MCGR PRACTICAL

Modelling of $G(r)$ for CS_2

All the files needed for this practical, including programs, are found in the file **`mcgr_cs2.zip`**. Extract them all into the same directory. You should have the following:

`coord.exe`
`mcgr_31.exe`
`rmcplot.exe`
`show.exe`
`cs2.fq`
`cs2_mcgr.dat`
`cs2_mcgr_0.dat`

The general approach in this practical is as follows:

- Calculate a pair distribution function *G(r)* from the measured structure factor of CS_2.
- Try different backgrounds to see how it affects the result.

The times given in this practical, for running MCGR and RMC is real time and NOT 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.

The neutron scattering data is contained in the file **cs2.fq**. Plot it with the program show.

```
File format (RAW, TEXT, DATA)? data
Full File name: cs2.fq
Blocks no: 1 to 1 exists.
> d 1
```

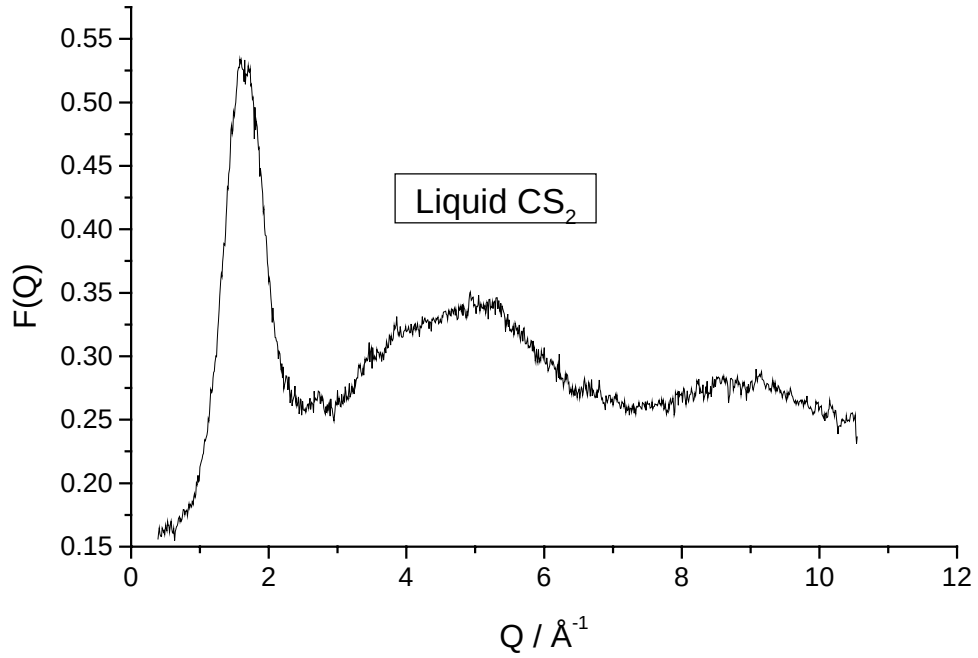
Now you should have a plot on the screen.

To plot with other limits:

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

To exit

```
> e
```



The data only reaches Q=10.5 Å^{-1}, and has a slope (due to bad background correction or Placzek correction). We will see how this affect the result.

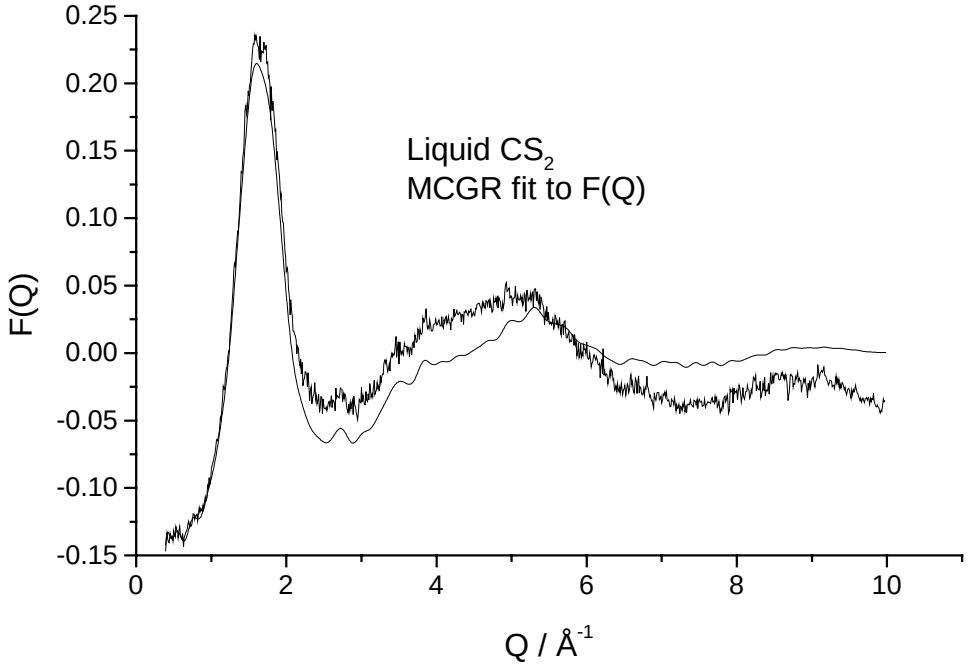
2. *G(r)* is produced using the MCGR program. The control data are in **cs2_mcgr_0.dat**. Use an editor (like Wordpad) to look at the control data.

```
Liquid CS2
.false.          ! rerun
.true.           ! plot
500              ! nplot
0.030            ! density
.false.          ! generate partials
1                ! no of partials
1                ! no of zero constr.
1 0 1.2
0.01             ! delta
6 30.            ! mr rmax
.false.         ! save
.false.         ! converge on
1               ! positively constr.
1 0 30
1               ! no of coord. constr.
1 1.2 1.9 0.667 0.0841 2. 0.01
.true.          ! smoothing
3               ! nsmooth
2               ! nchanges
0.1 1.9
0.6 31.         ! gau_sig,r_change
.false.         ! resolution
500             ! printing
60,5            ! time limits
1 0             ! no of data sets
cs2.fq
1 960           ! points used
0.0             ! const. to subtract
0.1692          ! coeff.
0.002           ! sigma
.false.         ! renormalise
.true.          ! background
1               ! nback
.false.         ! magnetic
cs2_mcgr
```

Here we only let the background be a constant level (nback = 1).
Run the program **mcgr_31** and give **cs2_mcgr_0.dat** as input file. This will take 60 minutes. On the screen you can see how χ^2 decreases as the fitted *F(Q)* approach the experimental *F(Q).* You can also see how the fit of *F(Q)* changes together with corresponding *G(r).*

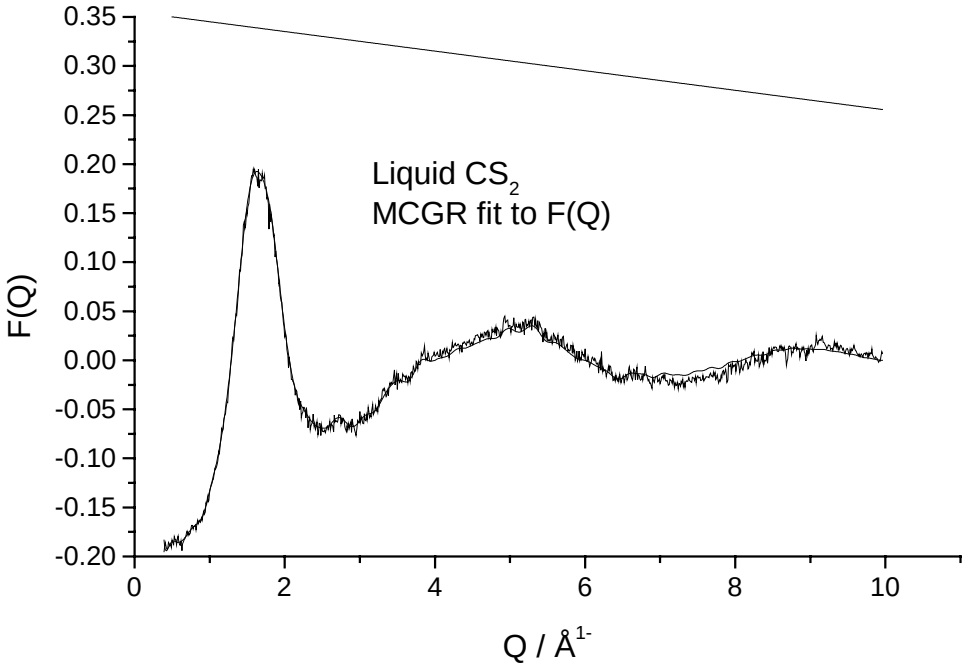
3. Plot the fit to *F(Q)* and the resulting *G(r)* from the MCGR run. Use the program **rmcplot**.

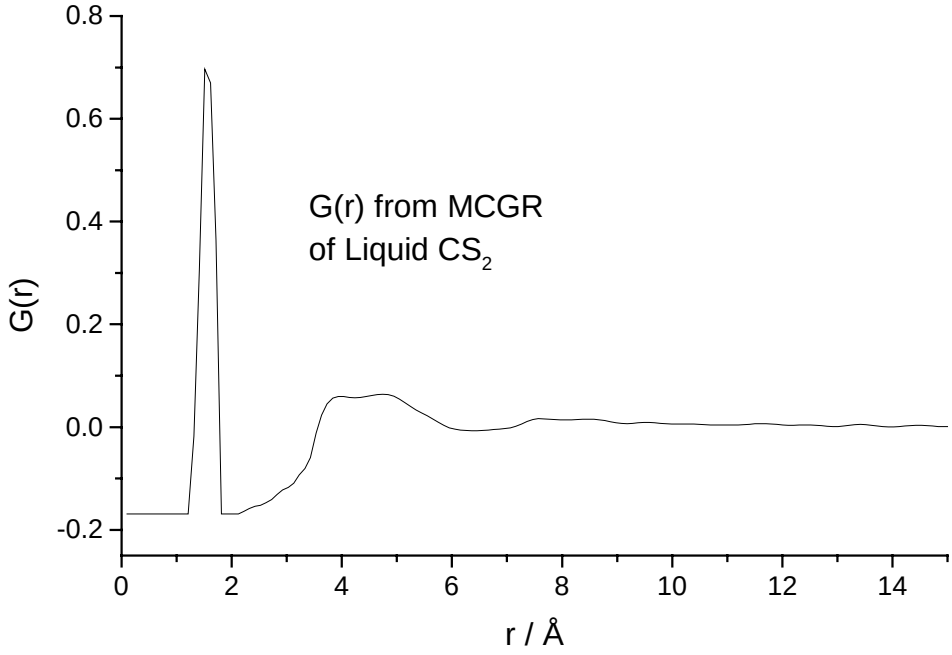
```
Graphics device/type (? to see list, default /NULL): /ws
File to plot (or RETURN to exit) > cs2.out
Input file contains   2 groups of plots:
  Group   1 contains   1 plots of  3 curves
  Group   2 contains   1 plots of  1 curves
Plot which group (enter 0 to exit) ? 1
```



MCGR is not able to make a good fit to *F(Q)*. We need to use a sloping background. Run **mcgr_31** again, this time with **cs2_mcgr.dat** as input. Here we use nback = 2, corresponding to a linear background. To save time we can continue from the previous result by letting rerun = .true.. Expected χ^2 ~10.

4. Plot the result in **cs2.out** again.





Now the fit is much better. In *G(r)* we have a very well defined peak from C-S pairs. This peak should have a coordination of 2 S-atoms around each C-atom. To check this use the program **coord** as shown below:

```
File containing g(r): cs2.g
Density: 0.030
Add constant [0.]: 0.1692
Concentration [1.]: 0.6667
Coefficient [1.]: 0.08409
Write a file with cumulative coordination (y/n)? n
Select min/max r-value G=Graphically or N=Numerically: n
Minimum r-value [0.]:
Maximum r-value [Max-r]: 2.0
Coordination=    2.10
```

The coordination of 2.10 is good. This was obtained from the data even though the background correction in the original data was bad and the *Q* range is relatively short.