Electronic supplementary data

Two Dimensional Indirect Fourier Transformation for Evaluation of Small Angle Scattering Data of Oriented Samples

GERHARD FRITZ-POPOVSKI*

Institute of Physics, Montanuniversitaet Leoben, 8700 Leoben, Austria.
E-mail: gerhard.popovski@unileoben.ac.at

The effect of various parameter settings for data evaluation using the two dimensional indirect Fourier transformation should be demonstrated using the example of a cuboid introduced in section 4 of the contribution.

1. Variation of the number of azimuthal splines

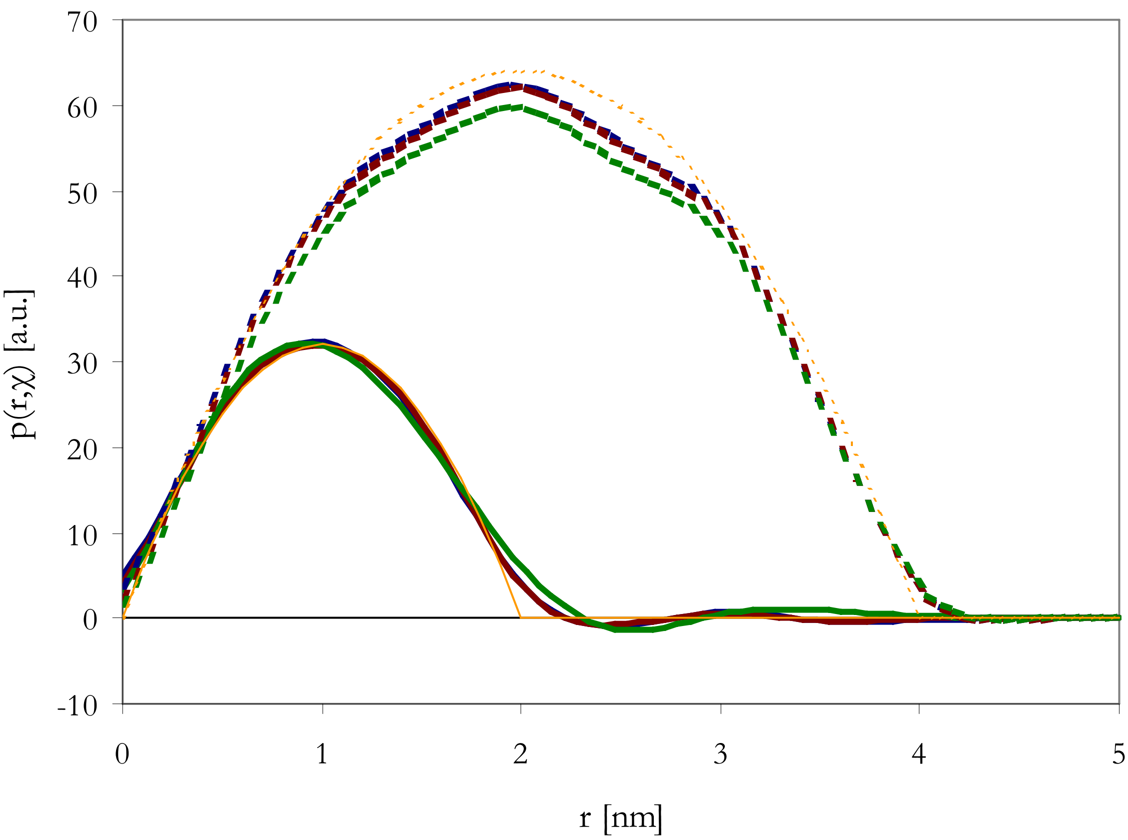

Figure 1: Cuts through the $p(r,\chi)$ functions at χ=0° (solid) and χ=90° (dotted). The number of azimuthal splines is set to n_A=50 (blue), n_A=25 (red), and n_A=10 (green). The orange lines are the theoretical curves.

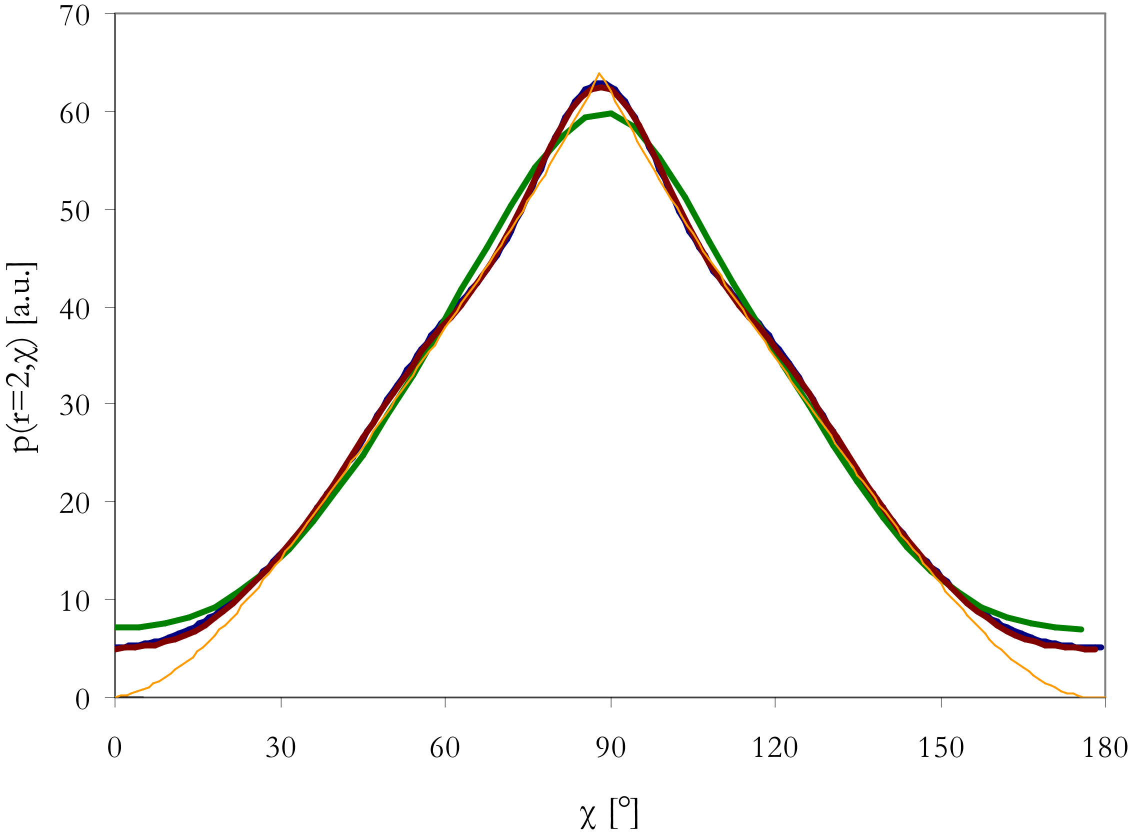

Figure 2: Cuts through the $p(r,\chi)$ functions at r=2 nm. The number of azimuthal splines is set to n_A=50 (blue), n_A=25 (red), and n_A=10 (green). The orange line is the theoretical curve.

Once a sufficient high number of azimuthal splines is found the result no longer depends on the ecact value of the parameter. If the value is too low, not all features can be approximated well.

2. Variation of the number of radial splines

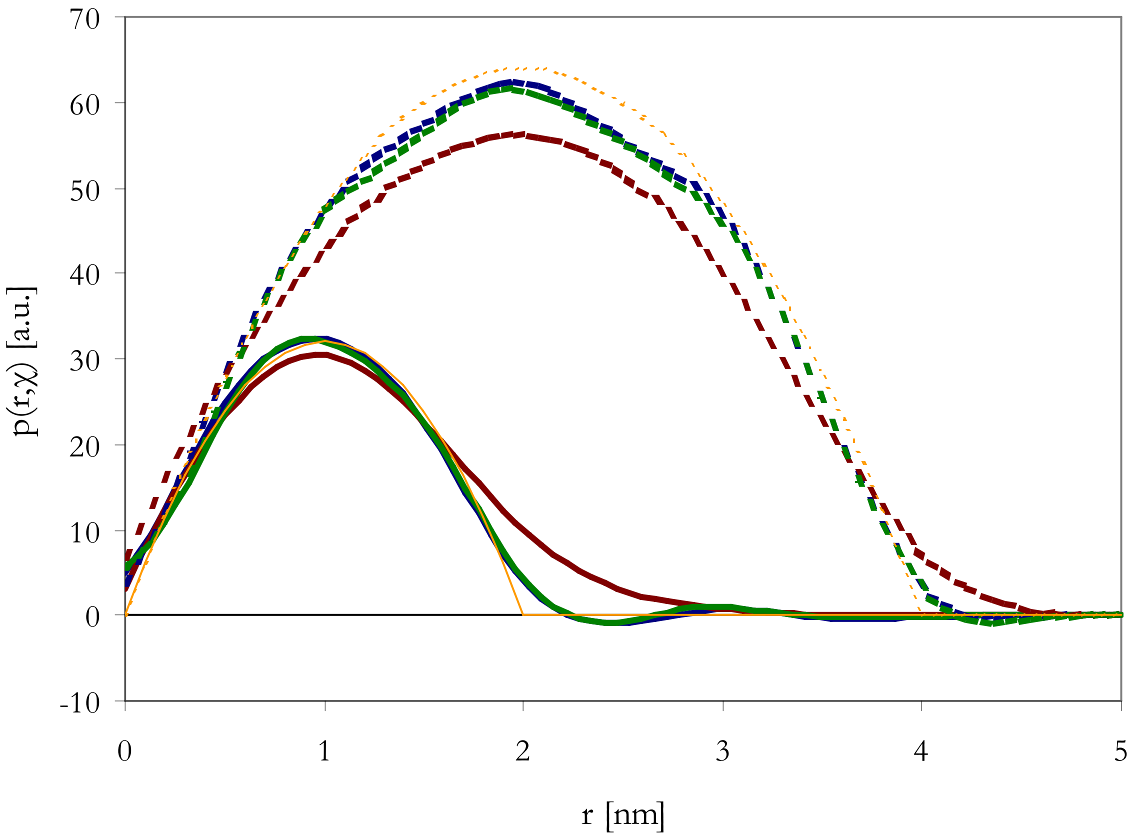

Figure 3: Cuts through the $p(r,\chi)$ functions at χ=0° (solid) and χ=90° (dotted). The number of radial splines is set to n_R=10 (blue), n_R=5 (red), and n_R=15 with 7 of them up to r=2 nm (green). The orange lines are the theoretical curves.

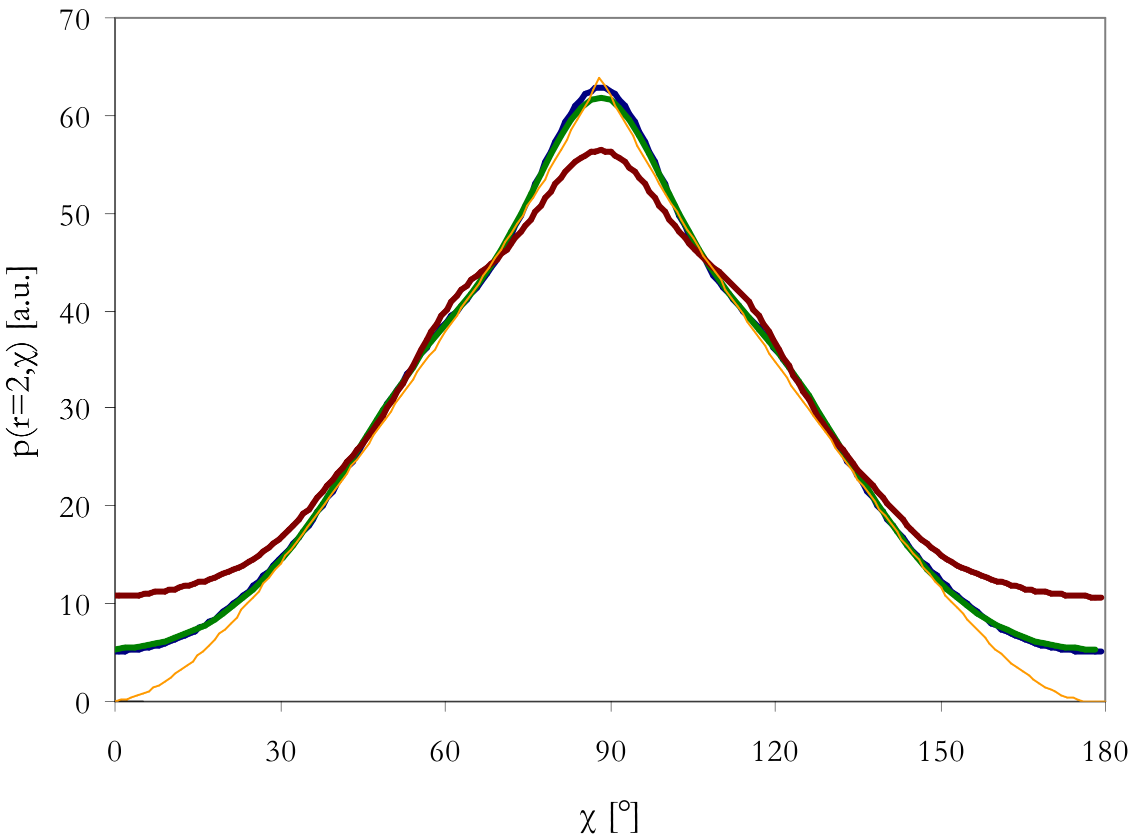

Figure 4: Cuts through the $p(r,\chi)$ functions at r=2 nm. The number of radial splines is set to n_R=10 (blue), n_R=5 (red), and n_R=15 with 7 of them up to r=2 nm (green). The orange line is the theoretical curve.

Like in the case of azimuthal splines the result is stable as soon as a sufficient number of radial splines is selected. Increasing the number of splines in the low r-regime does not influence the function in this case.

3. Variation of azimuthal Lagrange multiplier

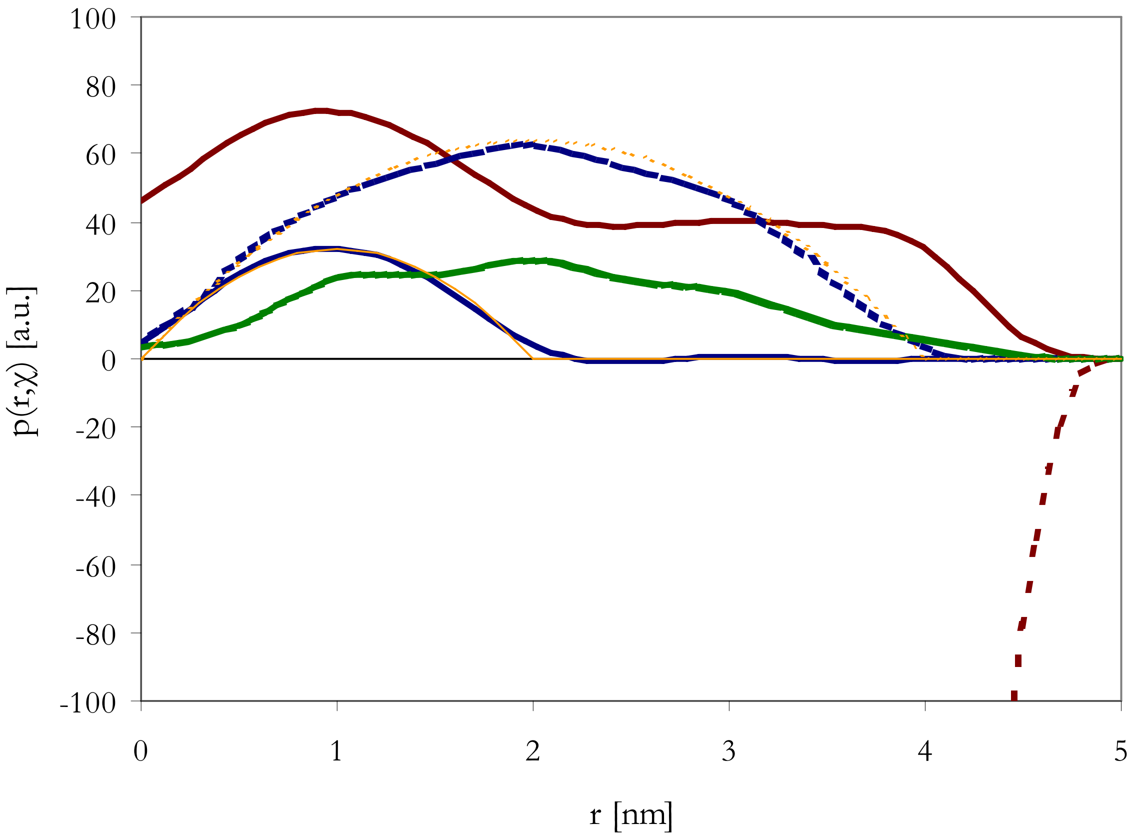

Figure 5: Cuts through the $p(r,\chi)$ functions at χ=0° (solid) and χ=90° (dotted). The azimuthal Lagrange multiplier is set to λ_A=-1 (blue), λ_A=-9 (red), and λ_A=+8 (green). The orange lines are the theoretical curves.

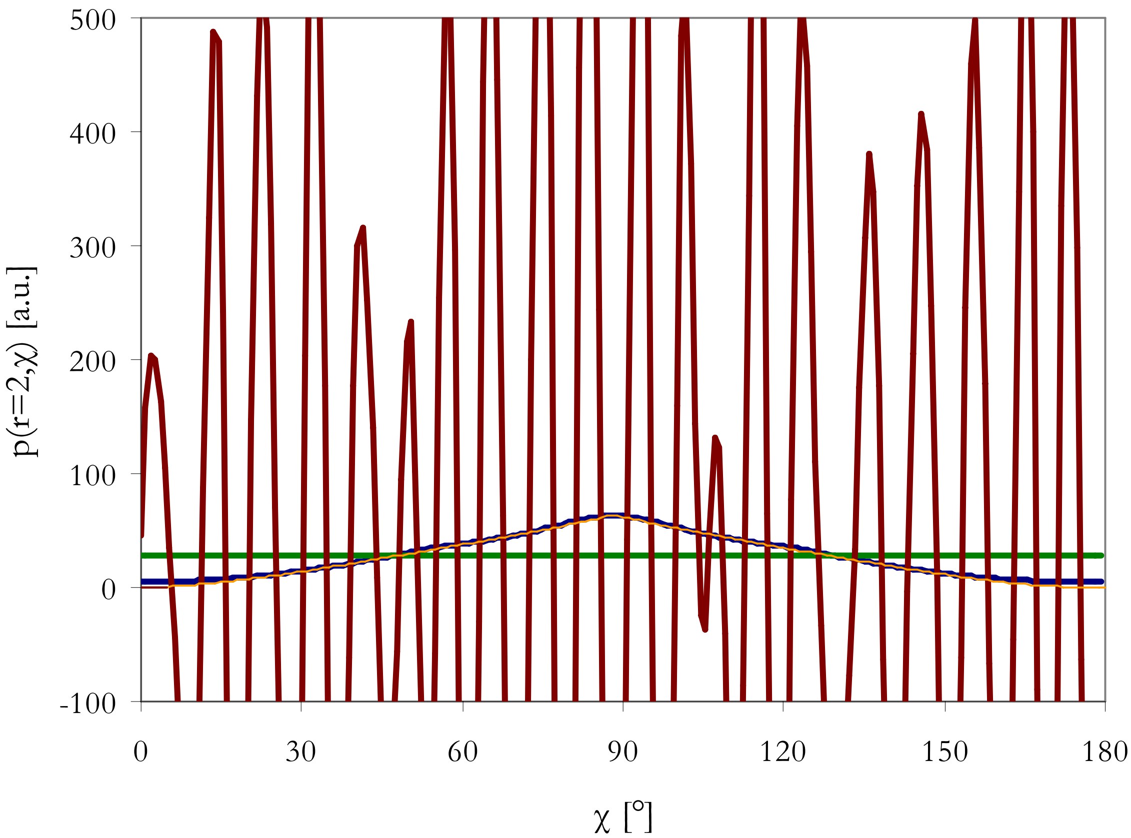

Figure 6: Cuts through the $p(r,\chi)$ functions at r=2 nm. The azimuthal Lagrange multiplier is set to λ_A=-1 (blue), λ_A=-9 (red), and λ_A=+8 (green). The orange line is the theoretical curve.

An azimuthal Lagrange multiplier that is too high results in a centrosymmatric real space curve, where the information of orientation is lost. Cuts through are nearly identical regardless of the angle χ . If the Langrage multiplier is, however, too small than there are strong oscillations in azimuthal direction.

4. Variation of radial Lagrange multiplier

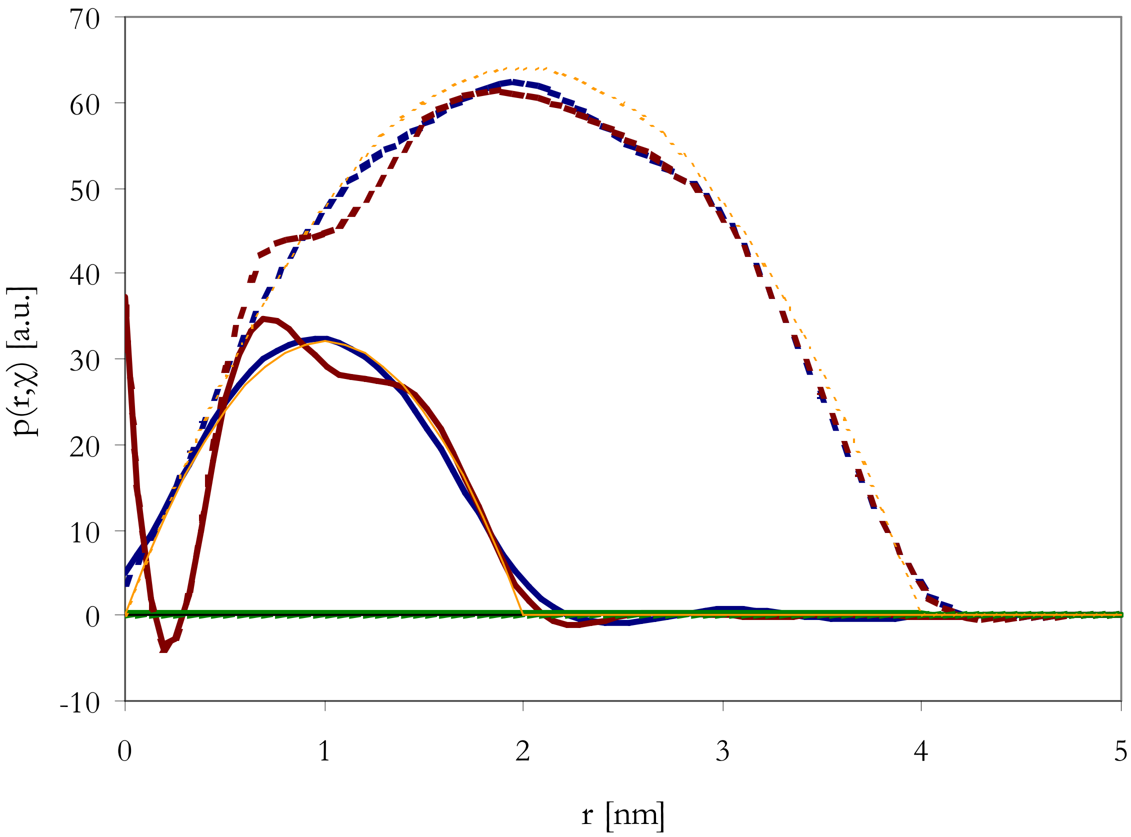

Figure 7: Cuts through the $p(r,\chi)$ functions at χ=0° (solid) and χ=90° (dotted). The radial Lagrange multiplier is set to λ_R=-2 (blue), λ_R=-10 (red), and λ_R=+6 (green). The orange lines are the theoretical curves.

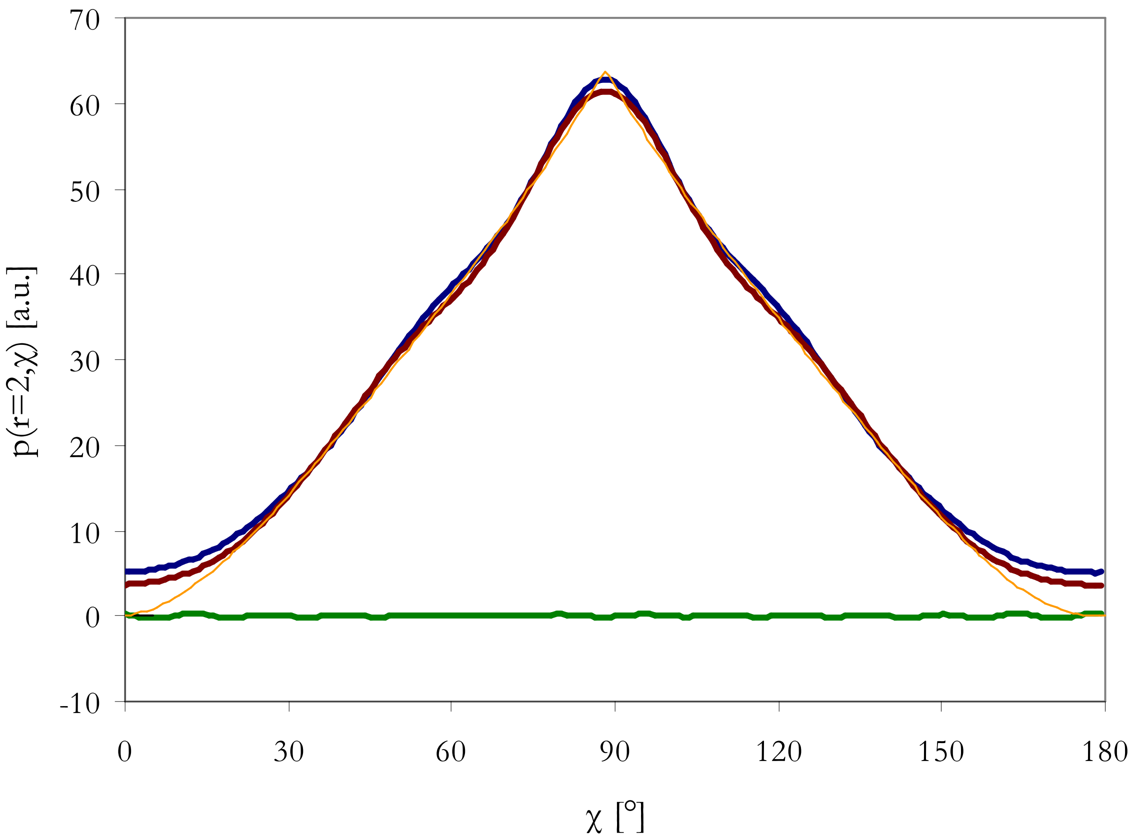

Figure 8: Cuts through the $p(r,\chi)$ functions at r=2 nm. The radial Lagrange multiplier is set to λ_R=-2 (blue), λ_R=-10 (red), and λ_R=+6 (green).. The orange line is the theoretical curve.

Radial Lagrange multipliers that are too high result in flat real space functions. If the radial Lagrange multiplier is too small then the cuts at a given angle show oscillations, which are strongest at small distances.