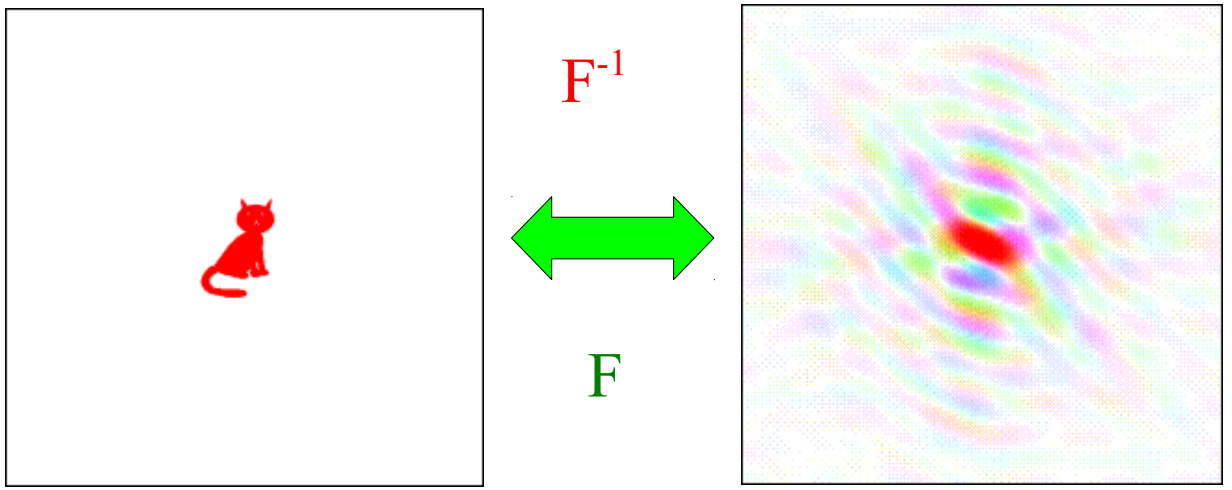
# Few slides on Form Factor

## (courtesy Jörg Evers)

# What is the form factor good for?

- In an experiment, the scattered light intensity is recorded
- This intensity is proportional to $|\text{form factor}|^2$
- Thus the scattered light contains information on the Fourier transformation of the structure of the object
- Goal: Obtain 3D structural information with high resolution

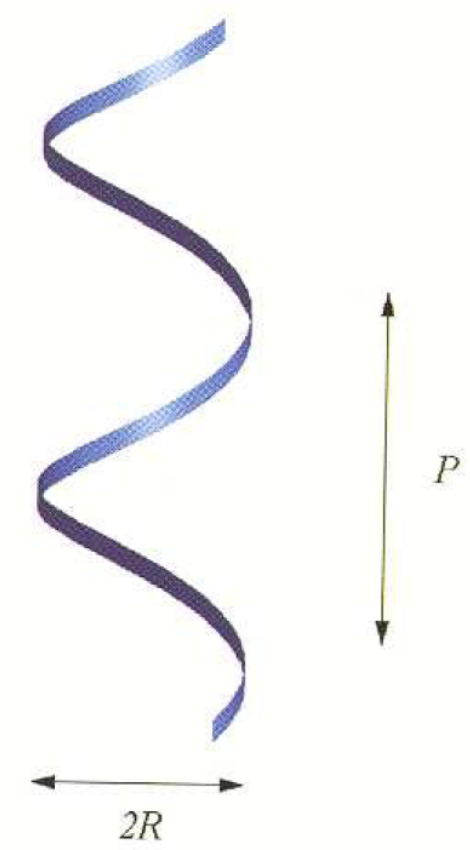


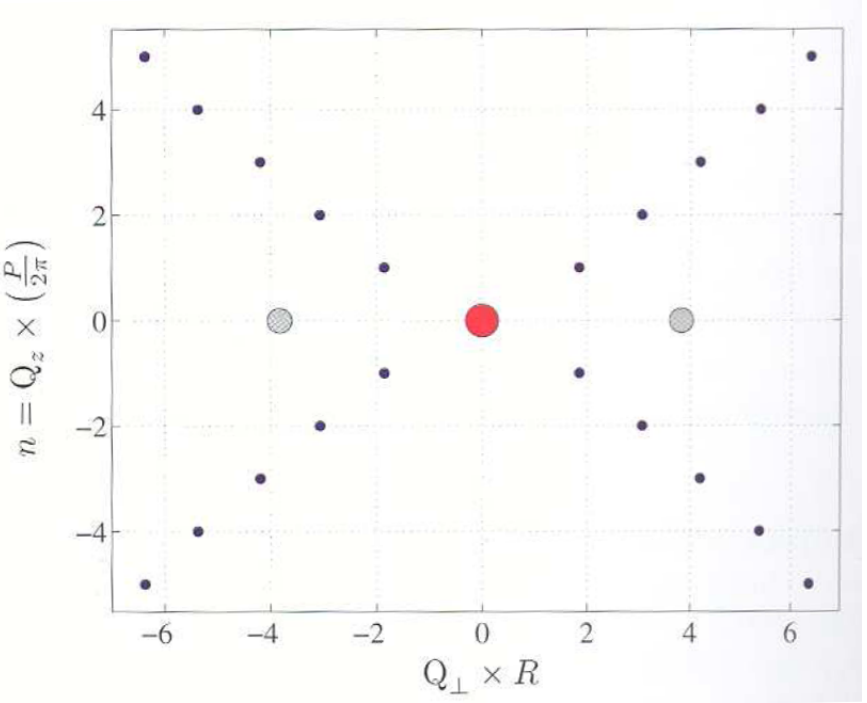

Images: Kevin Cowtan's Book of Fourier, Uni York (UK)

# Example: Scattering from complex structures

Single helix

Pauling 1951: Proteins form helix
Cochran 1952: Calculation of helix diffraction pattern

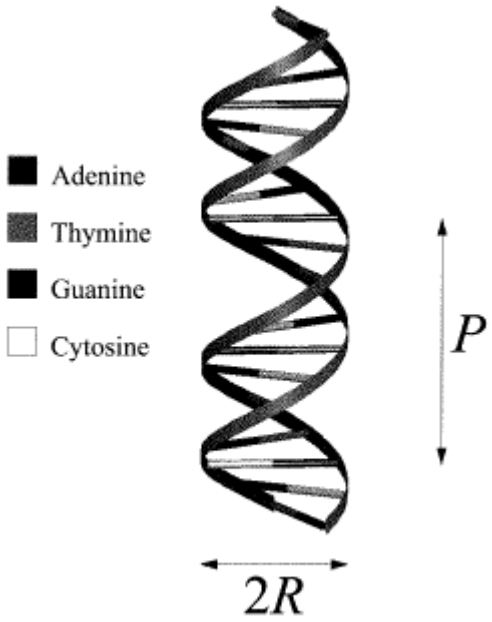


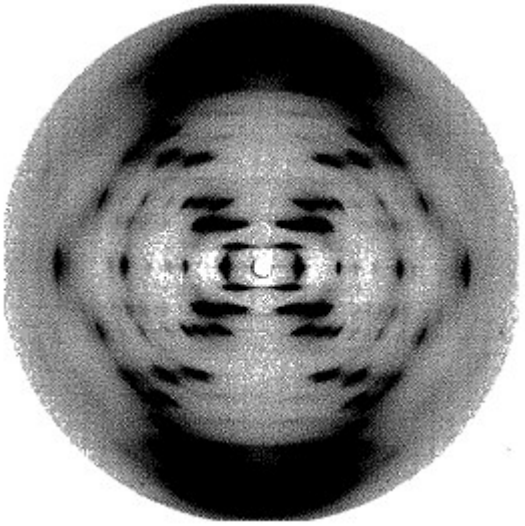



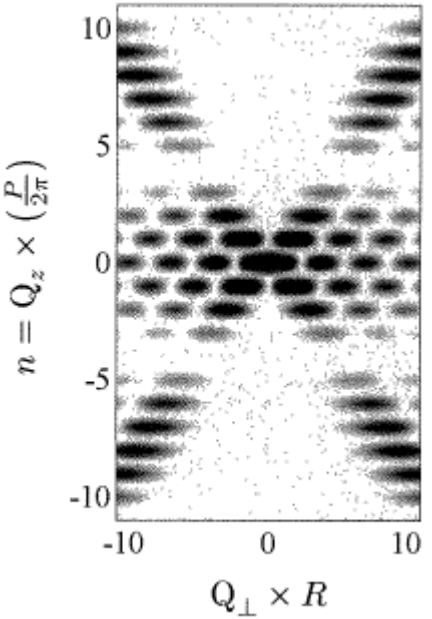

From "Elements of Modern X-Ray Physics" by J. Als-Nielsen and D. McMorrow

# Example: Scattering from complex structures

## Double helix






Structure Experiment Theory

Watson and Crick 1953: DNA forms double helix
Wilkins, Franklin, Gosling, ... 1953: X-ray diffraction experiments

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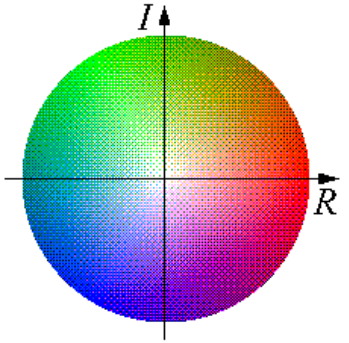
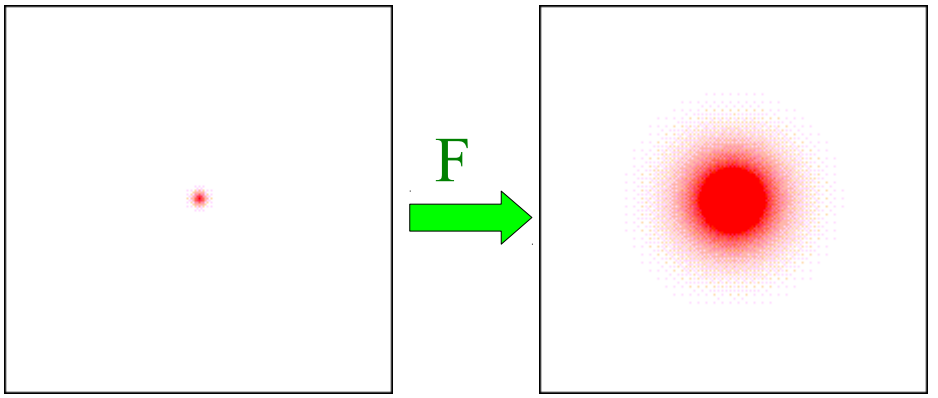
# How does the structure retrieval work?

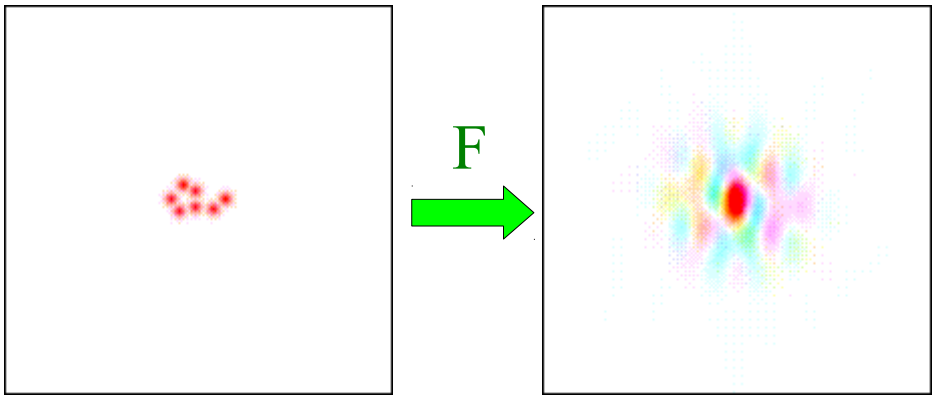
Color coding of magnitude and phase:




Example: Atom



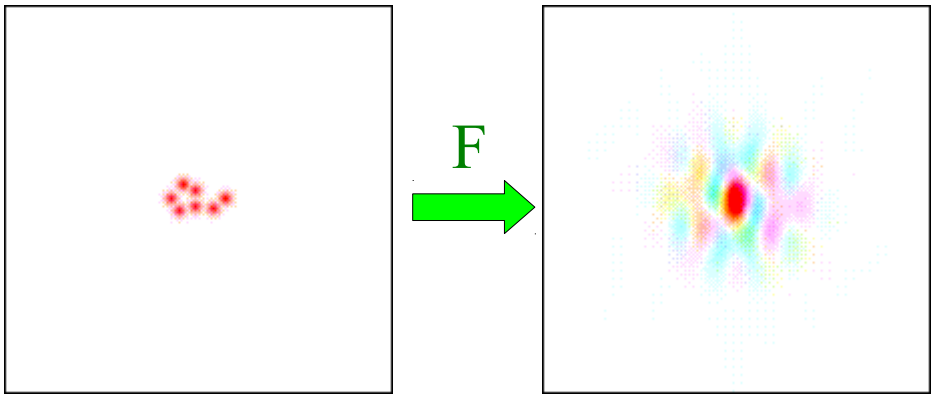

Example: Molecule



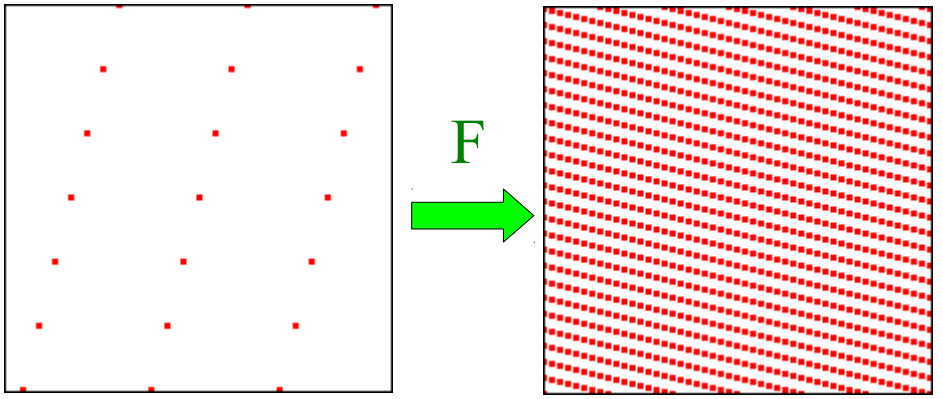

Examples from Kevin Cowtan's
Book of Fourier, Uni York (UK)
http://www.ysbl.york.ac.uk/~cowtan/fourier

# Fourier properties

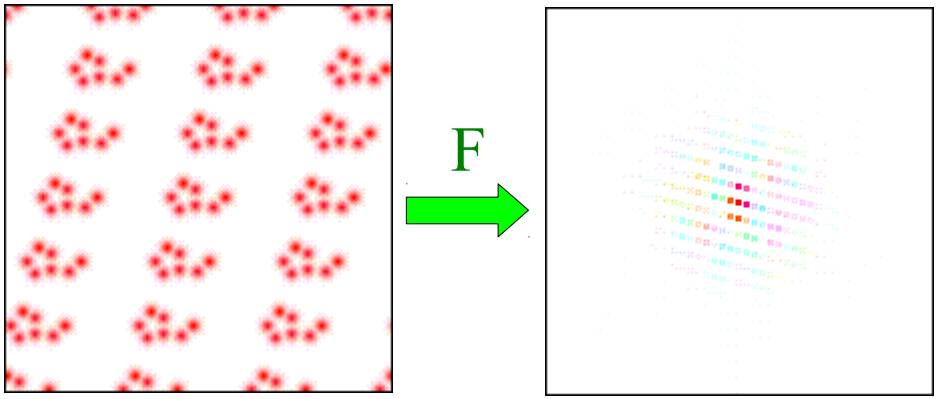
Molecule




Lattice

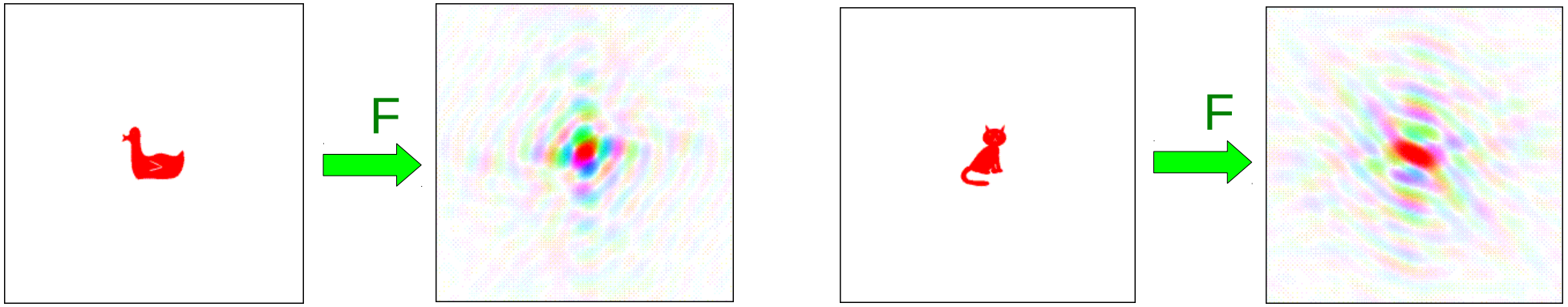



Molecule crystal: Convolution

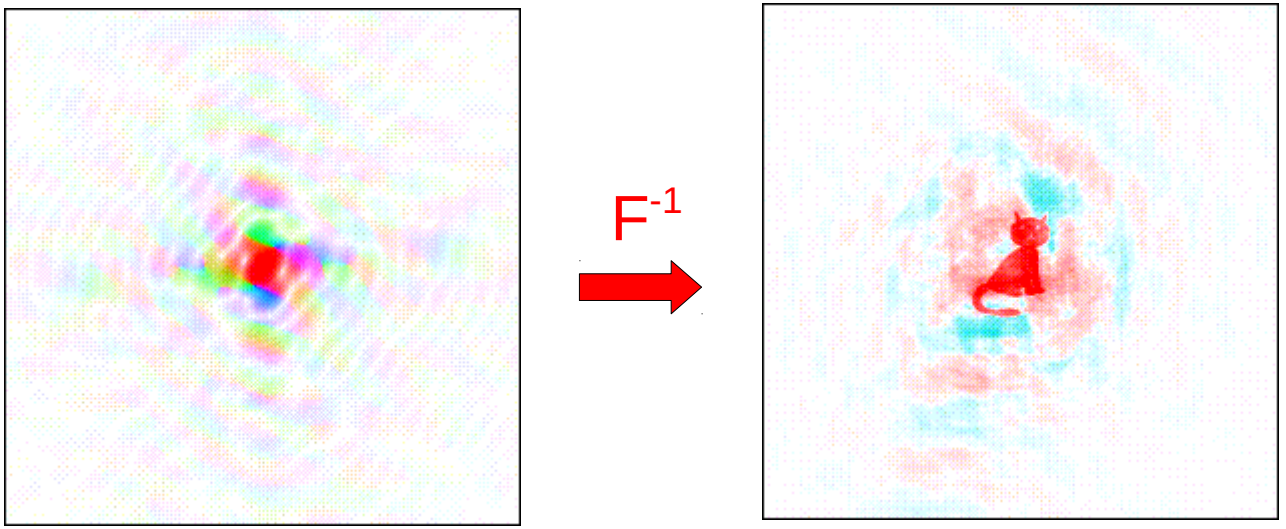



Examples from Kevin Cowtan's Book of Fourier, Uni York (UK)

# The phase problem




Combine Fourier magnitude of duck with Fourier phase of cat




Measurement gives mostly cat!

Examples from Kevin Cowtan's Book of Fourier, Uni York (UK)

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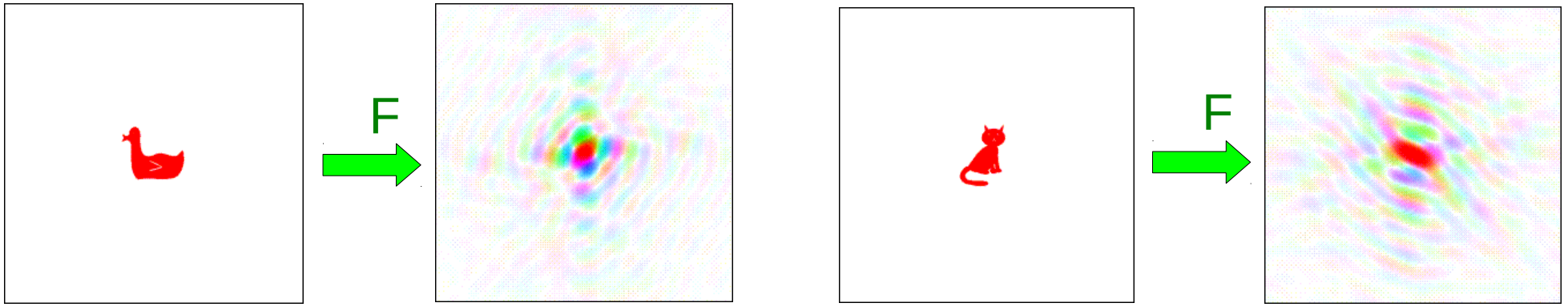


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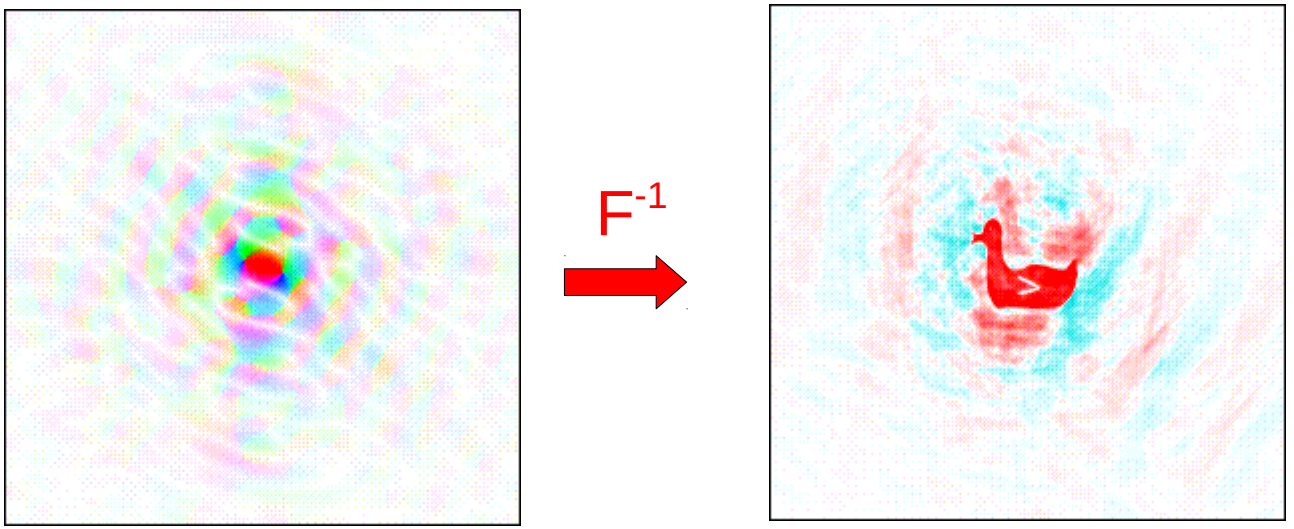
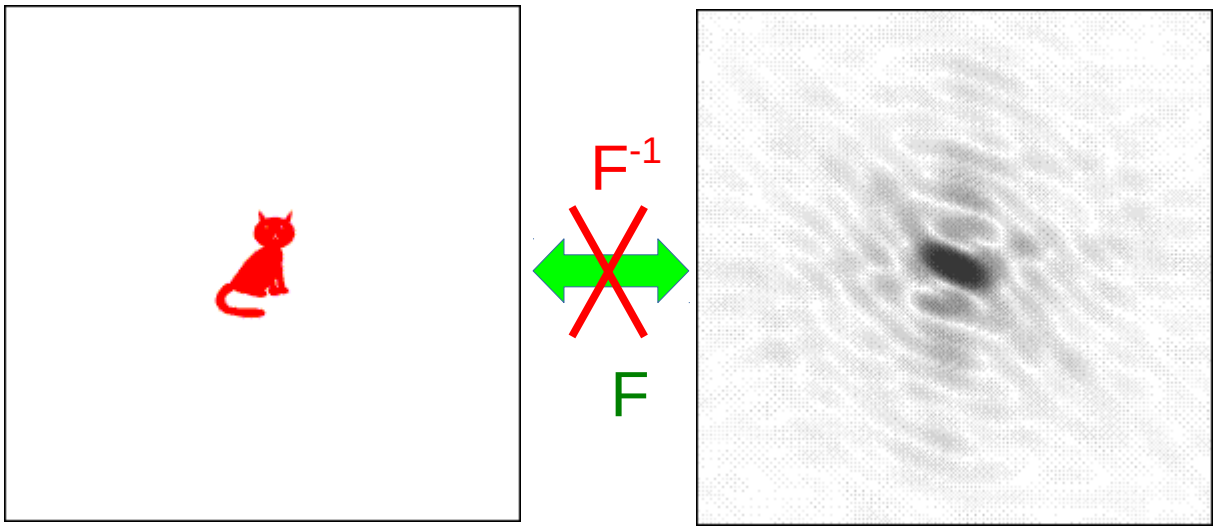



Measurement gives mostly duck!

Examples from Kevin Cowtan's Book of Fourier, Uni York (UK)

# The phase problem

- After the Fourier-backtransform, the image which contributed the phase dominates the result
- In general: Phases contain most of structural information
- Problem: Diffraction experiments only provide magnitudes, not the phases
- → Need method to reconstruct phases. This is the phase problem.




Object

Potential measurement

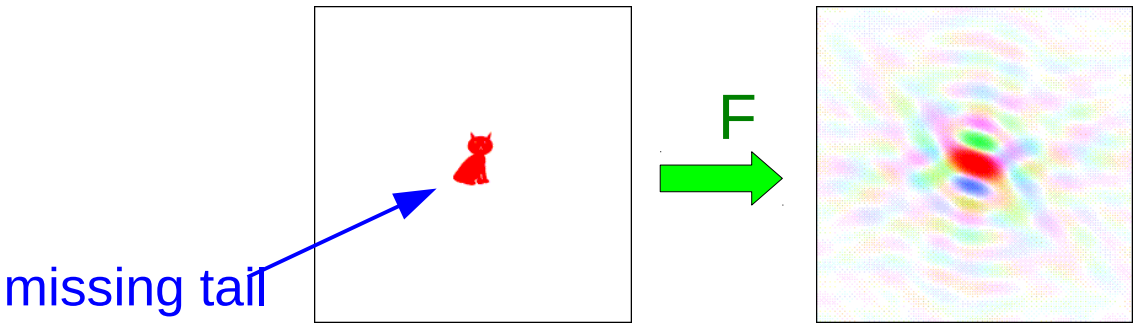
Examples from Kevin Cowtan's Book of Fourier, Uni York (UK)

# One solution: Use reference data

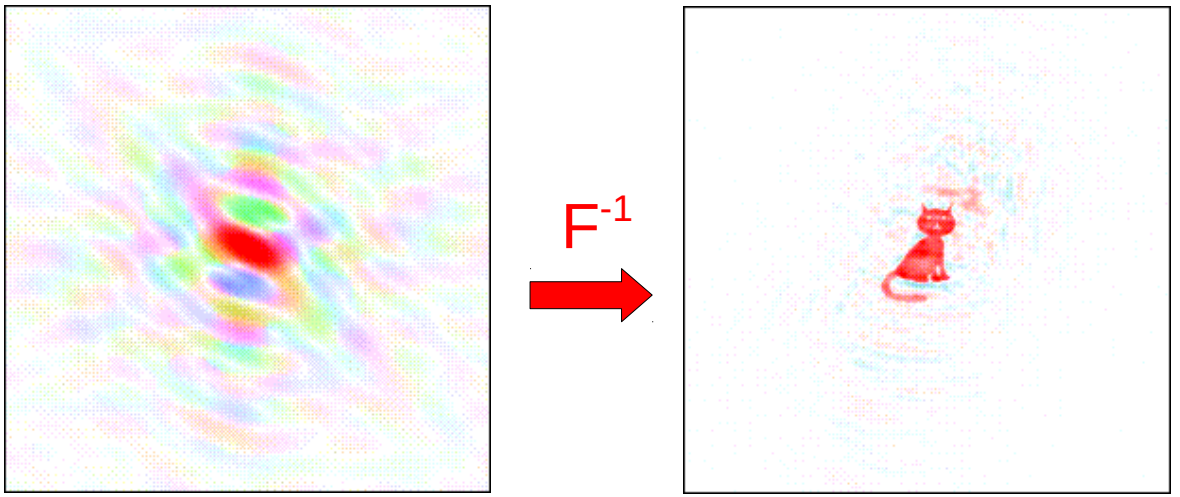
## Idea

- Often, part of a structure – e.g., half of a molecule – are known
- Then, the known part can be used as a model

## Model




## Combine measured magnitude of cat with phase from model:




- Missing tail recovered with 50% magnitude
- But some noise

Examples from Kevin Cowtan's Book of Fourier, Uni York (UK)

# Iterative phase retrieval

## Make use of constraints in Fourier and real space

- Mathematical properties (e.g. real non-negative density, symmetries)
- Object support / aperture as well-defined area of zero signal
- Oversampling (obtain more data in Fourier space to compensate for loss in phase information)

## Basic algorithm