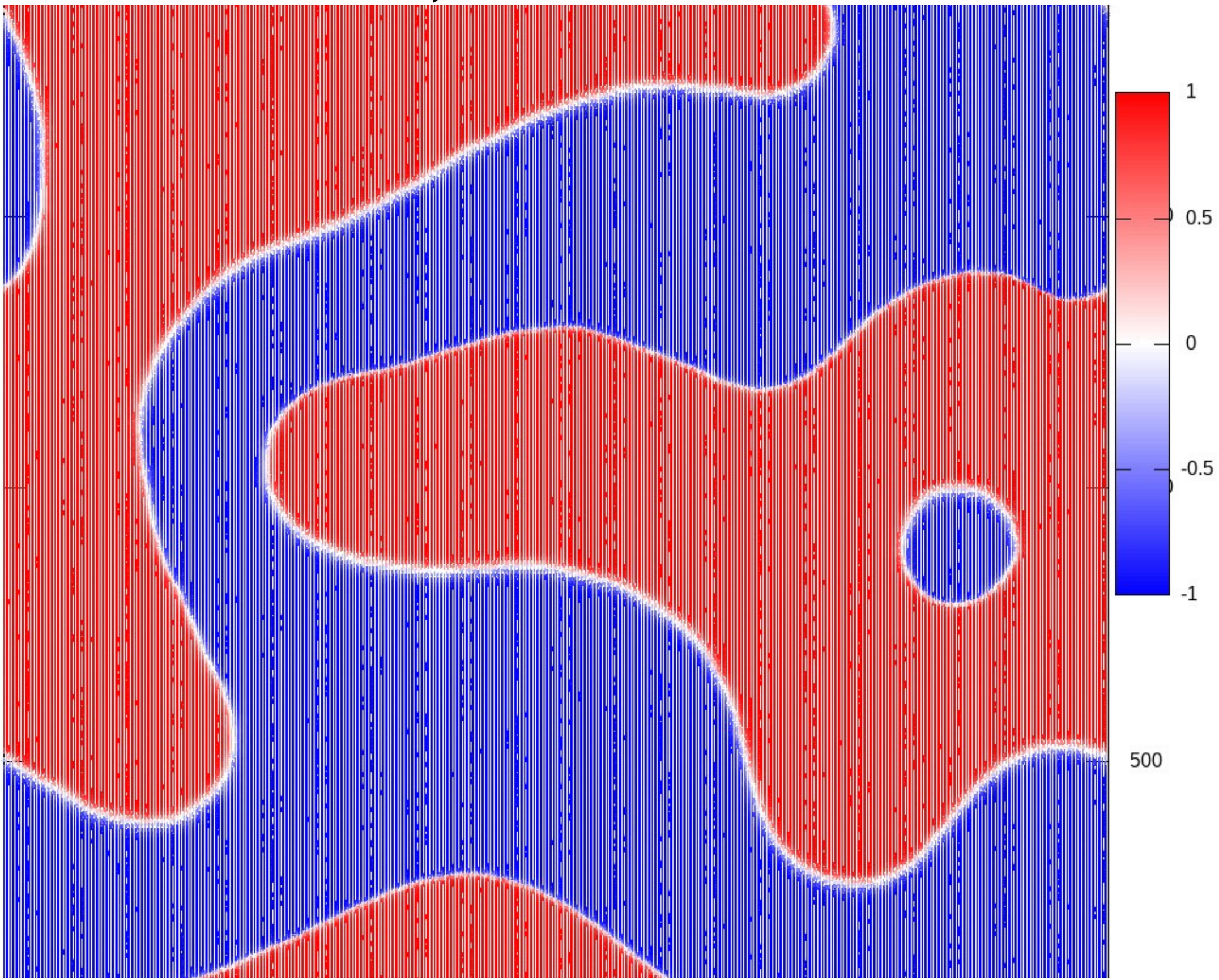
# FC, Remanent curves



**Bext = 0 T**

**DMI = 45 Deg (Y,Z)- plane**

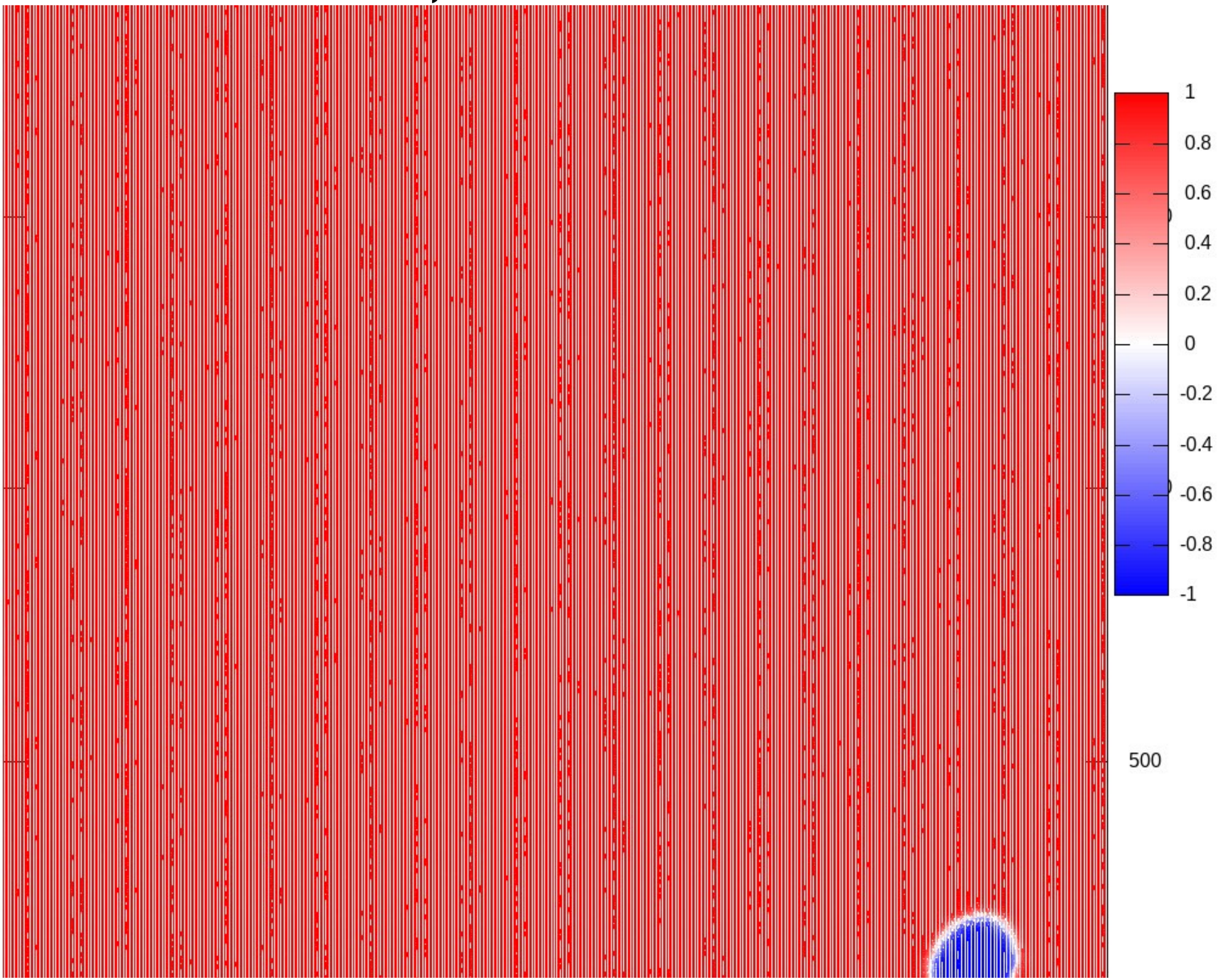
# FC, Remanent curves



**Bext = 0.1 T**

**DMI = 45 Deg (Y,Z)- plane**

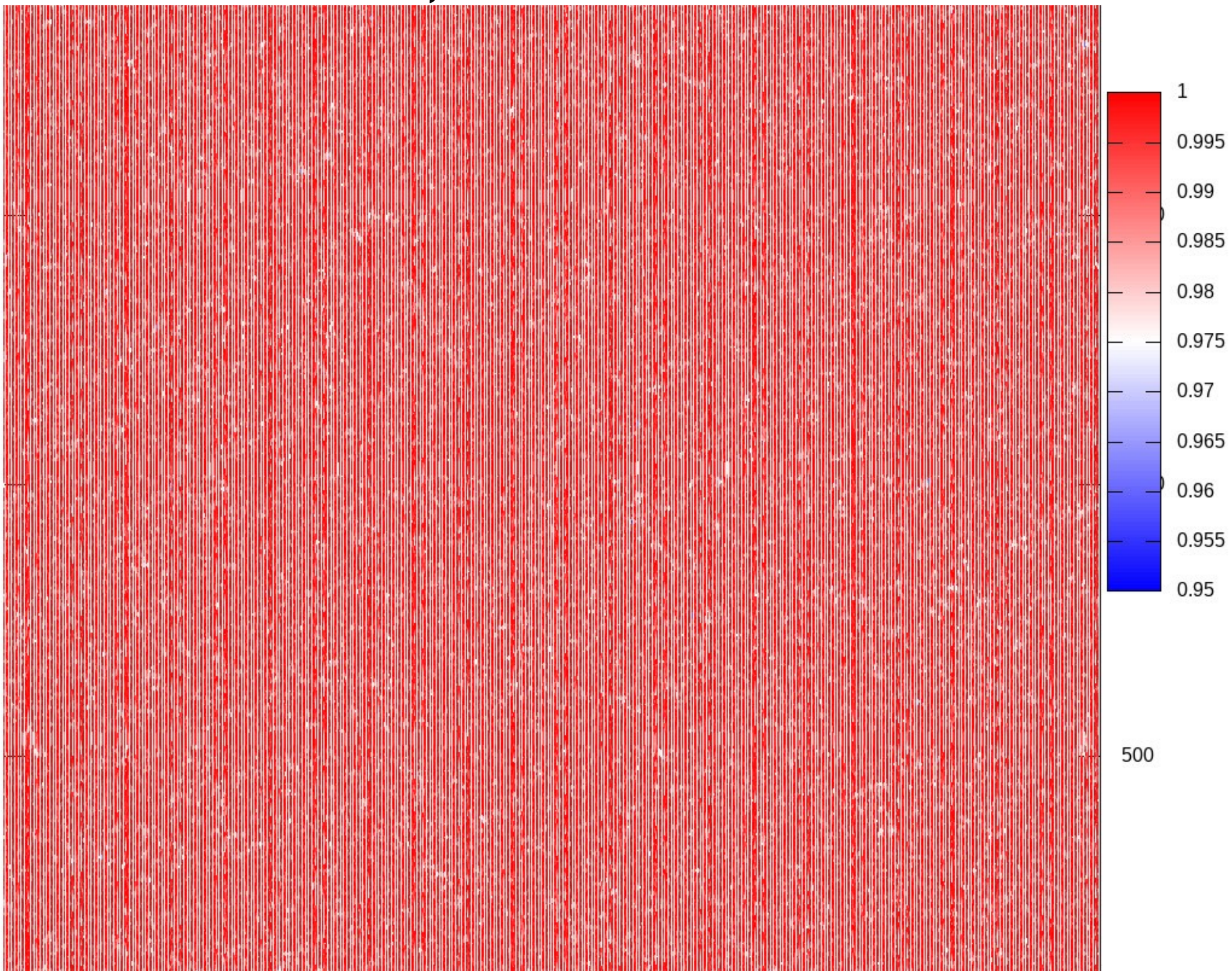
# FC, Remanent curves



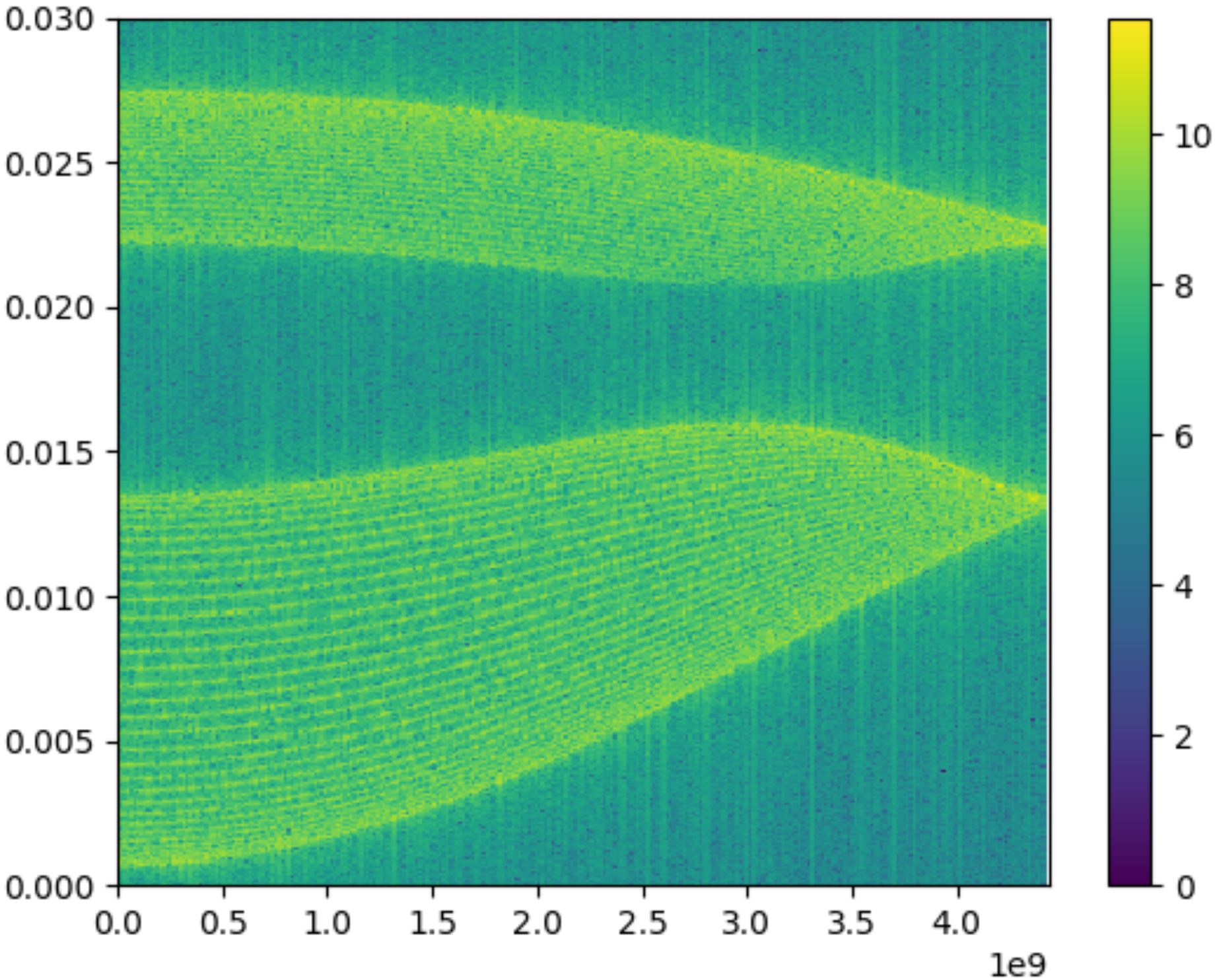
**Bext = 0.1 T**

**DMI = 45 Deg (Y,Z)- plane**

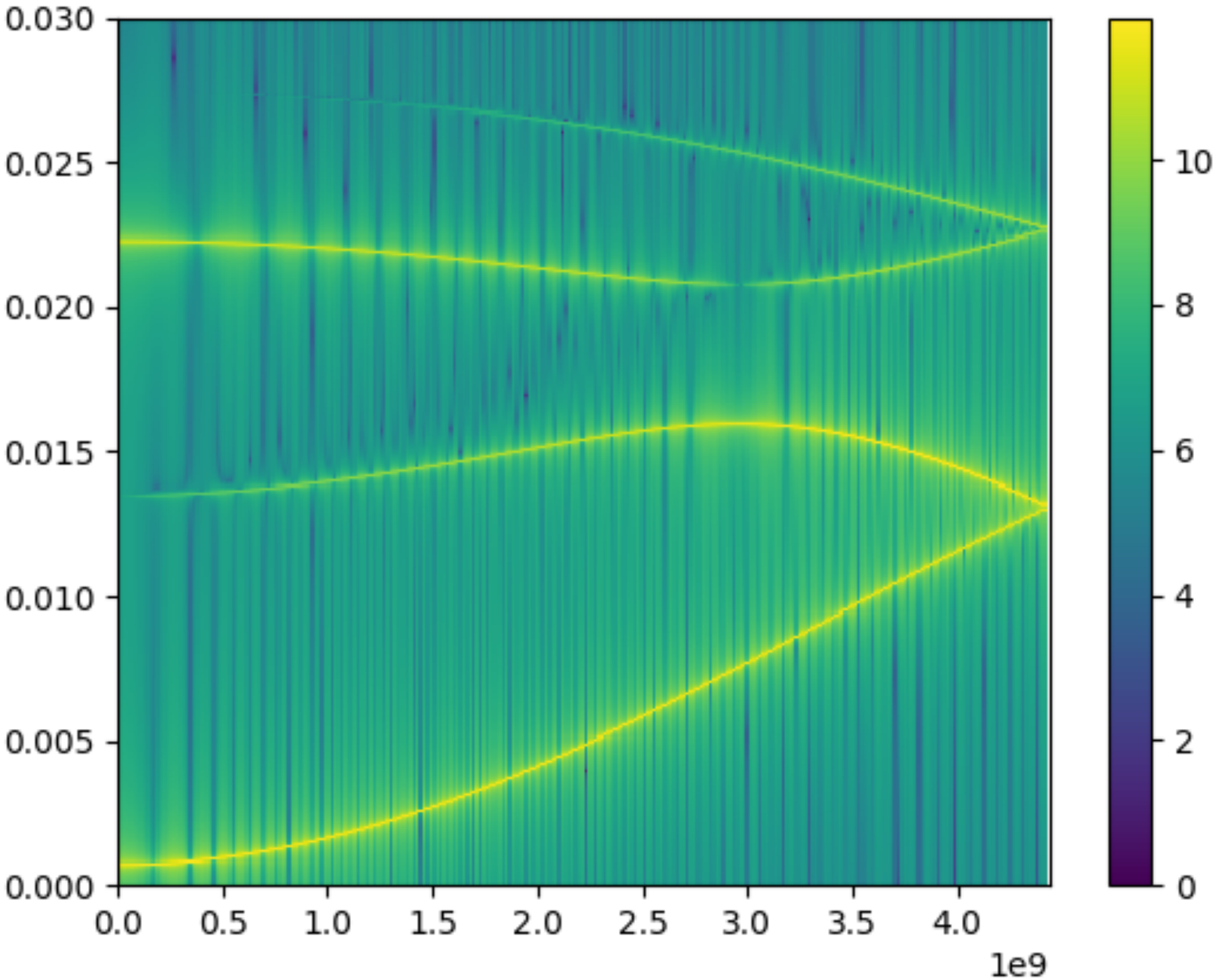
# FC, Remanent curves



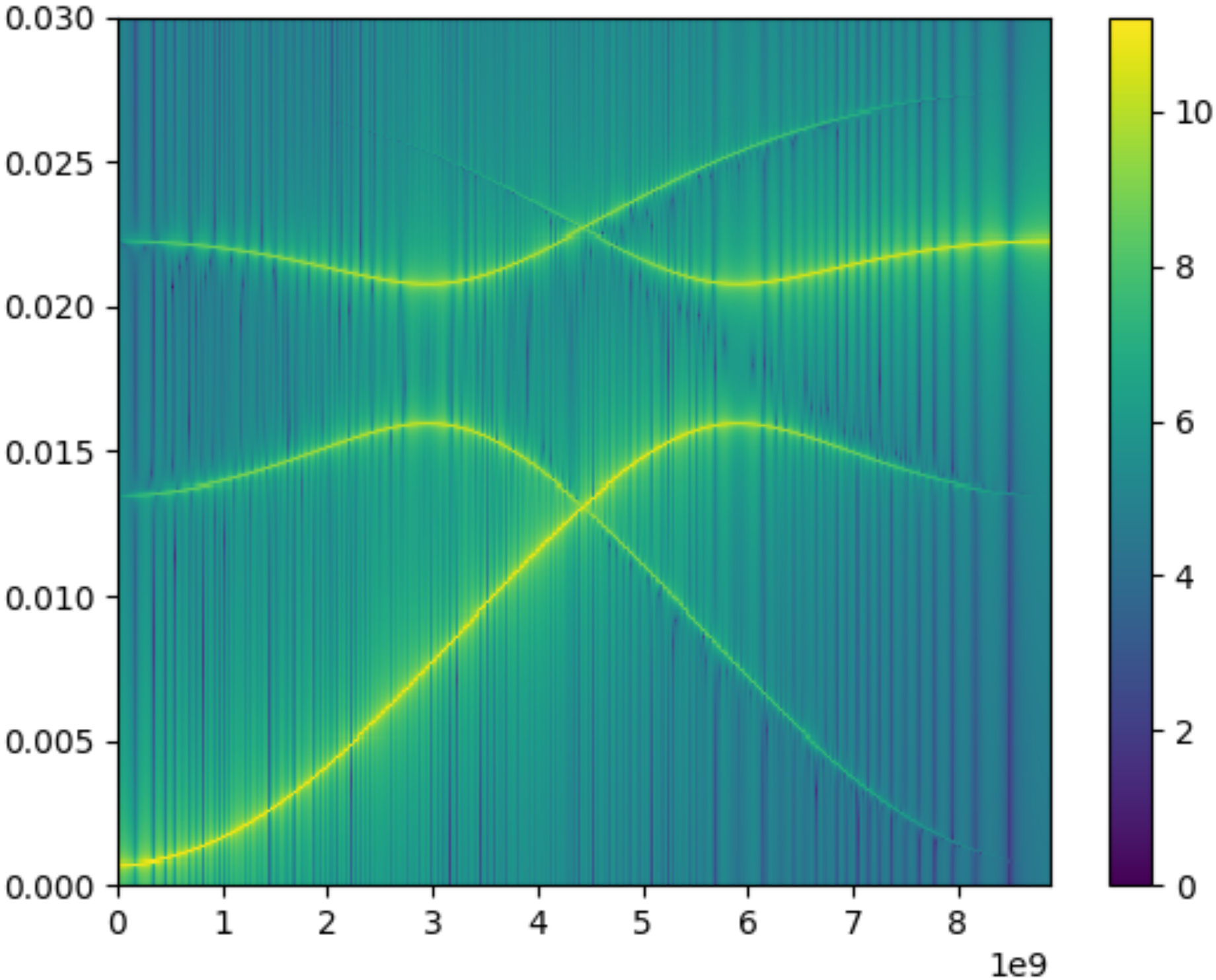
# All Bulk Modes of monolayer



# Bulk Modes of primitive cell

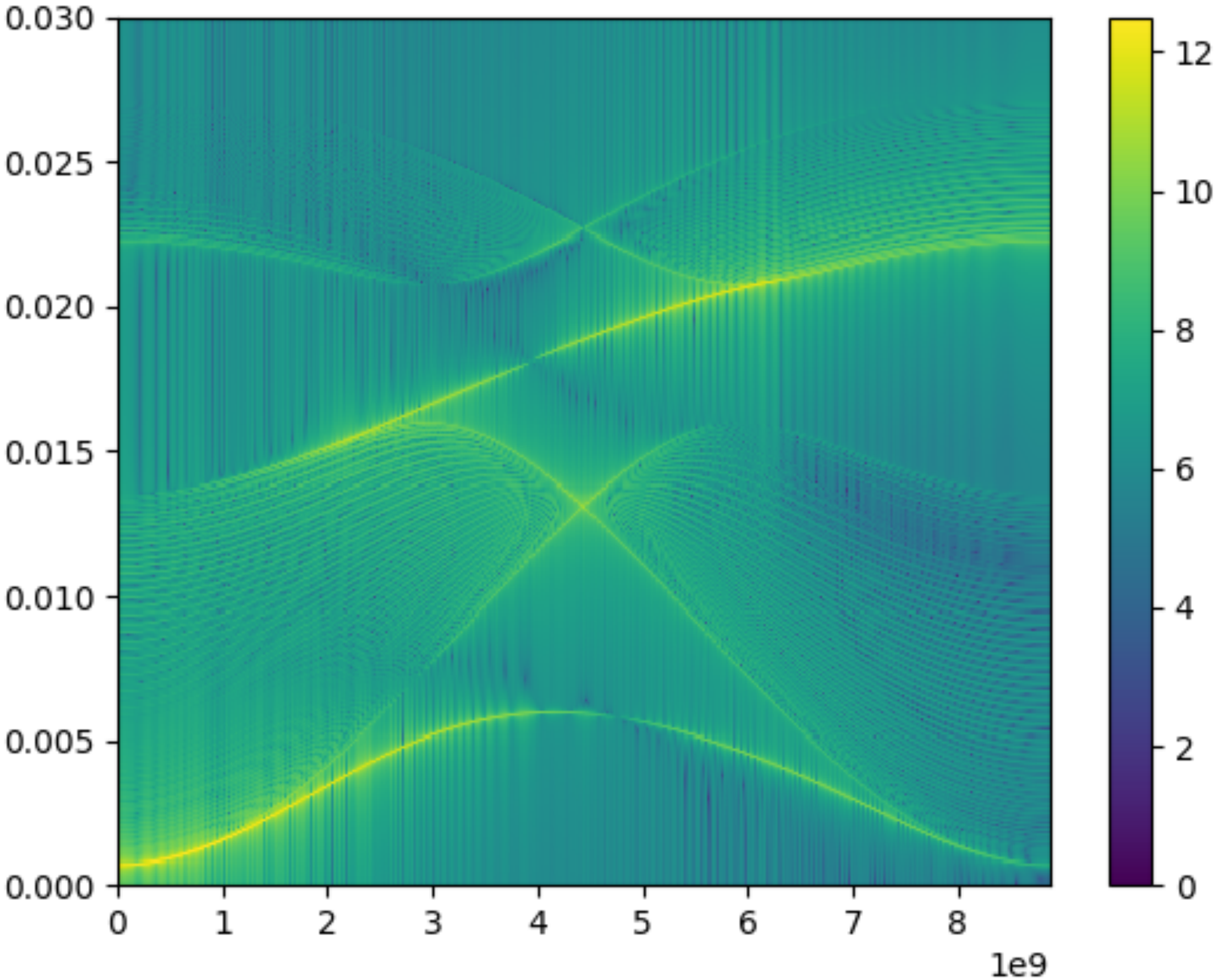


# Bulk Modes of primitive cell



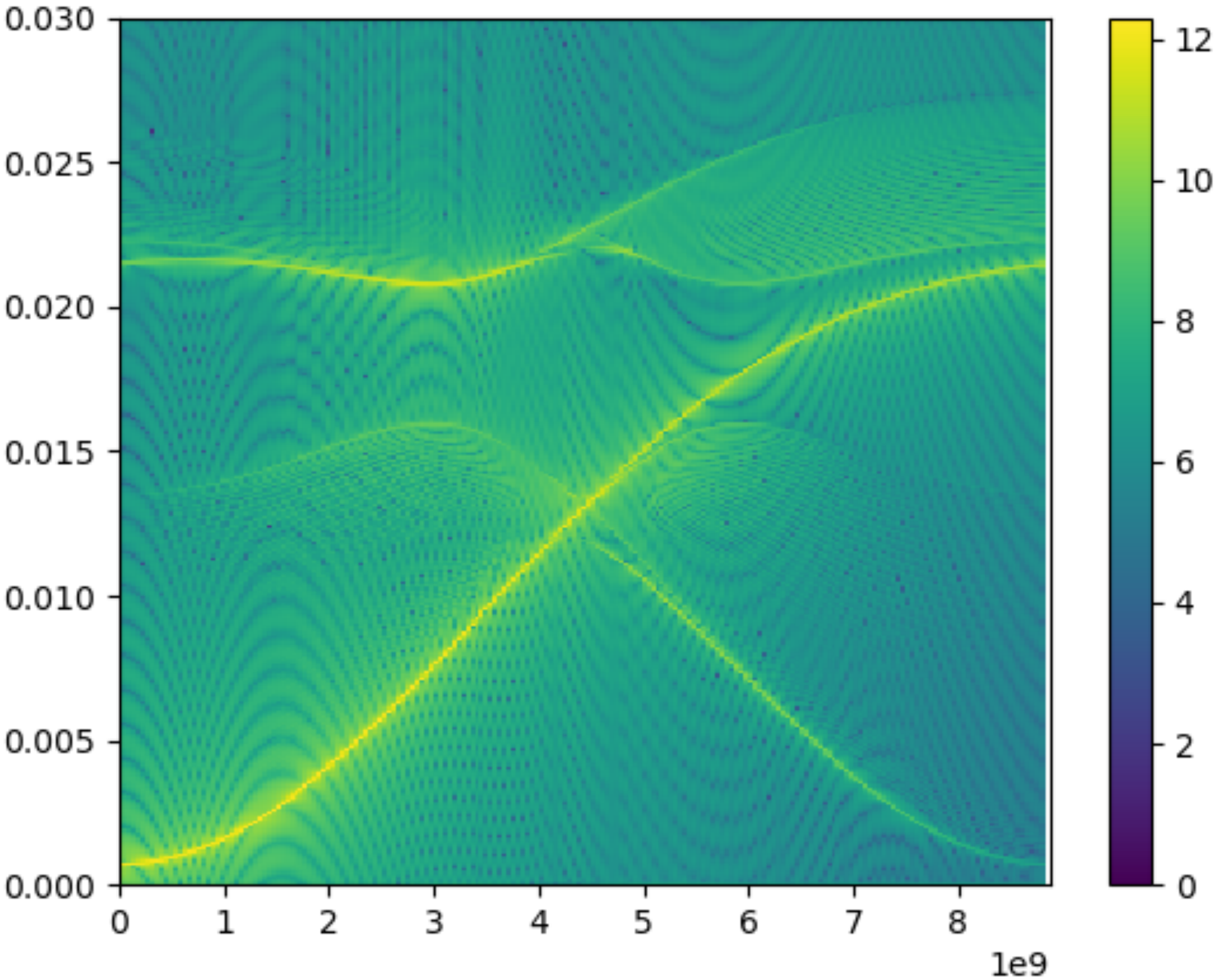
# Edge States of primitive cell

## Surface at X direction



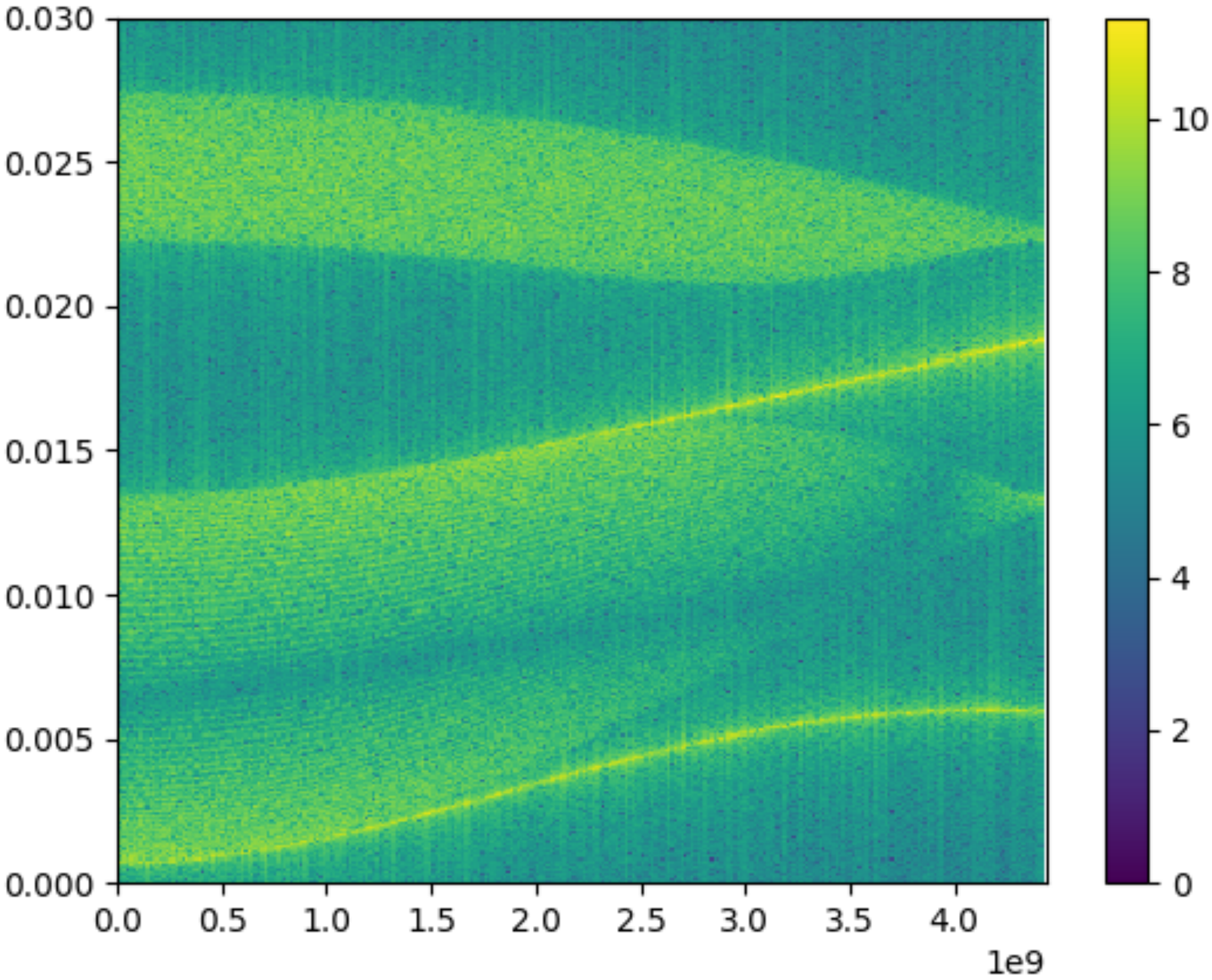
# Edge States of primitive cell (correct edge)

## Surface at X direction



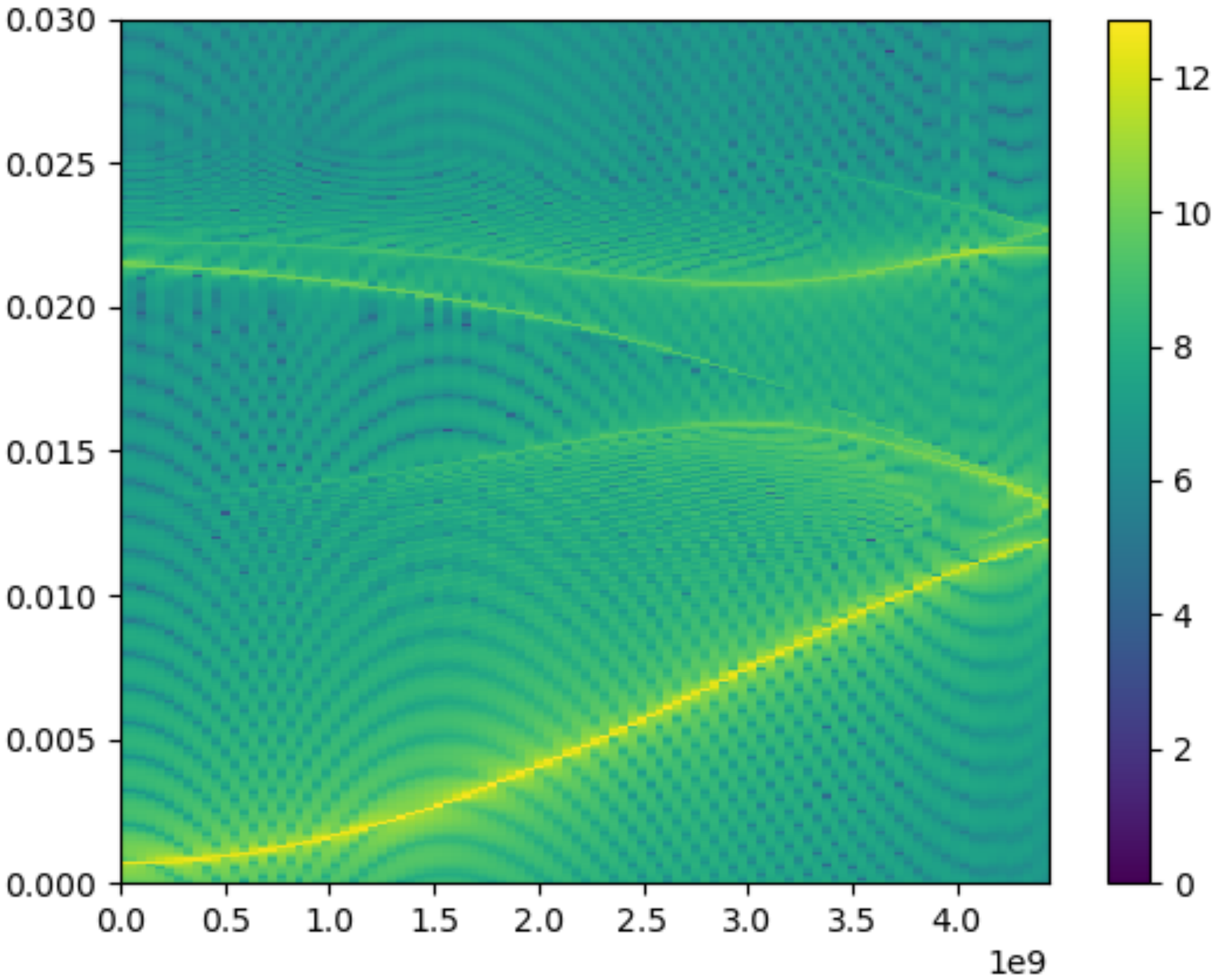
# Edge States of primitive cell

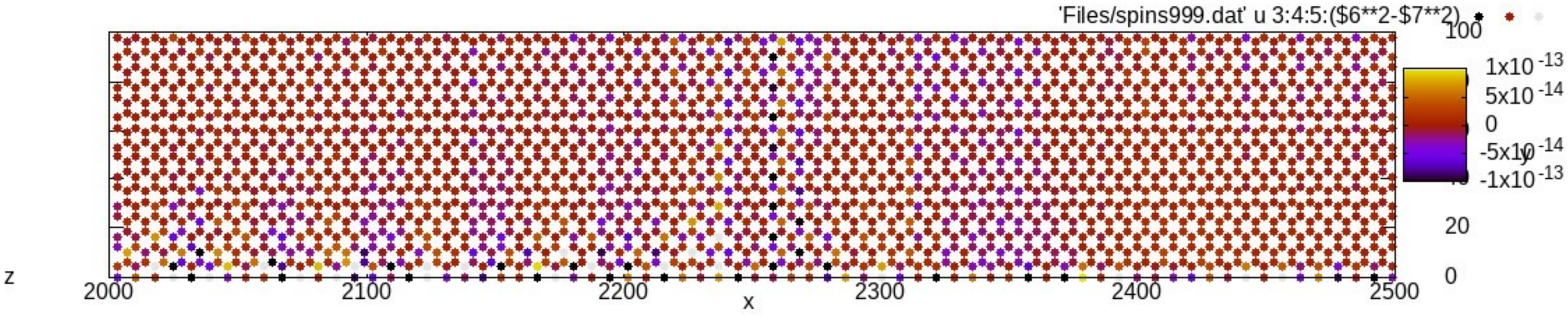
## Surface at X direction

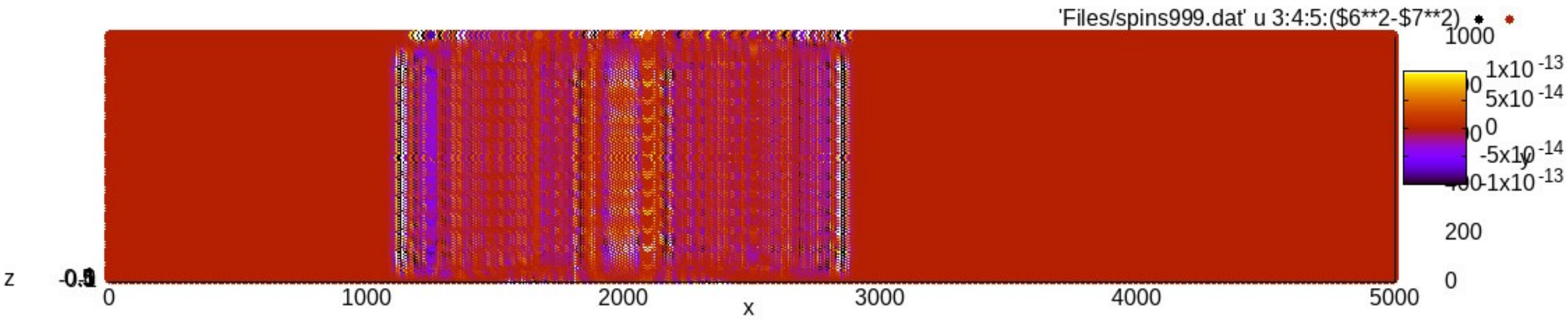


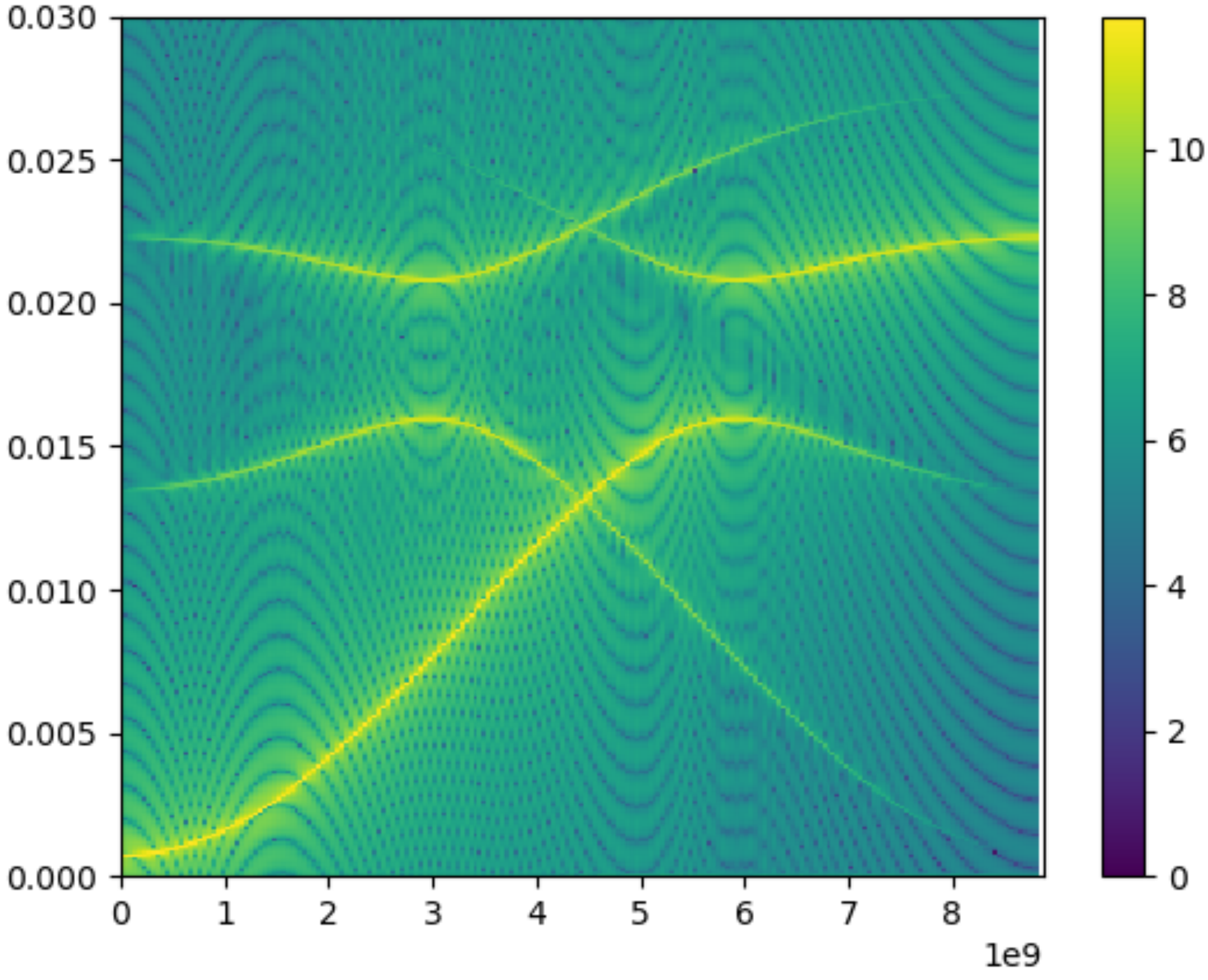
# Edge States of primitive cell
# (correct edge)

**Surface at X direction**




'Files/spins999.dat' u 3:4:5:($6**2-$7**2)
1x10 -13
5x10 -14
0
-5x10 -14
-1x10 -13
z
x
y
2000
2100
2200
2300
2400
2500
100
20
0


'Files/spins999.dat' u 3:4:5:($6**2-$7**2)
1x10 -13
5x10 -14
0
-5x10 -14
-1x10 -13
z
x
y
0
1000
2000
3000
4000
5000
1000
200
0


0.030
0.025
0.020
0.015
0.010
0.005
0.000
0
1
2
3
4
5
6
7
8
1e9
10
8
6
4
2
0

**Mean-magnetisation** **ZFC FC** **10T**

```
#---------------------------------------
# Simulation attributes:
#---------------------------------------
sim:total-time-steps=1000000
sim:equilibration-temperature=60
sim:equilibration-time-steps = 10000
sim:time-steps-increment = 1
sim:time-step=1e-16

sim:minimum-temperature=0
sim:maximum-temperature=60.0
sim:temperature-increment = 1
sim:applied-field-strength=10.0 !T
sim:cooling-time=100!ps
sim:cooling-function = linear
sim:integrator-random-seed= 123456

#---------------------------------------
# Program and integrator details
#---------------------------------------
sim:program=field-cool
sim:integrator=llg-heun
```