Methoden moderner Röntgenphysik: Streuung und Abbildung

Lecture 18	Vorlesung zum Haupt- oder Masterstudiengang Physik, SoSe 2021
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Location	online
Date	Tuesday 12:30 - 14:00 (starting 6.4.)
	Thursday 8:30 - 10:00 (until 8.7.)

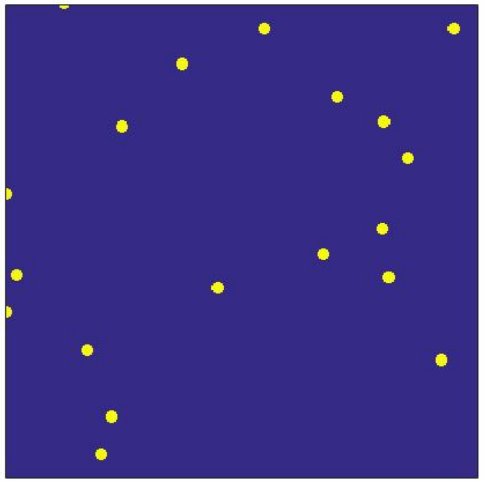
Soft Matter – Timeline

- Do 27.05.2021 Soft Matter studies I: Methods & experiments
  Definitions, complex liquids, colloids, storage ring and FEL experiments, setups, liquid jets, **…**
- Di 01.06.2021 Soft Matter studies II: Structure
  SAXS & WAXS applications, X-ray cross correlations, **…**
- Do 03.06.2021 Soft Matter studies III: Dynamics
  XPCS applications, diffusion, dynamical heterogeneities, …
- Di 08.06.2021 XPCS & XCCA simulations and modelling
- Do 10.06.2021 Case study I: Glass transition
  Supercooled liquids, glasses vs. crystals, glass transition concepts, structure-dynamics relations, …
- Di 15.05.2021 Case study II: Water
  Phase diagram, anomalies, crystalline and glassy forms, FEL studies, …
- Do 17.06.2021 Outlook: Opportunities at new facilities

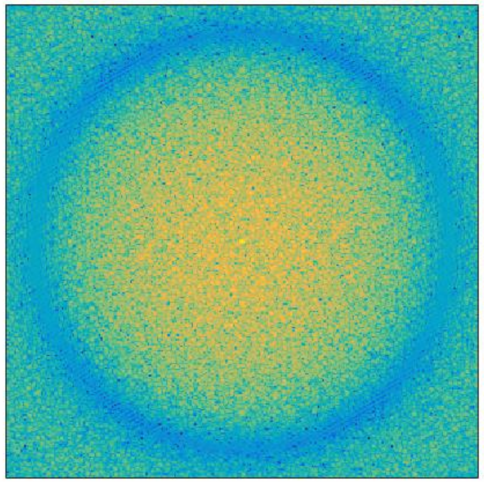
XPCS modelling

Diffusing particles
- Real space particle placement
- Model scattering – SAXS
- Correlation functions

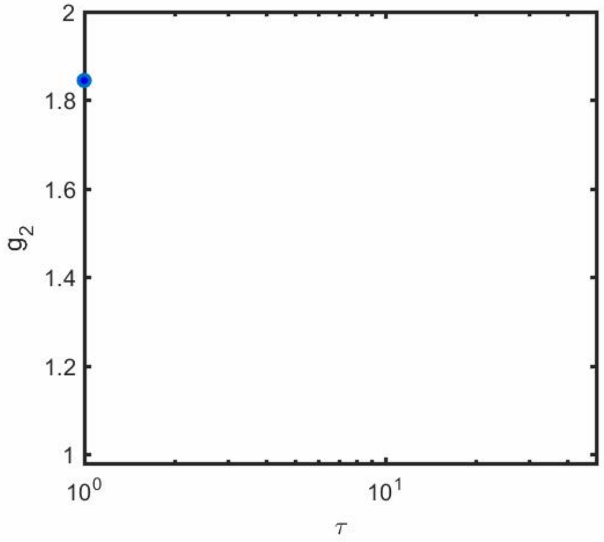
Use Matlab for simulation – many alternatives availble, e.g. Octave, FreeMat, Python



Diffusing particles



Speckle pattern



g_2 function

Matlab basics

Vector and matrices

- `v=[1,2,3]=[1 2 3]` is a linevector
- `w=[1;2;3]` is a row vector
- `A=[1,2;3,4;5,6]` generates 3x2 matrix
- Transpose: `v=w‘`
- Scalar: `x=1` as 1x1 vector

Basic algebra

- `A+B, A-B` : Addition/Subtraction of vectors/matrices of same type
- `A*B, A/B` : Matrixproduct/-division
- `A.*B, A./B` : point-wise Product/Division
- `.^` : point-wise exponent

- Example: `A=[1 2;0 4]; B=[-2 1;3 -1].`
  - `A*B=[4 -1;12 -4]` → Matrix-Multiplication
  - `A.*B=[-2 2;0 -4]` → point-wise Multiplication

Matlab basics

Functions

- Lots of basic vector/matrix functions, e.g.: `abs, max, min, size, length, sum, mean`, …
- In addition, pre-defined function such as: `sin, cos, tan, exp, log, log10`, … and many more
- How to use: `y=abs(x)`. `x` can be a number, vector, matrix etc. for most functions. Attention: operation may be done point-wise or column-wise!
  - Example: `B=[-2 1;3 -1]`.
    - `abs(B)=[2 1;3 1]` → absolute value of each entry
    - `mean(B)=[0.5 0]` → mean of each column
    - `min(B)=[-2 -1]` → minimum of each column
- One can define any type of function
- Information about any function can be obtained by typing „`help FUNCTIONNAME`“, e.g. `help mean`

Matlab basics

Scripts

Typically, scripts are used to work with matlab. Simple example:

```
% This is a comment.
x=[0:1:6]; % define vector x=[0 1 2 3 4 5 6]
y=sin(x); % calculate sinus of x
figure(1) % open a figure with number 1
plot(x,y,'o') % plot y vs. x as open circles
```

- Scripts are saved as .m file and can be called from the Command Window
- The same script can be written more flexible as function, e.g., to change input parameters

Matlab basics

Write simple functions

```
function y=plot_sin_square(x)

% This functions plots the squared sinus of x. y as defined in
% the function is the output.

y=(sin(x)).^2; % calculate squared sinus of x
figure(1) % open a figure
plot(x,y,'o') % plot y vs. x as open circles
```

- Like scripts, functions are stored as .m file, but input parameters.
- Example: `x=0:0.1:6; out=plot_sin_square(x);`

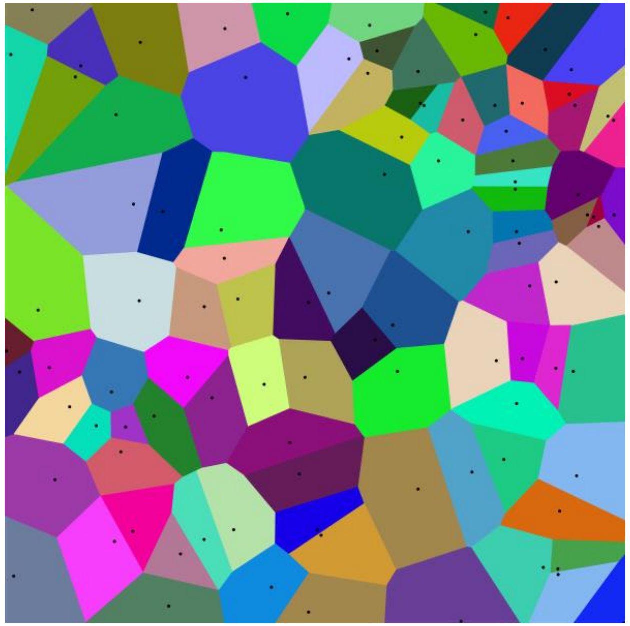
SAXS and XPCS from 2D diffusing discs

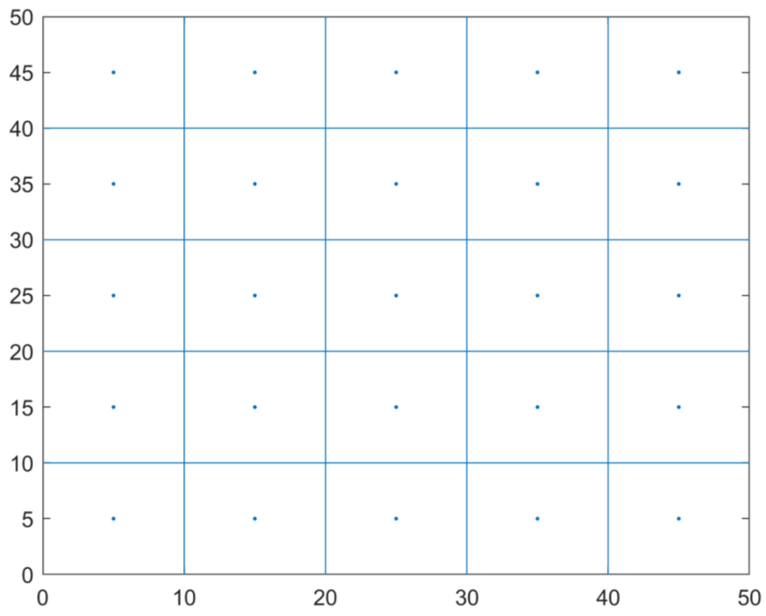
- How to design a 2D system?
- How to simulate diffusion?
- How to simulate scattering?
- How to analyze?

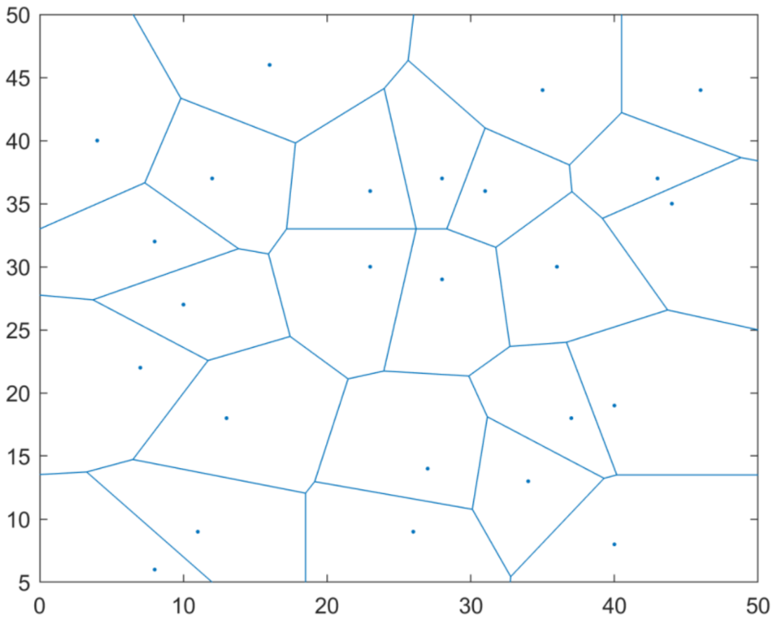
SAXS and XPCS from 2D diffusing discs

Placing particles in 2D

1. Place particles on lattice points
2. Iteratively move particles inside their Voronoi region
3. Repeat some times



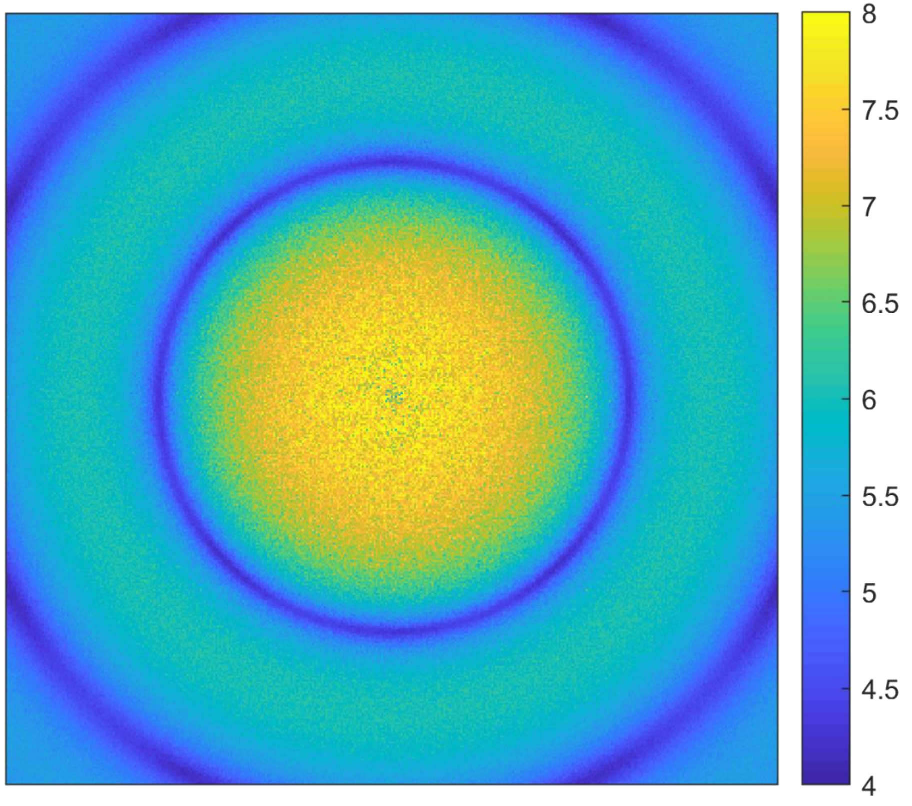




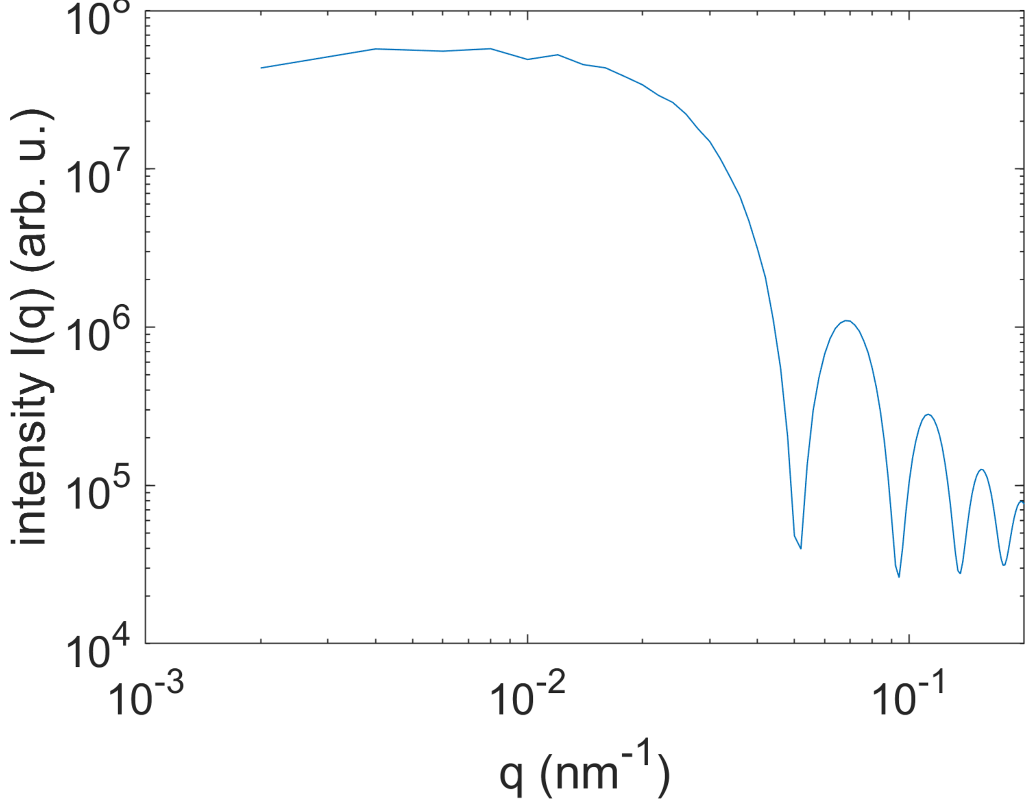
SAXS and XPCS from 2D diffusing discs

Results from xpcs.m

Summed 2D pattern



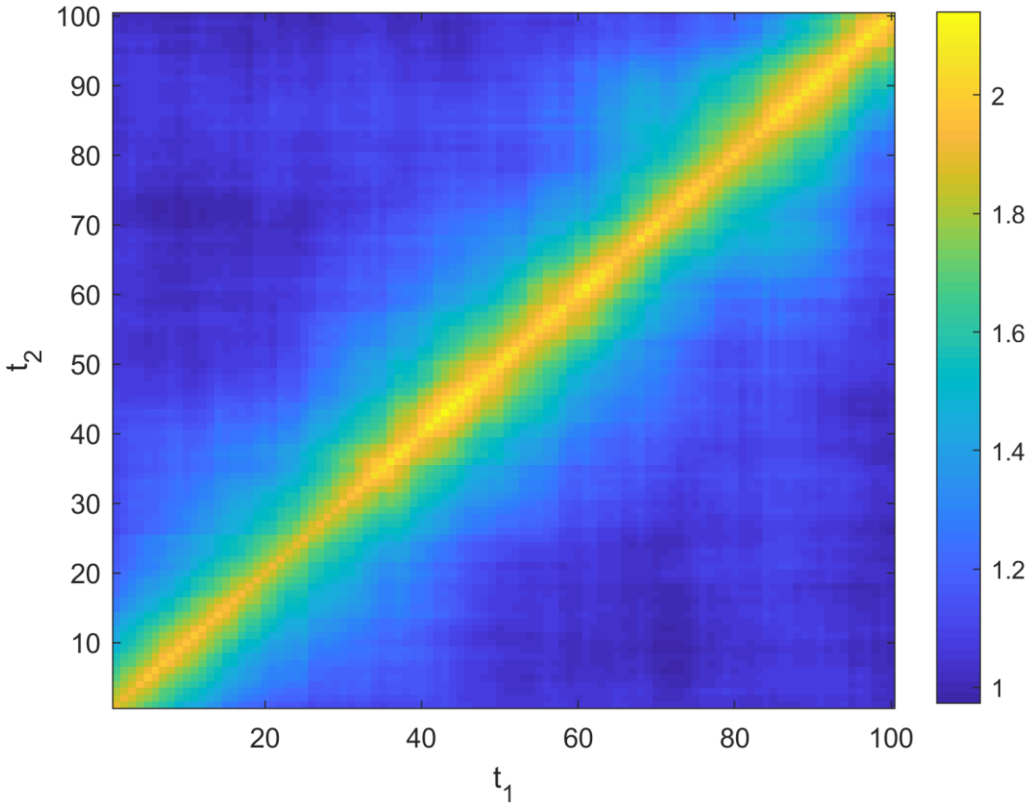
I(q)



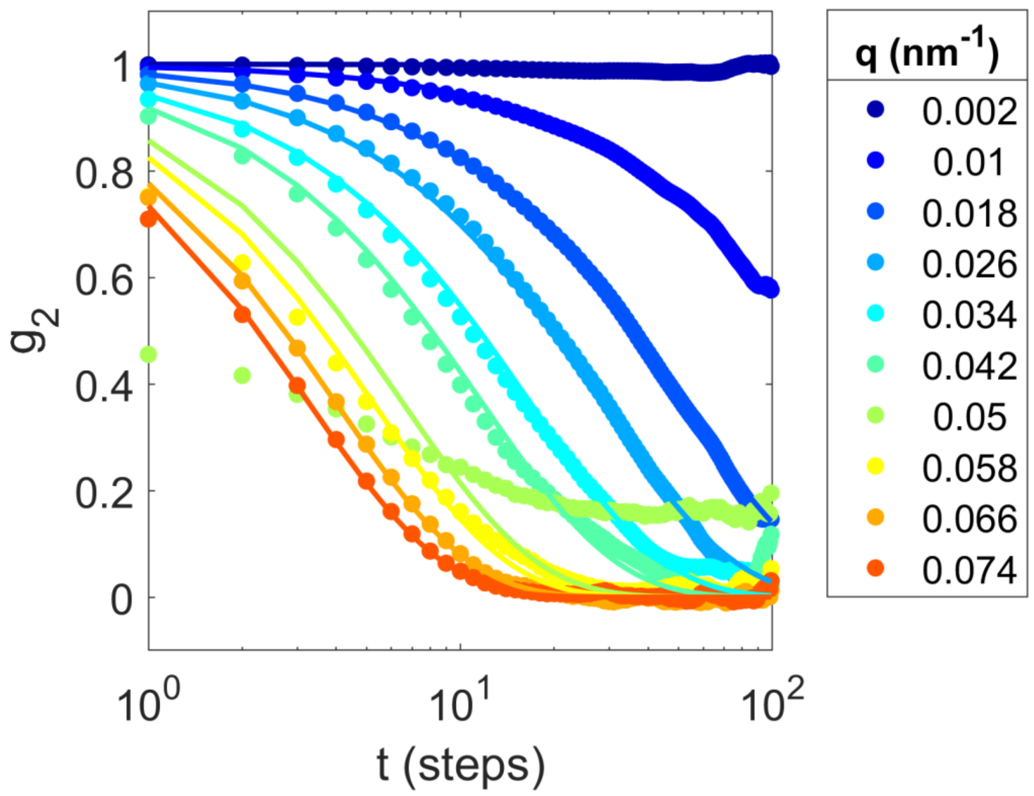
SAXS and XPCS from 2D diffusing discs

Results from xpcs.m

Two time correlation function



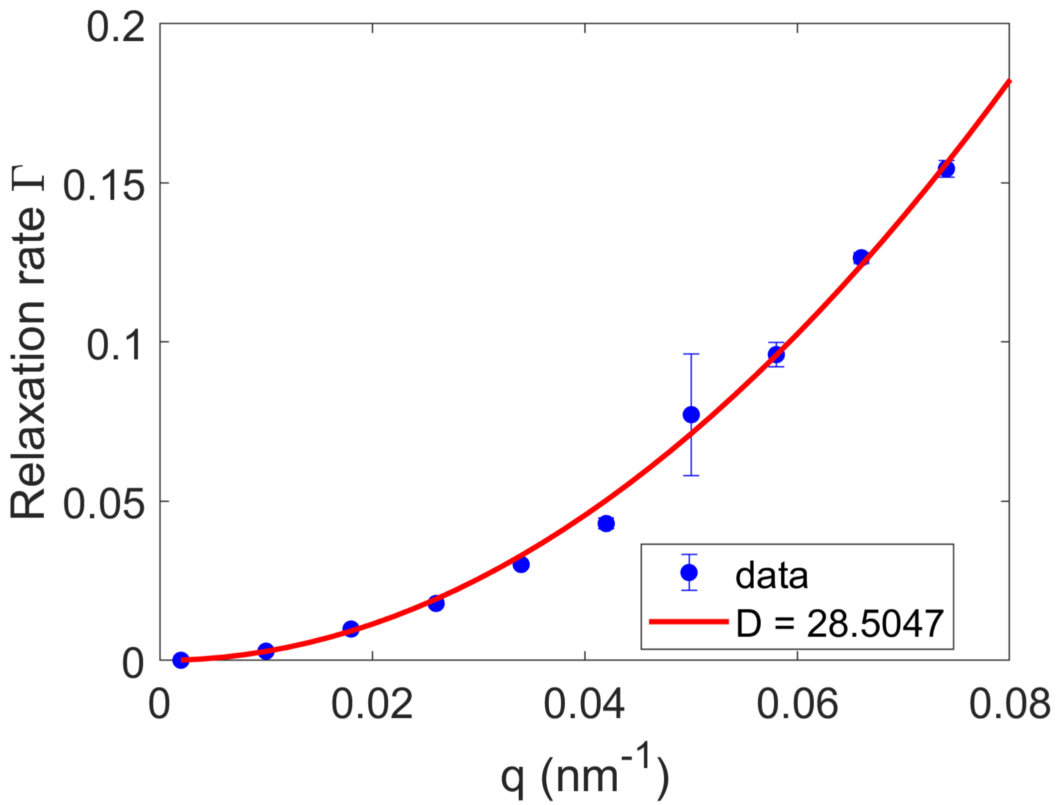
g_2 functions



SAXS and XPCS from 2D diffusing discs

Results from xpcs.m

Relaxation rate $\Gamma = Dq^2$



Further tasks could be:

- Change time scales
- How to model non-equilibrium dynamics, e.g., aging?
- How to obtain different dynamics, such as different q-dependence and/or different KWW exponent?
- How to implement XCCA?
- …