MCGR PRACTICAL

Modelling the *G*(*r*) from a bad *S*(*Q*) of molten Copper

All the files needed for this practical, including programs, are found in the file **mcgr_err_cu.zip**. Extract them all into the same directory. You should have the following:

mcgr_31.exe
rmcplot.exe
show.exe
cu_err_mcgr.dat
cusq_err.dat

The aim of this practical is to demonstrate how an error in the measured structure might be identified using MCGR.

The times given in this practical, for running MCGR and RMC is real time and <u>NOT</u> CPU time. The times may have to be increased on a slow computer. The outputs you get, will probably not be identical to the outputs in this example.

1. Neutron scattering data of molten copper is in the file **cusq_err.dat**. Plot it with the program **show**.

```
File format (RAW, TEXT, DATA)? data
Full File name: cusq_err.dat
Blocks no: 1 to 1 exists.
> d 1
```
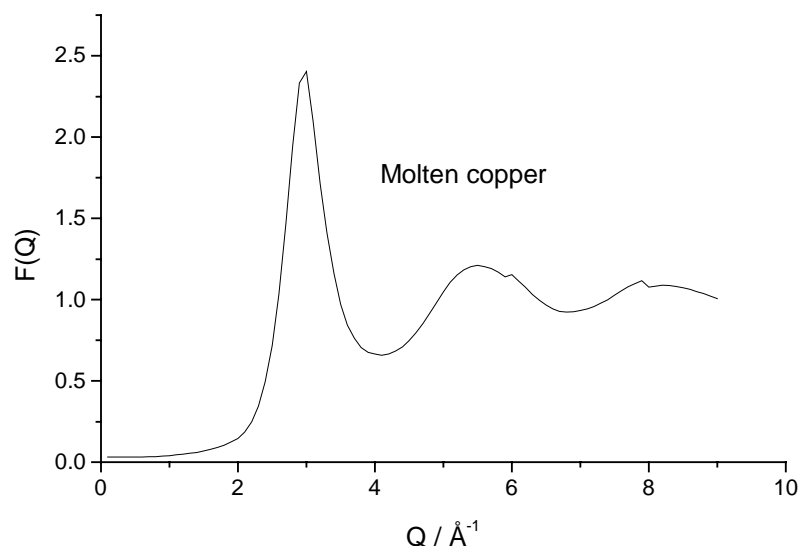
Now you should have a plot on the screen.

To plot with other limits

```
> d 1 Xlow Xhigh Ylow Yhigh
```

To exit

```
> e
```

We see that there must be an error after merging different detectors for Q values between 6 and 8 Å^{-1}. In the present case the error is obvious, but the same error for a crystalline material would be much less obvious.

2. To see how this affects the radial distribution function $G(r)$ we run the program MCGR with control data from the file **cu_err_mcgr.dat**. First look at **cu_err_mcgr.dat** (use an editor like Wordpad):

```
Liquid copper (test MCGR control file)
.false.            ! rerun
.true.             ! plot
2000               ! nplot
0.0721             ! density
.false.            ! generate partials
1                  ! no of partials
1                  ! no of zero constr.
1 0. 2.0
0.05               ! delta
5   20.            ! mr rmax
.false.            ! save
.false.            ! converge only
1                  ! no of positivity constr.
1 0. 20.1
0                  !no of coord. constr.
.true.             ! smoothing
3                  ! nsmooth
1                  ! nchanges
0.1,21.            ! gau_sig,r_change
.false.            ! resolution
1000               ! printing
15 5               ! time limits
1 0                ! no of data sets
cusq_err.dat
1 90               ! points to use
1.                 ! constant
1.0                ! coefficients
0.005              ! sigma
.false.            ! renormalise
.true.             ! background
1                  ! npar
.false.            ! magnetic
cu_err_mcgr
```

Here we vary a horizontal background (npar = 1). Run **mcgr_31** with this control data.

3. Plot the fit with the **rmcplot** program:

```
Graphics device/type (? to see list, default /NULL): /ws
File to plot (or RETURN to exit) > cu_err_mcgr.out
Input file contains 2 groups of plots:
 Group 1 contains 1 plots of 3 curves
 Group 2 contains 1 plots of 1 curves
Plot which group (enter 0 to exit) ? 1
```
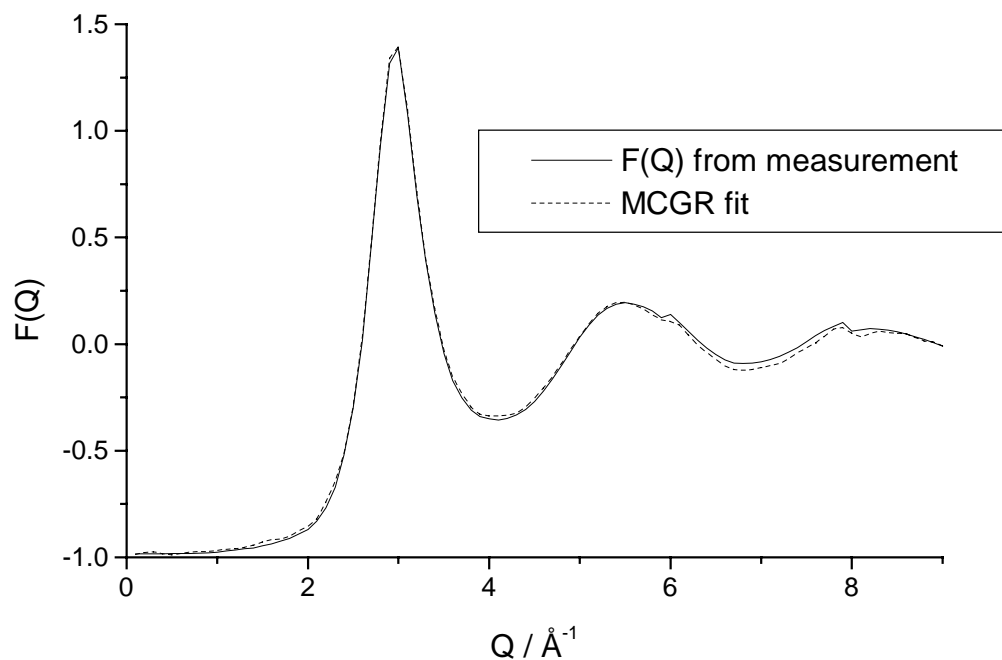
Change plot limits to see how the error in *F(Q)* affects the fit. Below we have plotted the difference (no program for this is supplied to do this you have to do it yourself).
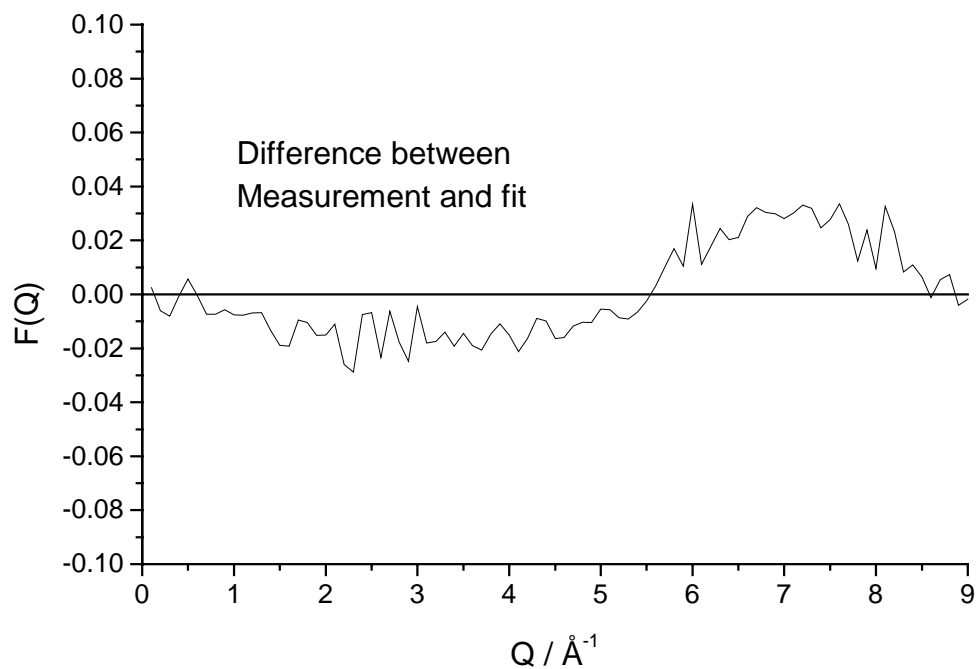
Even if there is a tendency to fit the step between 6 and 8 Å^{-1}, the fit stays at the "correct" level. The rest of the data and constraints on the model do not support the error in the data. In this way it is easy to find problems in data.
Look at *G(r)* from the same fit.
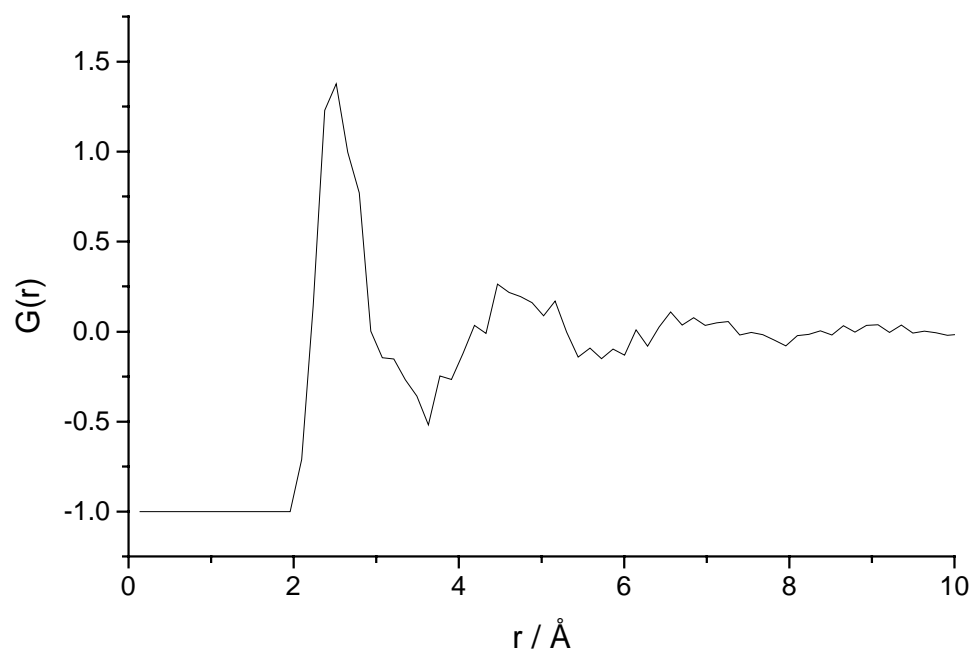
G(r) a look reasonable but it is spikier than the results obtained with the RMC practical of molten copper.