

Kai

$\chi(\mathbf{q})$ Calculation from Tight-Binding Energy Band Calculation

\mathbf{q} -Dependent susceptibility $\chi(\mathbf{q})$ is calculated on the basis of energy band $E(\mathbf{k})$.

$$\chi(\mathbf{q}) = g^2 \mu_B^2 / 2V \sum n_{\mathbf{k}}(1-n_{\mathbf{k}+\mathbf{q}}) / (E(\mathbf{k}+\mathbf{q}) - E(\mathbf{k})).$$

The computer gives $\chi(\mathbf{q}) / g^2 \mu_B^2$, which has the same dimension (states/eV) as the density of states. This program is a specialized modification of tmap, so that the input data are mostly the same as tmap.dat.

Input data: tmap.dat
Source: kai.f
Indy: kai.out
PC: kai.exe

This program generates the following output files:

Output: tmap.out
Output: tmap.gra for input of gnuplot
Output: tmap.kai for input of gnuplot

Test Data

The supplied input files are for λ -(BETS)₂FeCl₄.

(1) Download tmap.kai.dat and the kai executable program suitable for your computer.

(2) Change the filename tmap.kai.dat to tmap.dat.

(2) Run kai. This program generates tmap.out, tmap.gra, and tmap.kai. Open tmap.out and check the calculation is OK.

(3) Run gnuplot to draw $\chi(\mathbf{q})$. The following is the example of the procedure.

```
set parametric
view 40,120,,2.0
splot "tmap.kai" with lines
set terminal postscript
set output "tmap.kai.ps"
replot
quit
```

Input Data

The following is an example of input data in tmap.kai.dat.

The input data are the same as tmap.dat except the final one line.

```

16.164    18.358    6.5928    98.40    96.67    112.52
  4  0.0  0.0  0.0
0
0.03332   0.01861   0.01561   -0.00334   -0.00938   0.01283
0.01786   0.002665

  0.0      0.0      0.0
0 0 2 1 0 0 1 0 2 1 0 0 1 0 0 0
  0.0      0.0      1.0
5 0 0 6 0 4 6 0 7 0 5 0 0 0 0 4
  1.0      0.0      0.0
0 0 0 0 0 0 0 0 0 0 0 0 0 3 0 0
  1.0      0.0      1.0
0 0 0 0 0 0 0 0 0 0 0 0 0 8 0 0
10.0
  3    1    2    20  -20    1
0.02   -0.7    1.0    0.75
1
0 10  0.0  0.0  0.0
0  5 -1.0  0.0  1.0
1  5 -1.0  0.0  1.0  0.0  0.0  1.0  2  0.0
0 10  0.0  0.0  1.0
0 10  0.0  0.0  0.0
0 10  1.0  0.0  0.0
1 10  1.0  0.0  0.0  1.0  0.0  1.0  2  0.0
10
11
  1    2

```

Line 14 **1** **2** (2I2)
 Include from the **1**-st (upper) energy level to the **2**-nd energy level for the calculation of $\chi(\mathbf{q})$. These energy levels are those having the Fermi surfaces.