

30 jobs
Radial Centered
Gamma

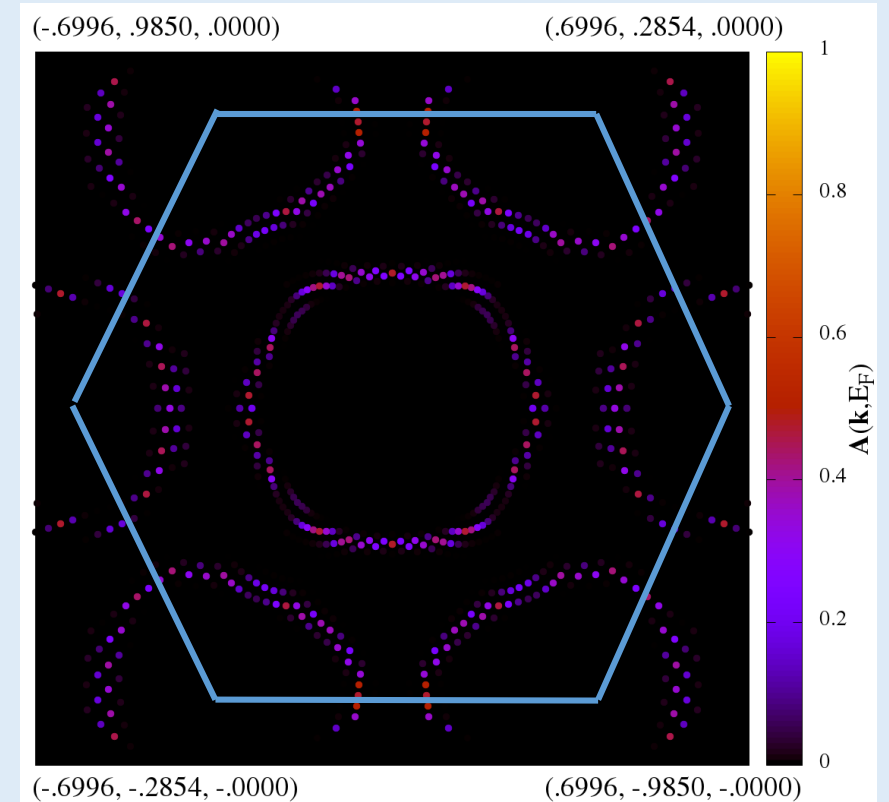
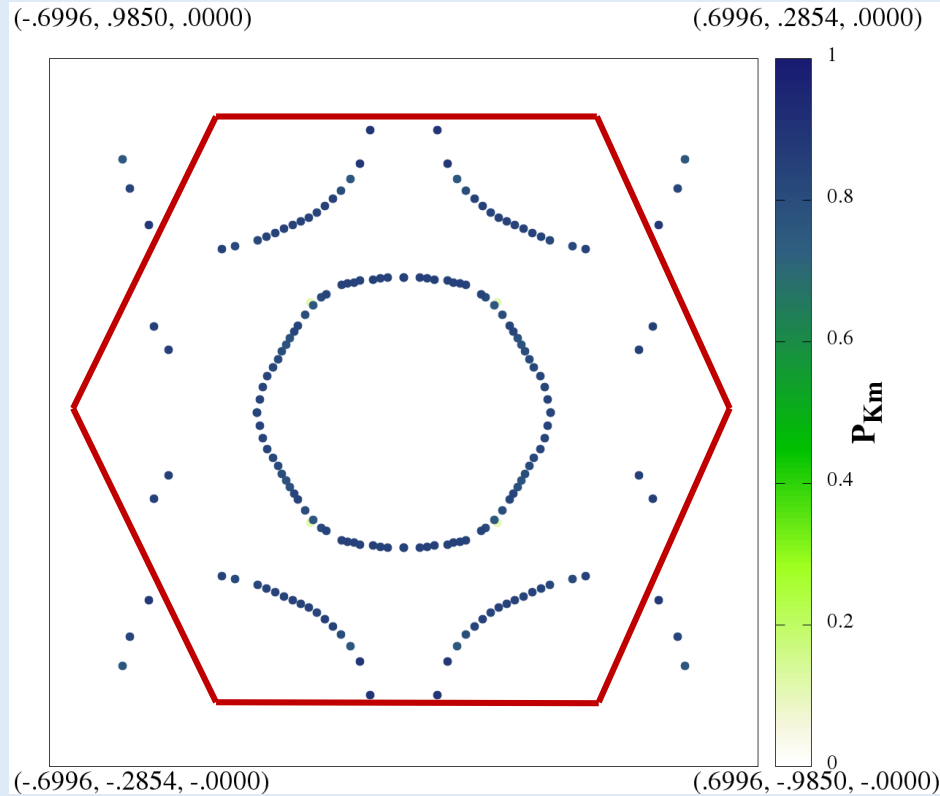
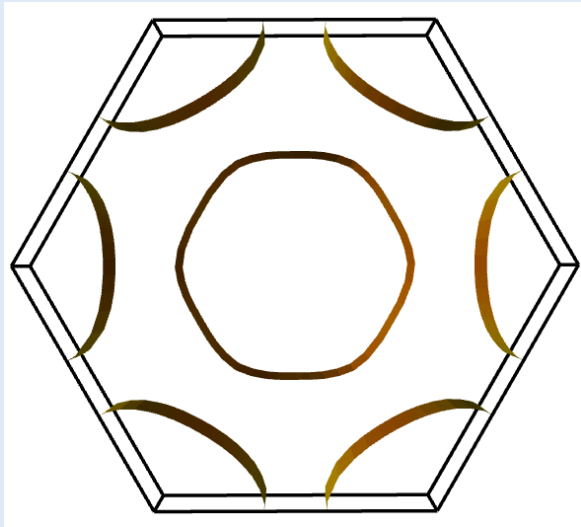
```
k-gen  
30  
p  
line  
rec  
#makepath  
0.000000 0.000000 0.000000 ! Center  
0.666666 -0.333333 0.000000 ! Start Kbar  
0.000000 0.500000 0.000000 ! End Mbar
```

INPAR

```
SIGMA = 0.03  
SPECDELTA = 0.001
```

```
SYMPOINT1 = 0.0 0.0 0.0
```

```
EDELTA1 = 3.0  
EDELTA2 = 3.0
```



Fermi Surface (NbSe2 unit)

Fermi Surface (Unfolded)

Fermi Surface Spectral Function (Unfolded)

30 jobs
Radial Centered
Gamma

```
k-gen  
30  
p  
line  
rec  
#makepath  
0.000000 0.000000 0.000000 ! Center  
0.666666 -0.333333 0.000000 ! Start Kbar  
0.000000 0.500000 0.000000 ! End Mbar
```

INPAR

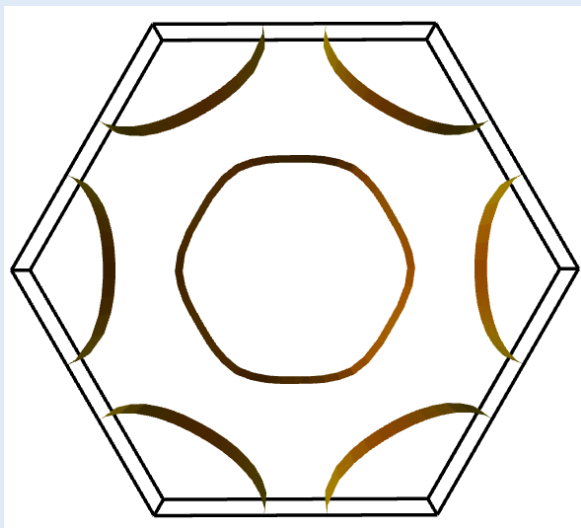
```
SIGMA = 0.03  
SPECDELTA = 0.001
```

SLIMSPEC = .FALSE.

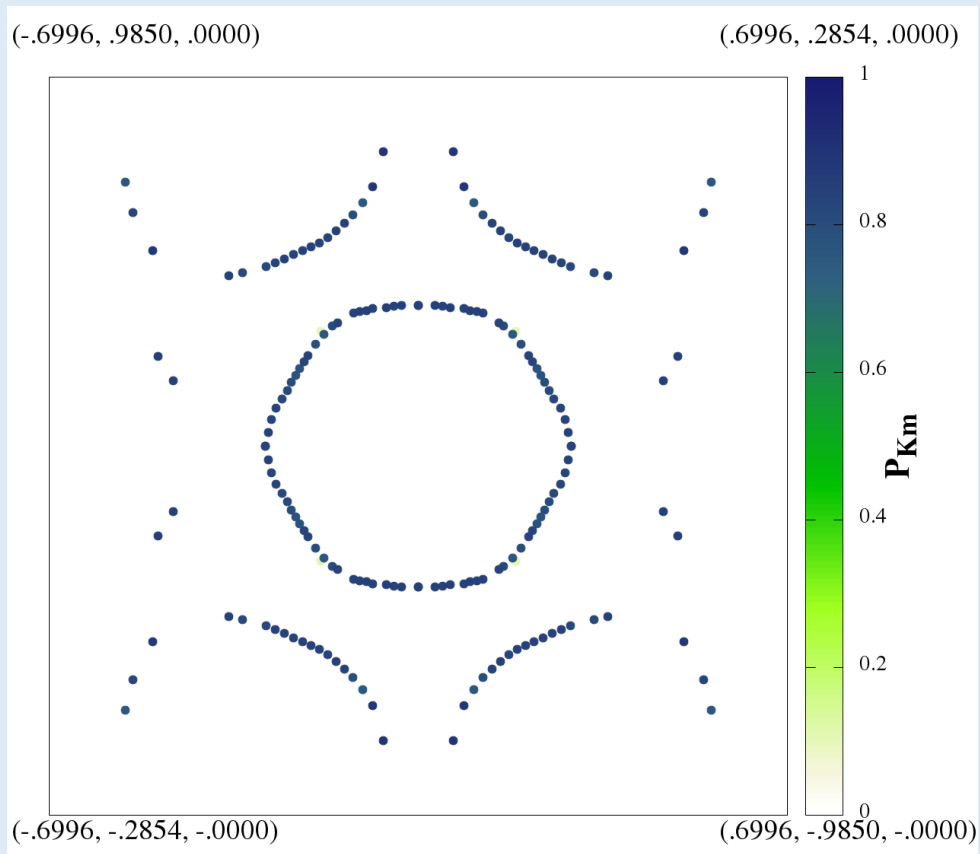
SYMPOINT1 = 0.0 0.0 0.0

EDELTA1 = 3.0

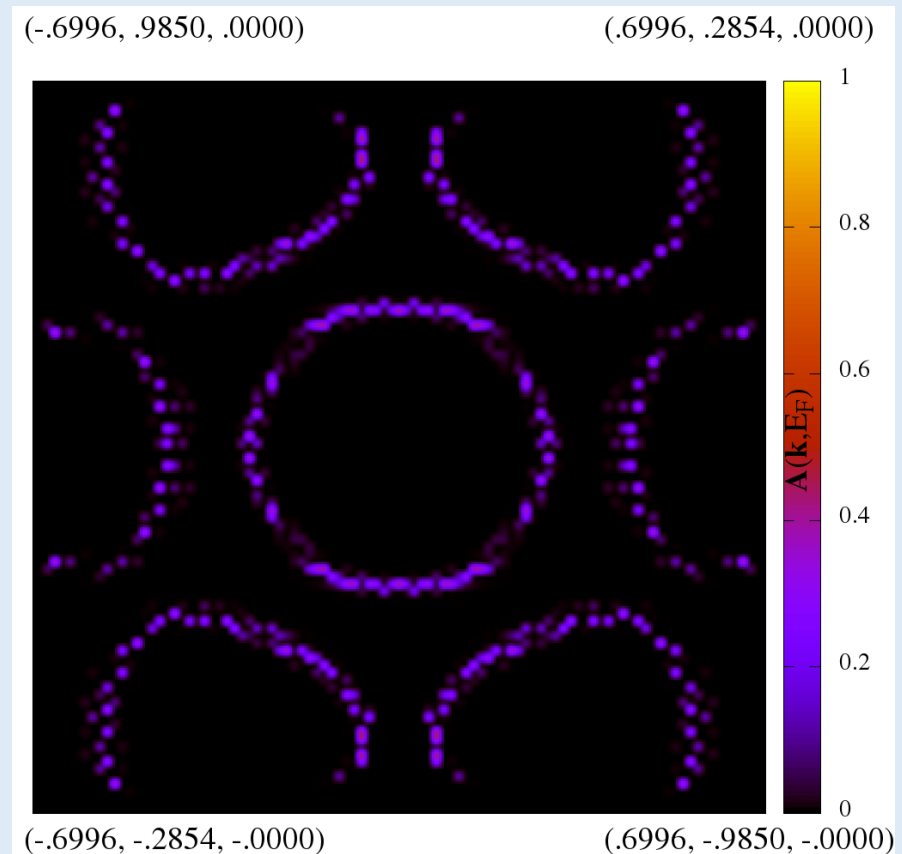
EDELTA2 = 3.0



Fermi Surface (NbSe2 unit)



Fermi Surface (Unfolded)



Fermi Surface Spectral Function (Unfolded)

30 jobs
Radial Centered
Gamma

```
k-gen  
30  
p  
line  
rec  
#makepath  
0.000000 0.000000 0.000000 ! Center  
0.666666 -0.333333 0.000000 ! Start Kbar  
0.000000 0.500000 0.000000 ! End Mbar
```

INPAR

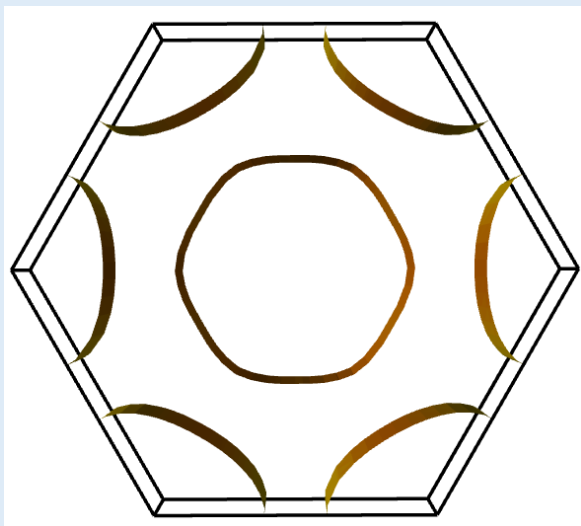
```
SIGMA = 0.04  
SPECDELTA = 0.0001
```

SLIMSPEC = .FALSE.

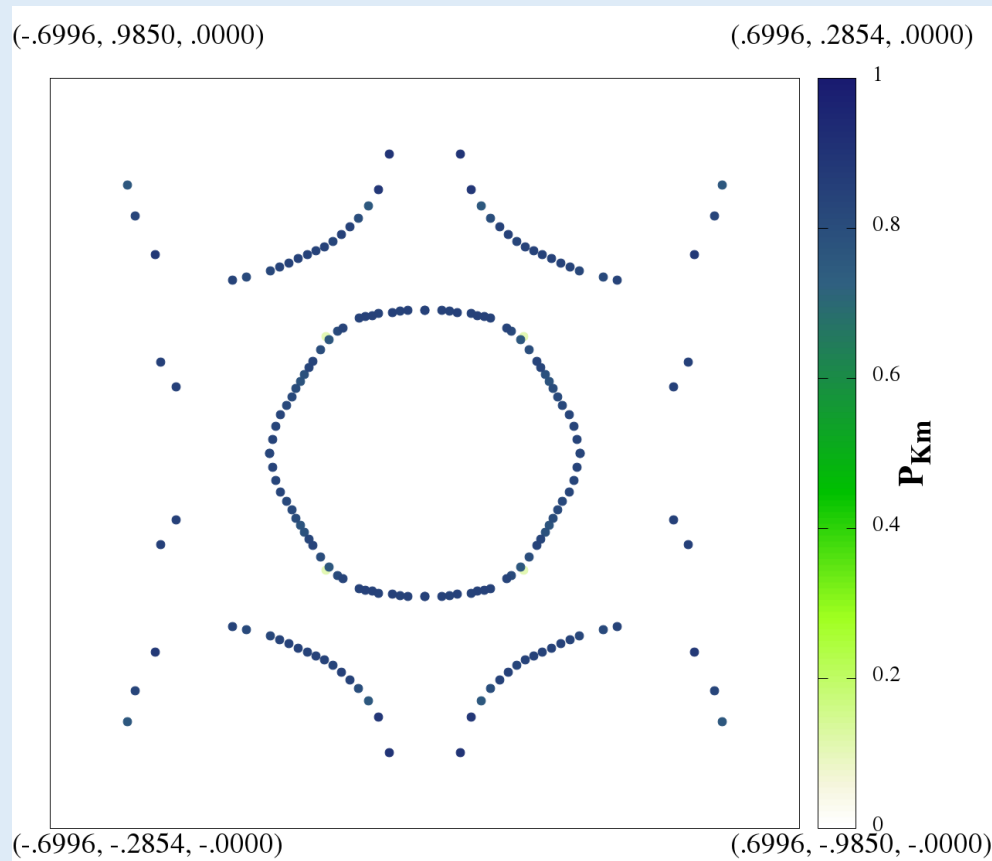
SYMPOINT1 = 0.0 0.0 0.0

EDELTA1 = 3.0

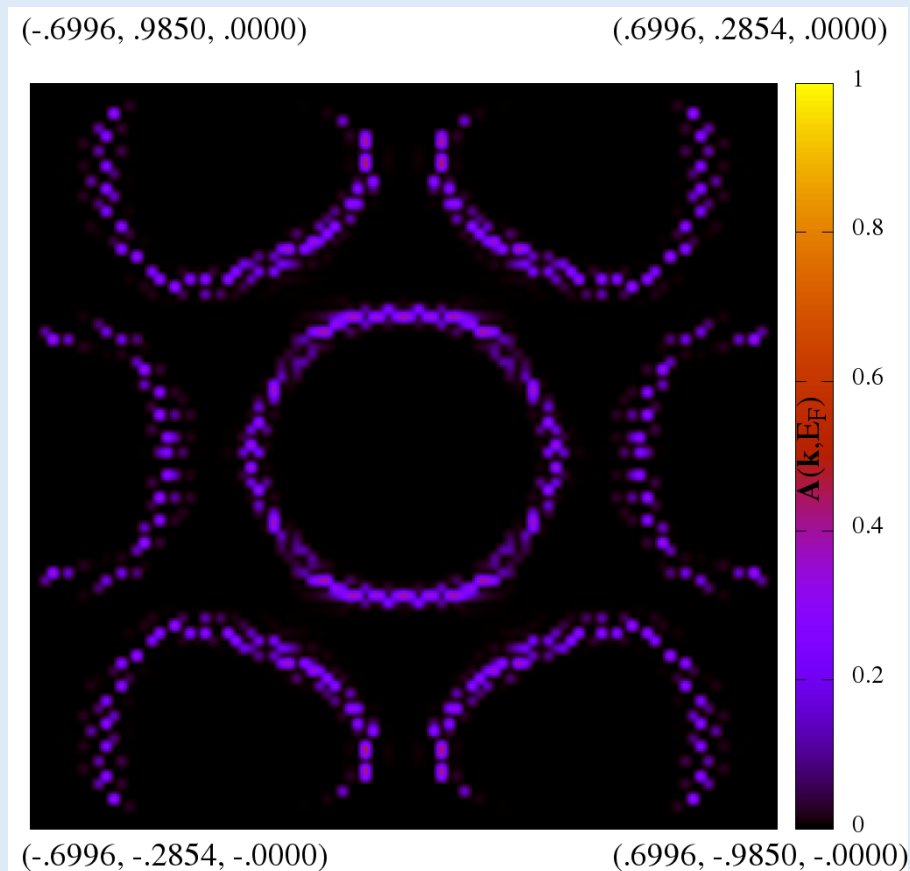
EDELTA2 = 3.0



Fermi Surface (NbSe₂ unit)

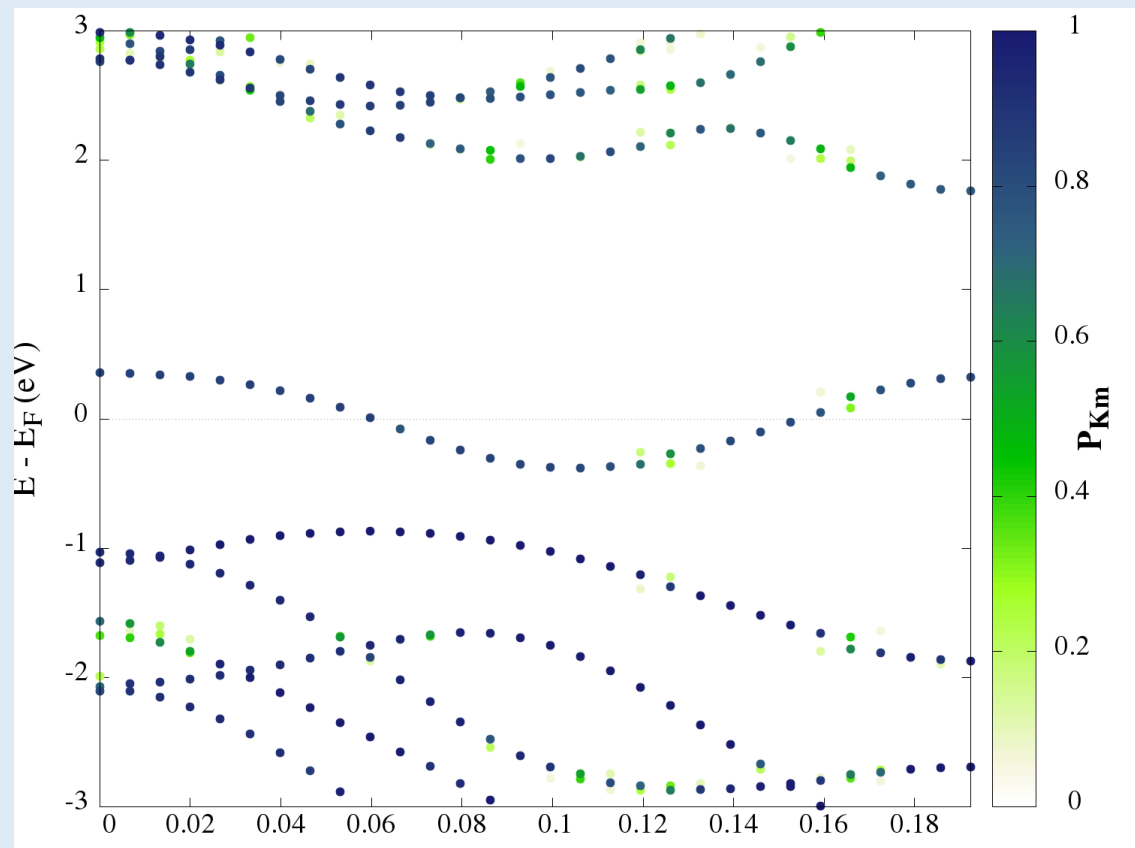


Fermi Surface (Unfolded)

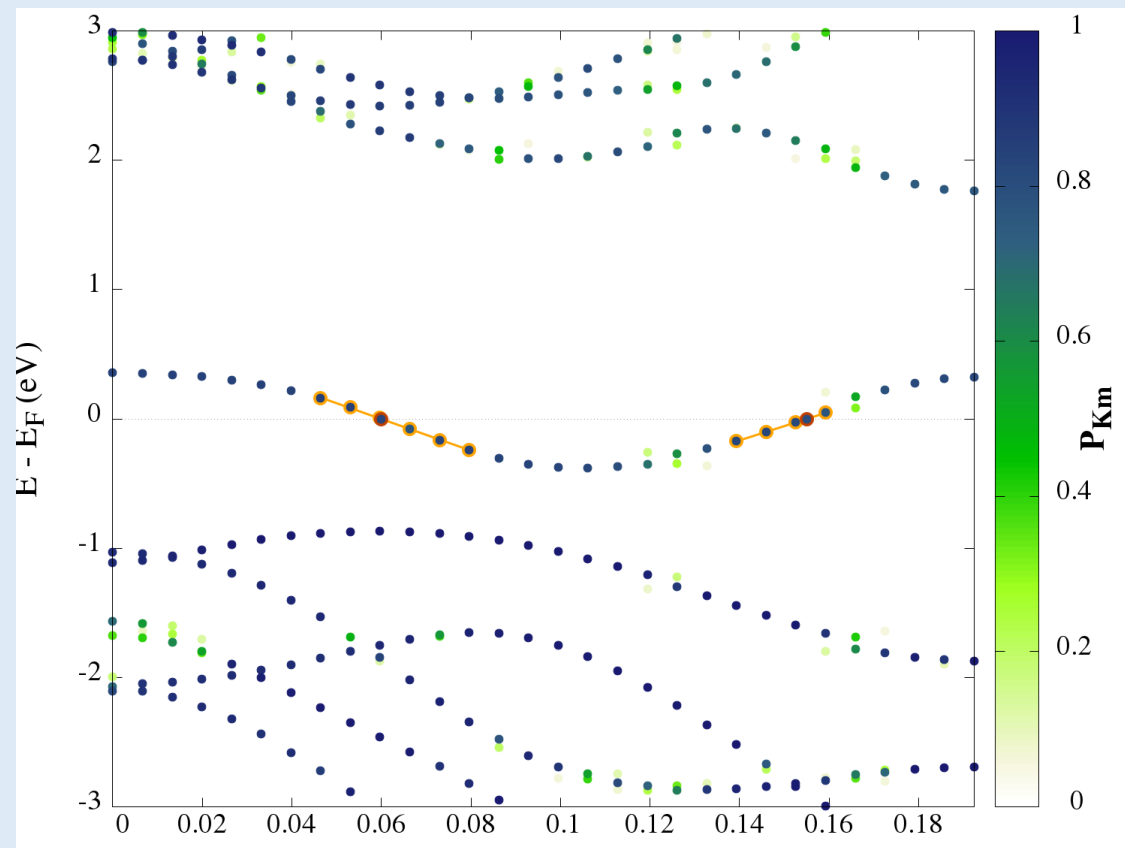


Fermi Surface Spectral Function (Unfolded)

EBSbloch



EBSbloch.processed



30 jobs
Radial Centered
Gamma

```
k-gen  
30  
p  
line  
rec  
#makepath  
0.000000 0.000000 0.000000 ! Center  
0.666666 -0.333333 0.000000 ! Start Kbar  
0.000000 0.500000 0.000000 ! End Mbar
```

INPAR

```
SIGMA = 0.04  
SPECDELTA = 0.0001
```

SLIMSPEC = .FALSE.

SYMPOINT1 = 0.0 0.0 0.0

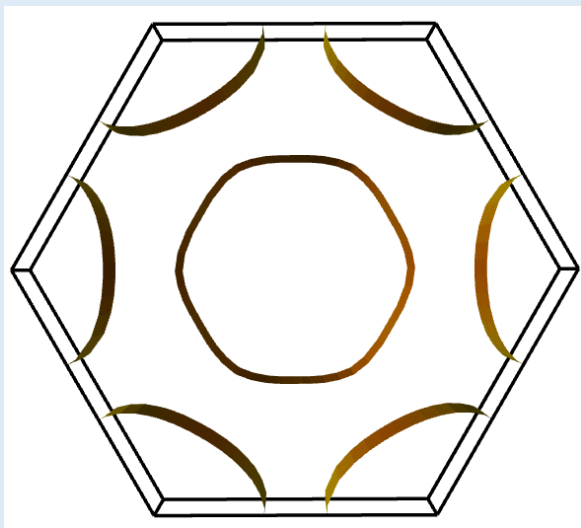
EDELTA1 = 3.0

EDELTA2 = 3.0

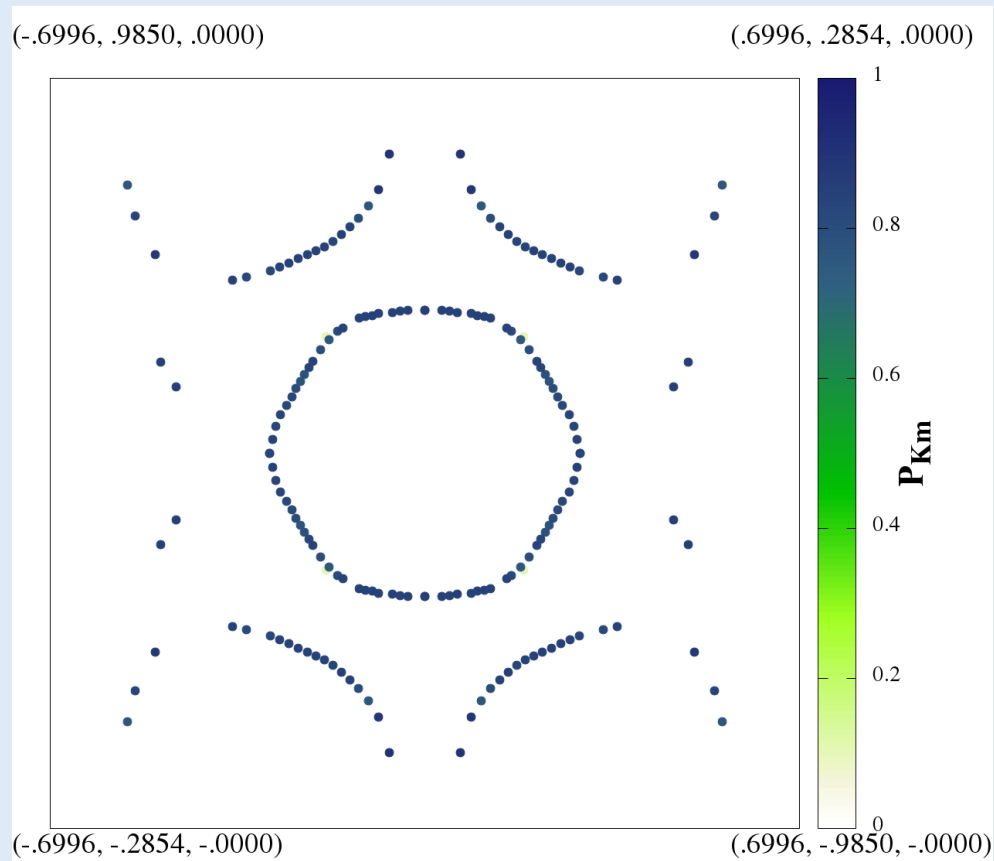
DBLOCH = 0.2

EGAP = 0.2

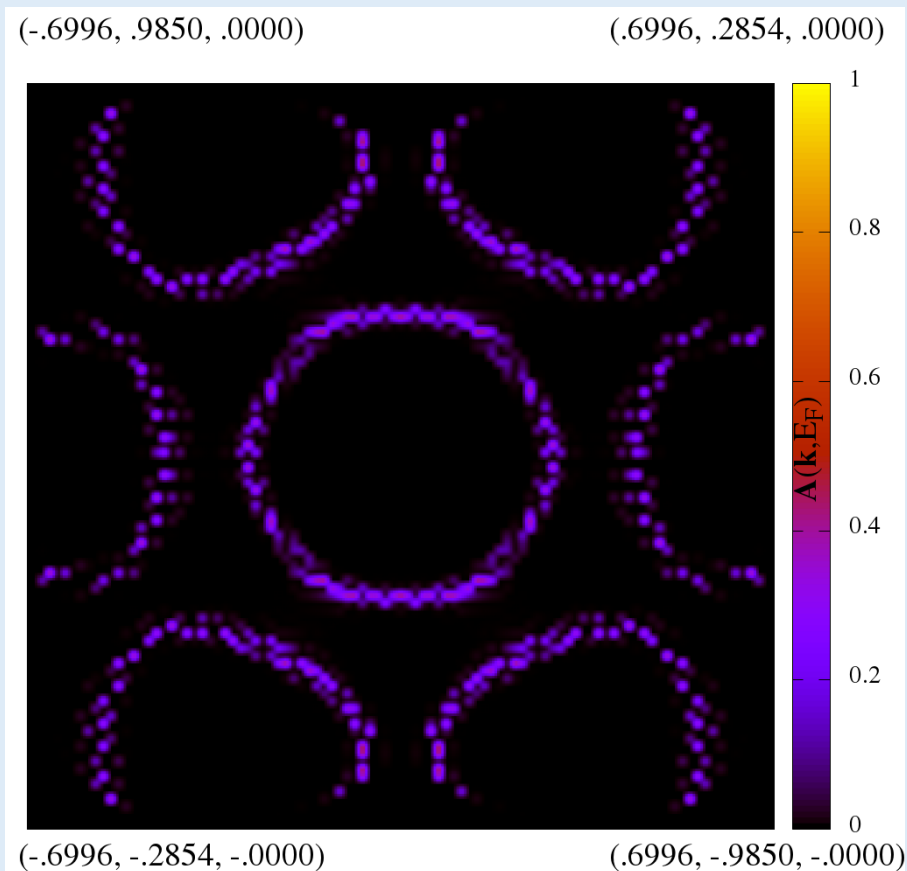
BLOCH_THRESHOLD = 0.05



Fermi Surface (NbSe2 unit)



Fermi Surface (Unfolded)



Fermi Surface Spectral Function (Unfolded)

30 jobs
Radial Centered
Gamma

```
k-gen  
30  
p  
line  
rec  
#makepath  
0.000000 0.000000 0.000000 ! Center  
0.666666 -0.333333 0.000000 ! Start Kbar  
0.000000 0.500000 0.000000 ! End Mbar
```

INPAR

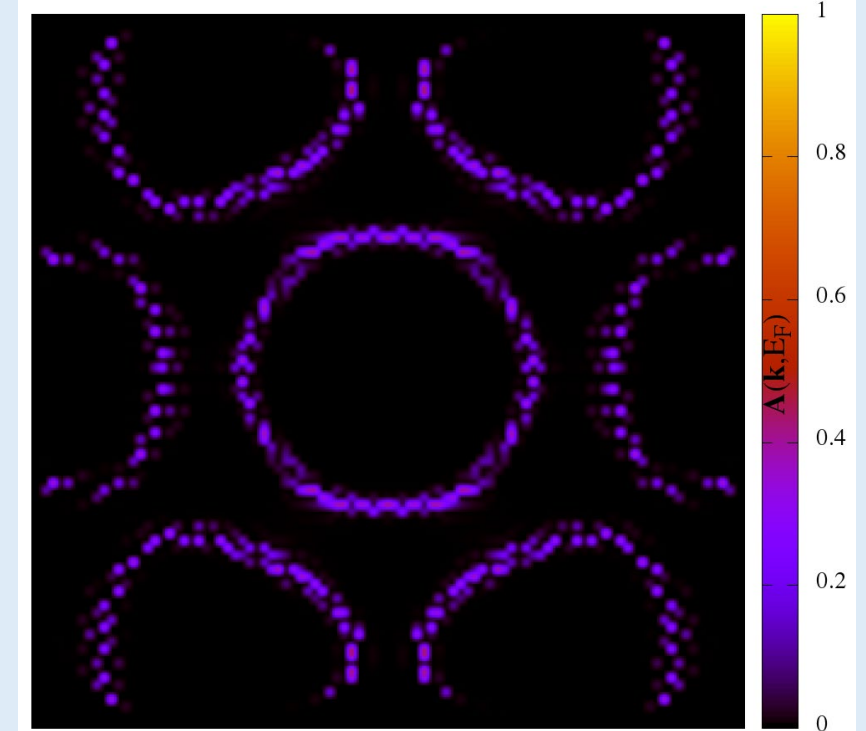
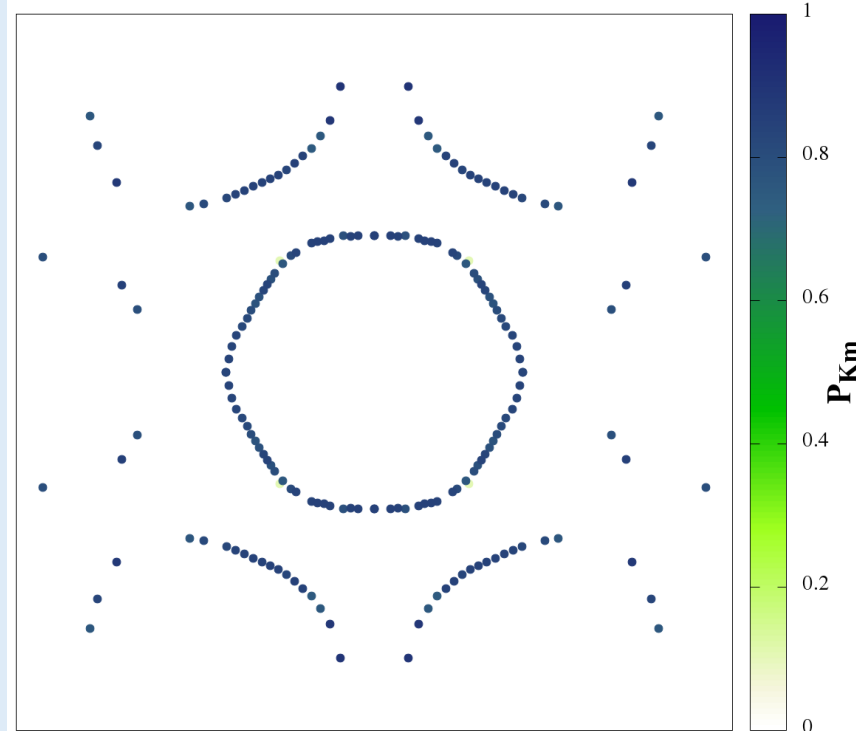
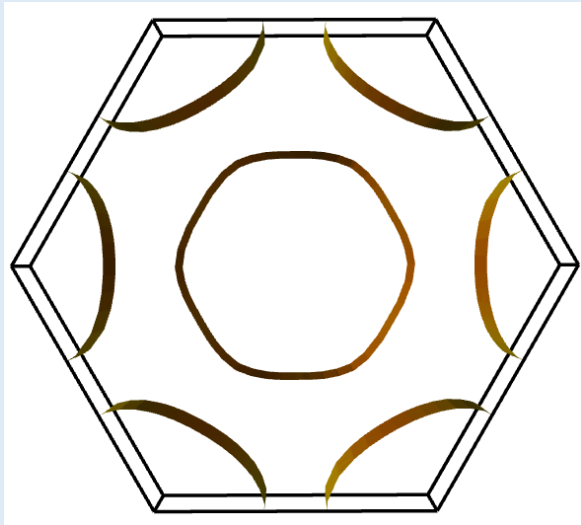
```
SIGMA = 0.04  
SPECDELTA = 0.0001
```

```
SLIMSPEC = .FALSE.
```

```
SYMPOINT1 = 0.0 0.0 0.0
```

```
EDELTA1 = 3.0  
EDELTA2 = 3.0
```

```
DBLOCH = 0.3  
EGAP = 0.2  
BLOCH_THRESHOLD = 0.05
```



Fermi Surface (NbSe2 unit)

Fermi Surface (Unfolded)

Fermi Surface Spectral Function (Unfolded)

30 jobs
Radial Centered
Gamma

```
k-gen  
30  
p  
line  
rec  
#makepath  
0.000000 0.000000 0.000000 ! Center  
0.666666 -0.333333 0.000000 ! Start Kbar  
0.000000 0.500000 0.000000 ! End Mbar
```

INPAR

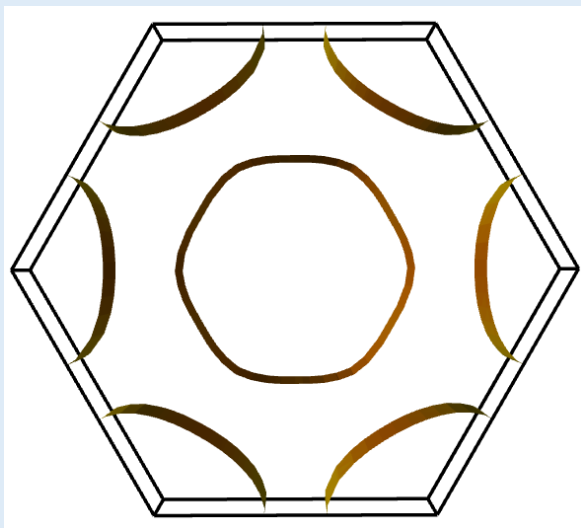
```
SIGMA = 0.04  
SPECDELTA = 0.0001
```

```
SLIMSPEC = .FALSE.
```

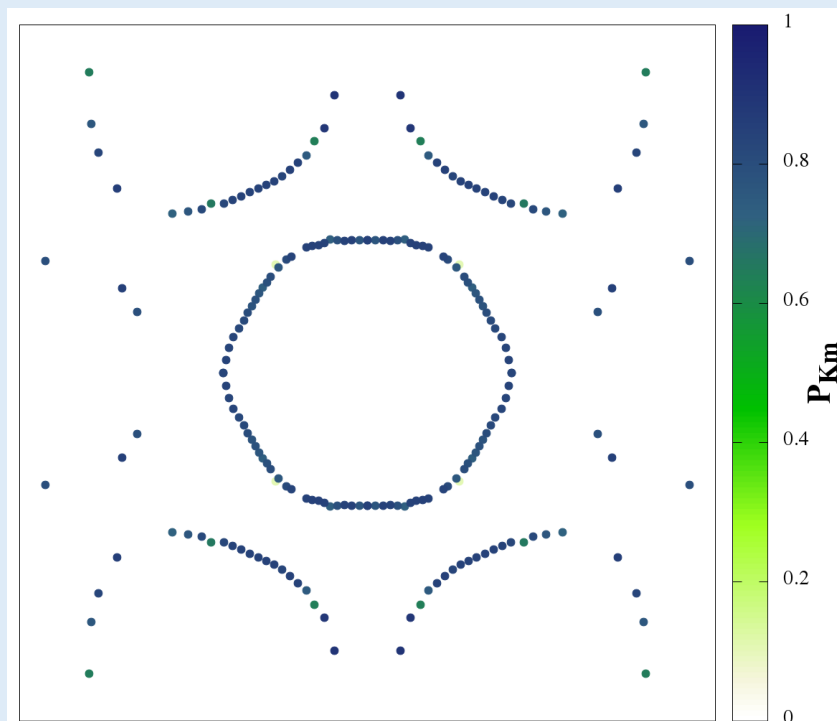
```
SYMPOINT1 = 0.0 0.0 0.0
```

```
EDELTA1 = 3.0  
EDELTA2 = 3.0
```

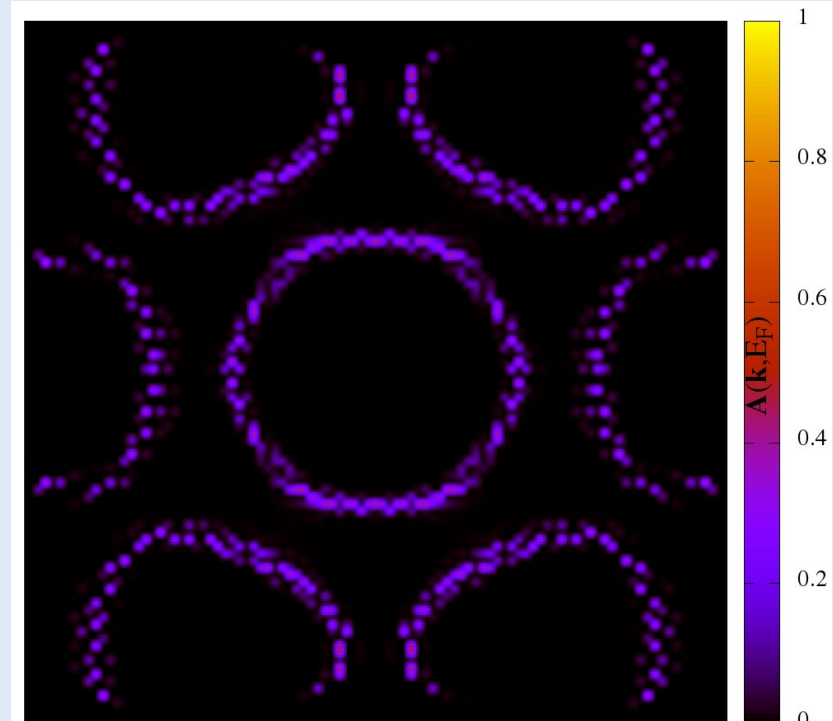
```
DBLOCH = 0.6  
EGAP = 0.2  
BLOCH_THRESHOLD = 0.05
```



Fermi Surface (NbSe2 unit)



Fermi Surface (Unfolded)



Fermi Surface Spectral Function (Unfolded)

30 jobs
Radial Centered
Gamma

```
k-gen  
30  
p  
line  
rec  
#makepath  
0.000000 0.000000 0.000000 ! Center  
0.666666 -0.333333 0.000000 ! Start Kbar  
0.000000 0.500000 0.000000 ! End Mbar
```

INPAR

```
SIGMA = 0.04  
SPECDELTA = 0.0001
```

```
SLIMSPEC = .FALSE.
```

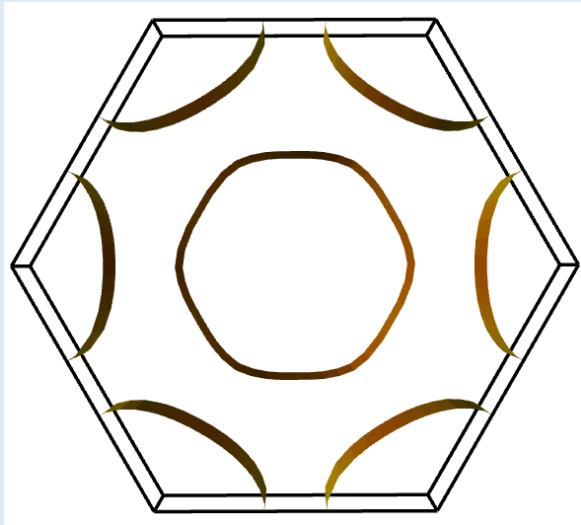
```
SYMPOINT1 = 0.0 0.0 0.0
```

```
EDELTA1 = 3.0  
EDELTA2 = 3.0
```

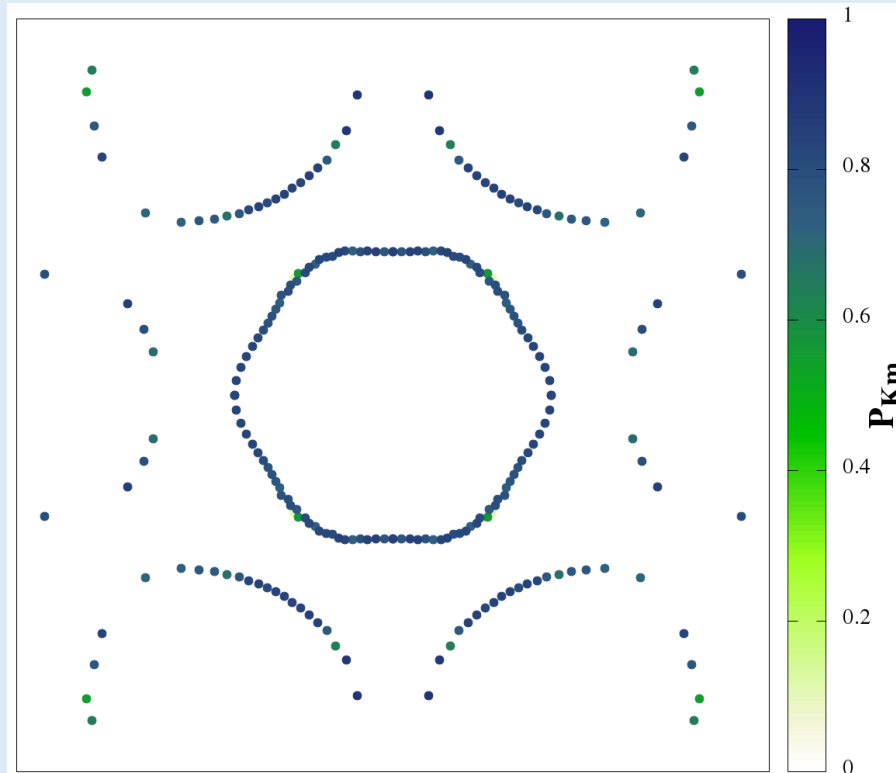
```
DBLOCH = 0.6
```

```
EGAP = 0.3
```

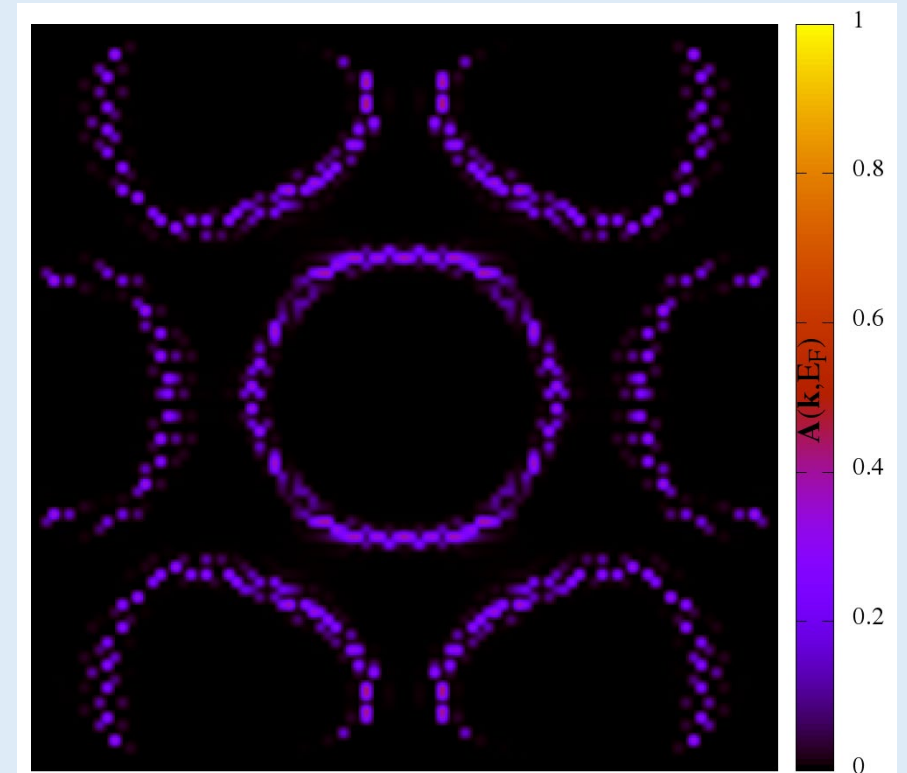
```
BLOCH_THRESHOLD = 0.05
```



Fermi Surface (NbSe2 unit)



Fermi Surface (Unfolded)



Fermi Surface Spectral Function (Unfolded)

30 jobs
Radial Centered
Gamma

```
k-gen  
30  
p  
line  
rec  
#makepath  
0.000000 0.000000 0.000000 ! Center  
0.666666 -0.333333 0.000000 ! Start Kbar  
0.000000 0.500000 0.000000 ! End Mbar
```

INPAR

```
SIGMA = 0.04  
SPECDELTA = 0.0001
```

```
SLIMSPEC = .FALSE.
```

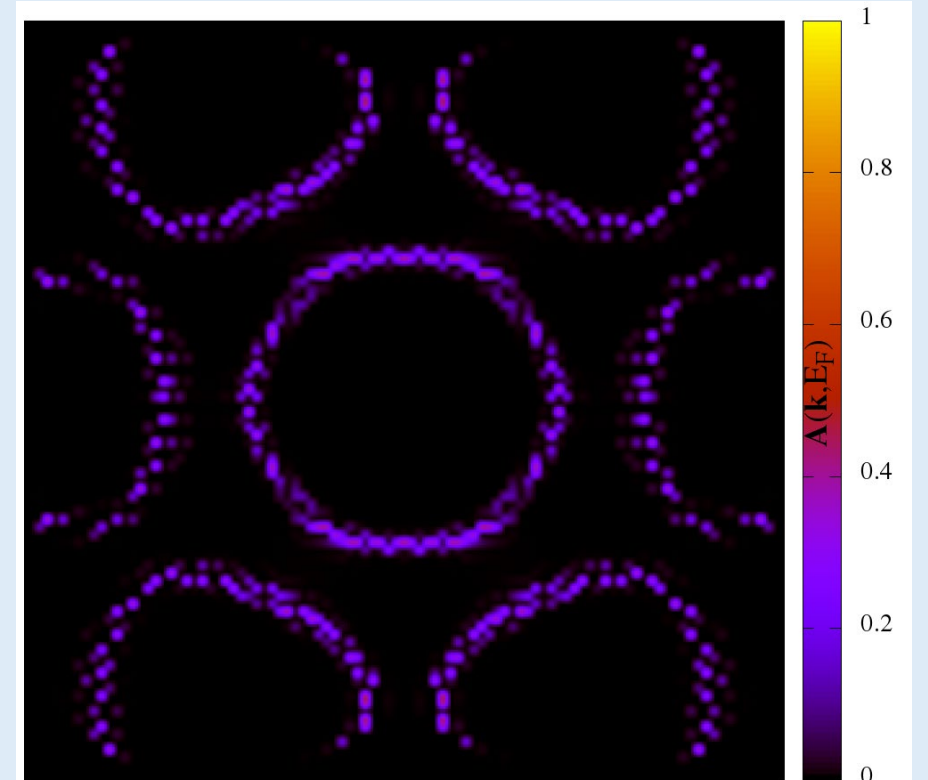
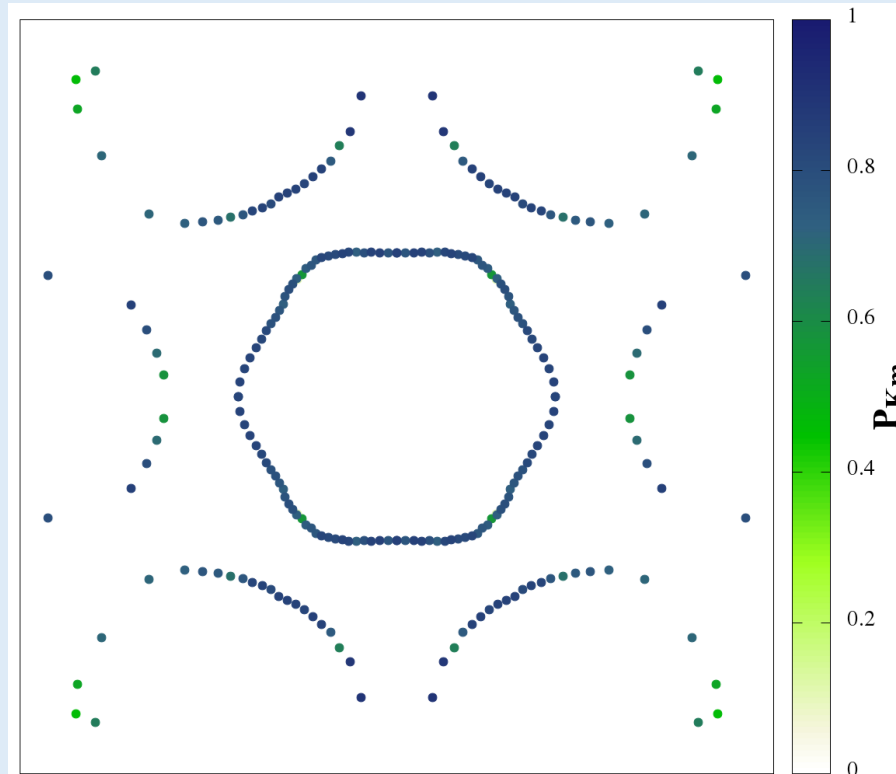
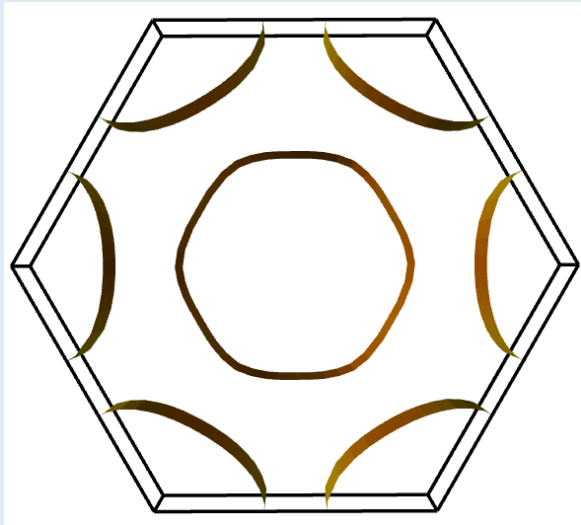
```
SYMPOINT1 = 0.0 0.0 0.0
```

```
EDELTA1 = 3.0  
EDELTA2 = 3.0
```

```
DBLOCH = 0.6
```

```
EGAP = 0.4
```

```
BLOCH_THRESHOLD = 0.05
```



Fermi Surface (NbSe2 unit)

Fermi Surface (Unfolded)

Fermi Surface Spectral Function (Unfolded)

30 jobs
Radial Centered
Gamma

```
k-gen  
30  
p  
line  
rec  
#makepath  
0.000000 0.000000 0.000000 ! Center  
0.666666 -0.333333 0.000000 ! Start Kbar  
0.000000 0.500000 0.000000 ! End Mbar
```

INPAR

```
SIGMA = 0.04  
SPECDELTA = 0.0001
```

```
SLIMSPEC = .FALSE.
```

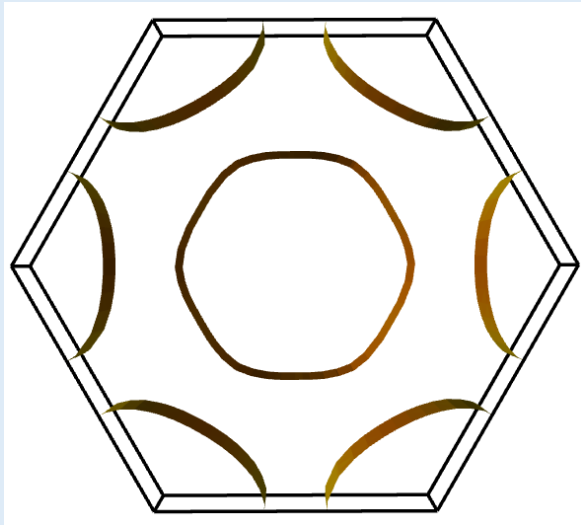
```
SYMPOINT1 = 0.0 0.0 0.0
```

```
EDELTA1 = 3.0  
EDELTA2 = 3.0
```

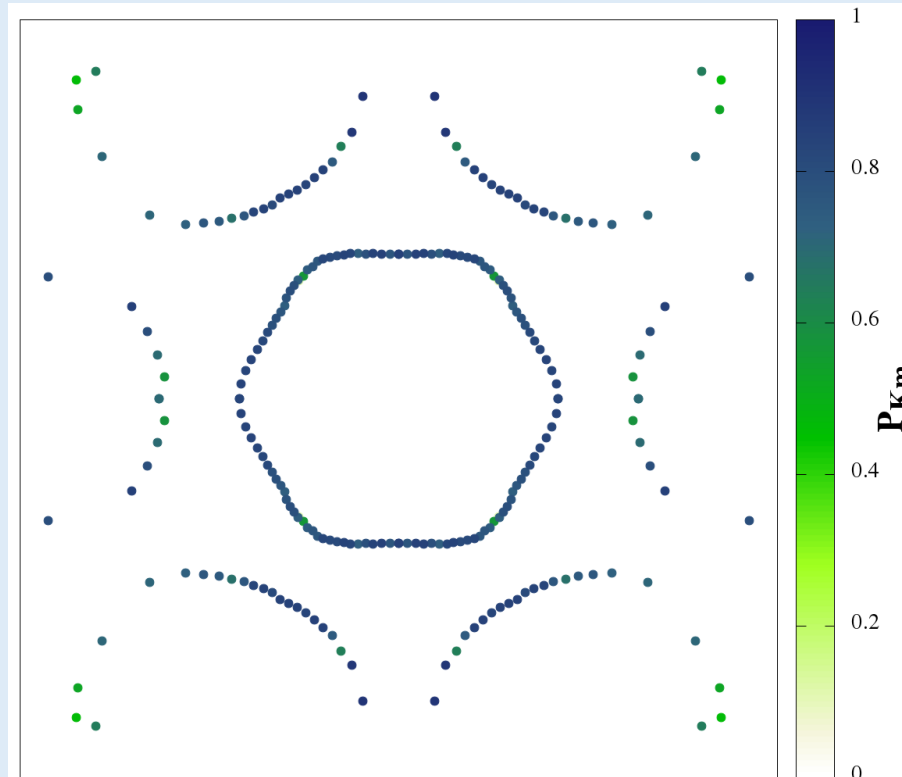
```
DBLOCH = 0.6
```

```
EGAP = 0.5
```

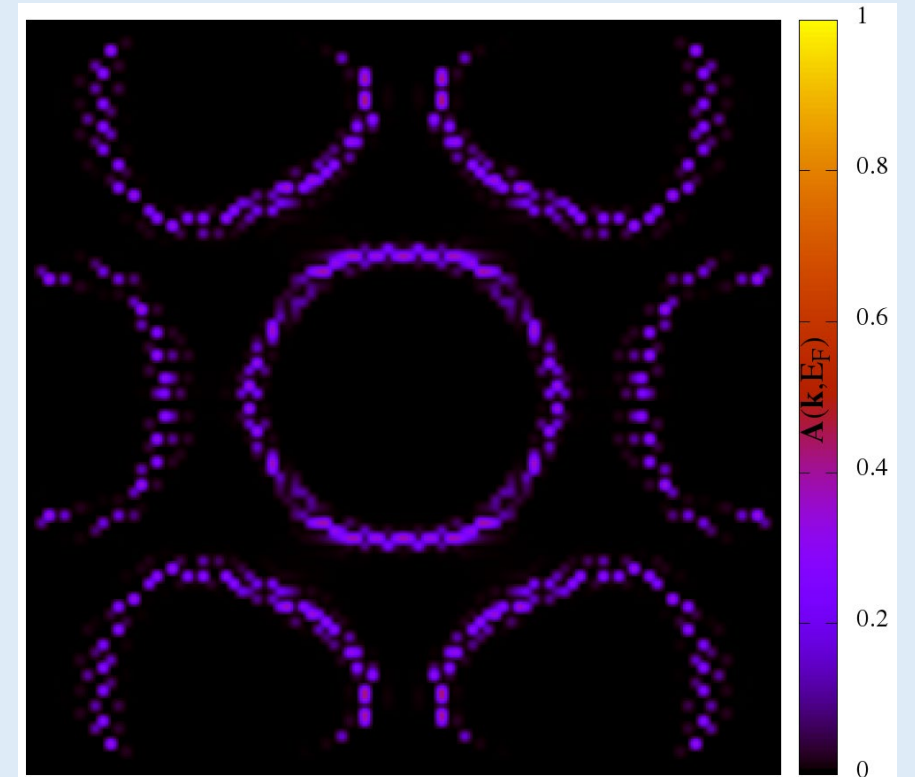
```
BLOCH_THRESHOLD = 0.05
```



Fermi Surface (NbSe2 unit)

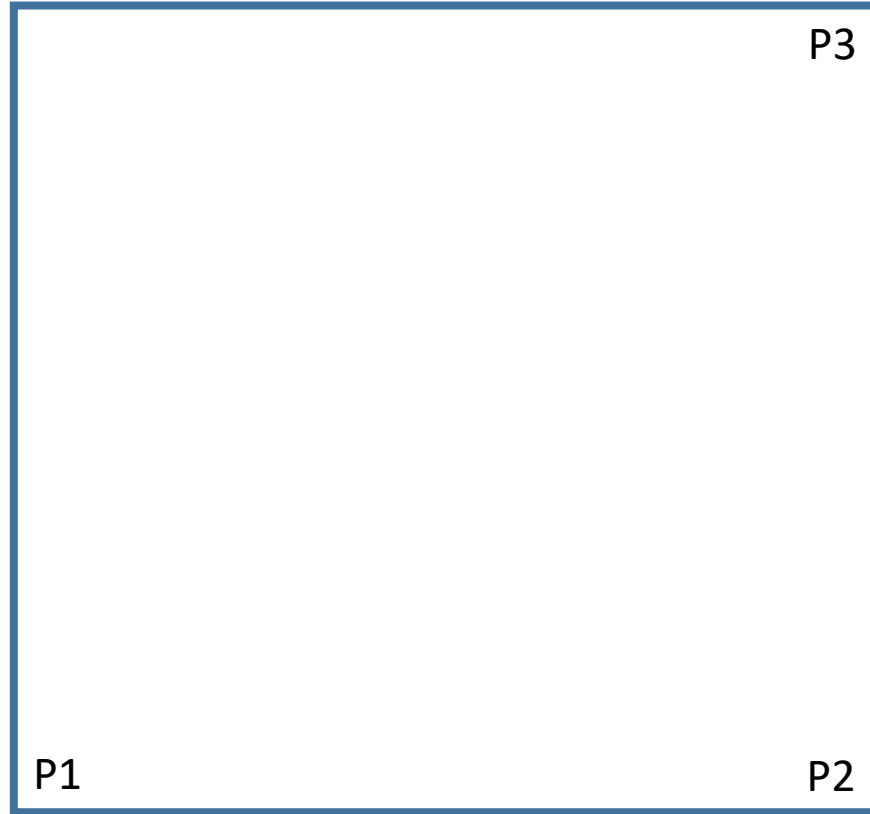


Fermi Surface (Unfolded)



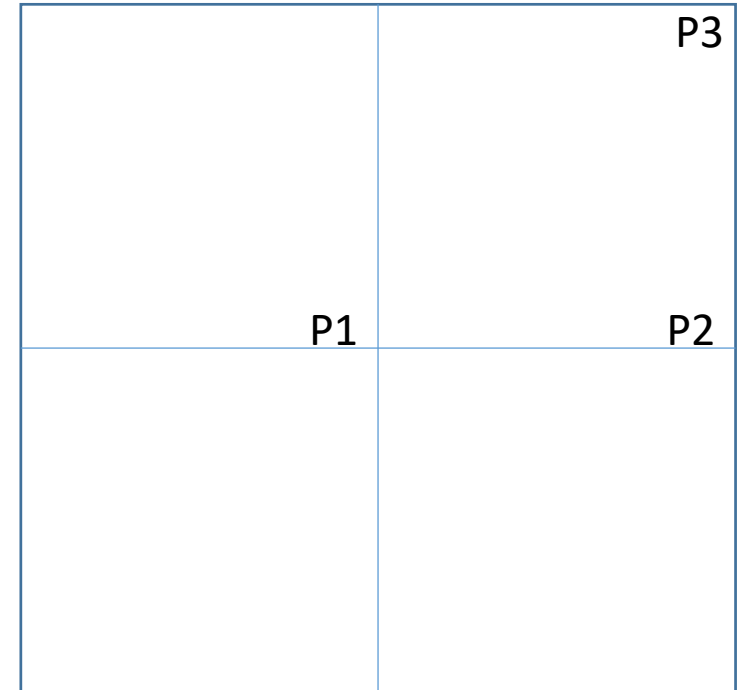
Fermi Surface Spectral Function (Unfolded)

3rd Corner of Rectangle
Defines translational direction of lines



1st Corner of Rectangle
Calculation Start

2nd Corner of Rectangle
Defines path of line calculation



90 jobs
Radial Centered
Gamma

```
k-gen  
60  
p  
line  
rec  
#makepath  
0.000000000 0.000000000 0.000000000 ! Center  
1.520233900 -0.760116950 0.000000000 ! Start Kbar_extended  
0.000000000 1.699673171 0.000000000 ! End Mbar_extended
```

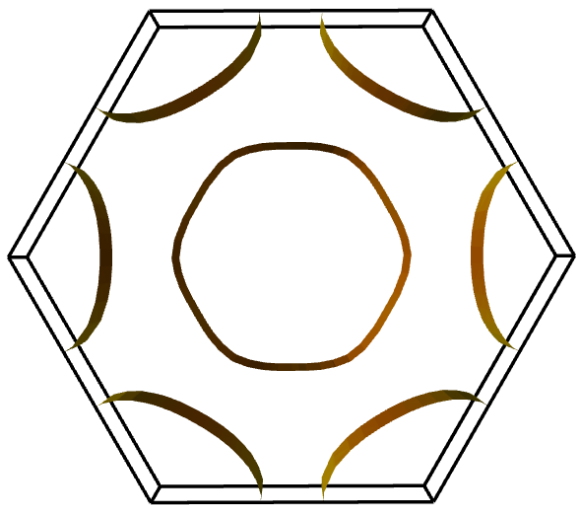
INPAR

SIGMA = 0.03
SPECDELTA = 0.001

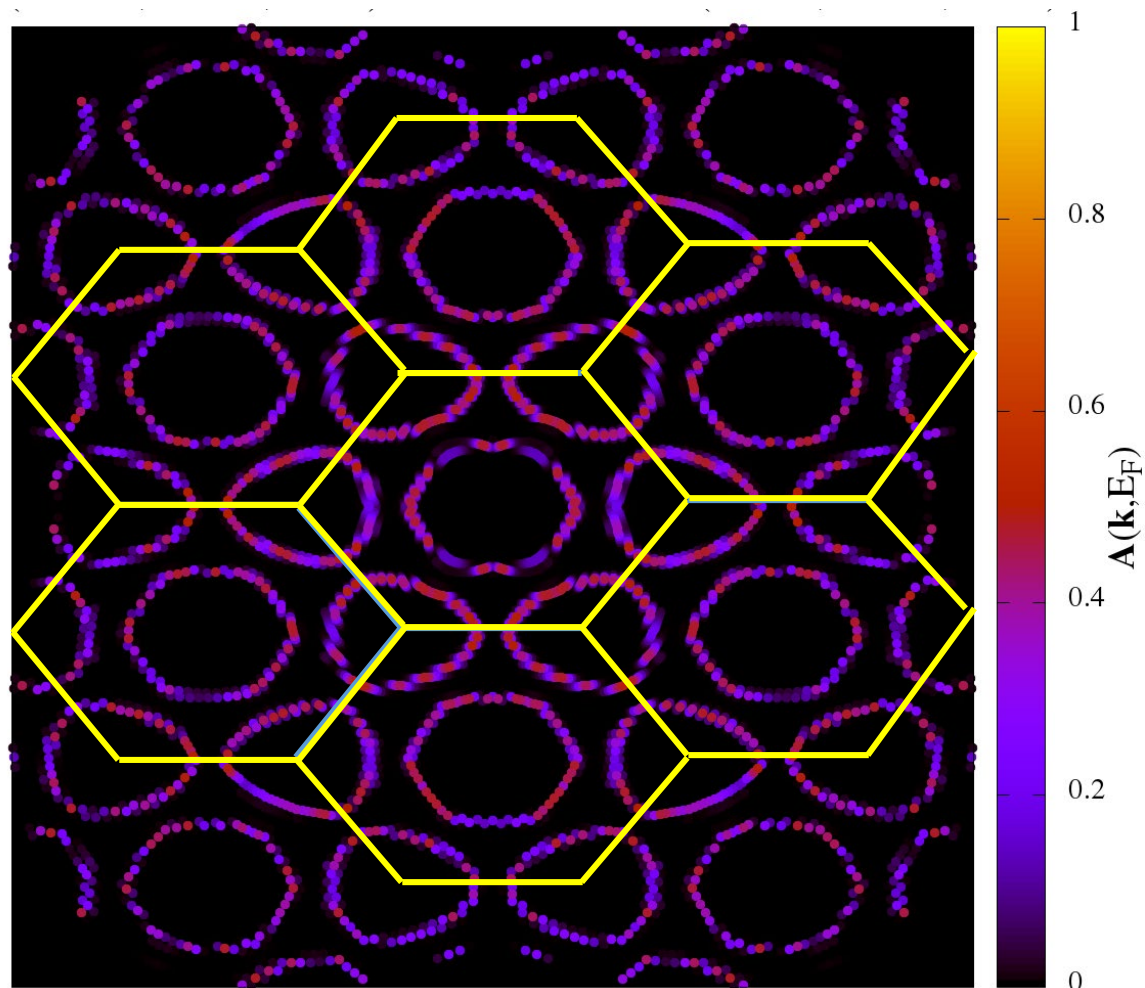
SYMPOINT1 = 0.0 0.0 0.0

EDELTA1 = 3.0
EDELTA2 = 3.0

SLIMSPEC = .TRUE.



Fermi Surface (NbSe2 unit)



Fermi Surface Spectral Function
(Unfolded)