

Direct methods for the 21st century

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The phase reconstruction problem, for periodic structures, is under-constrained by a factor of **two**.

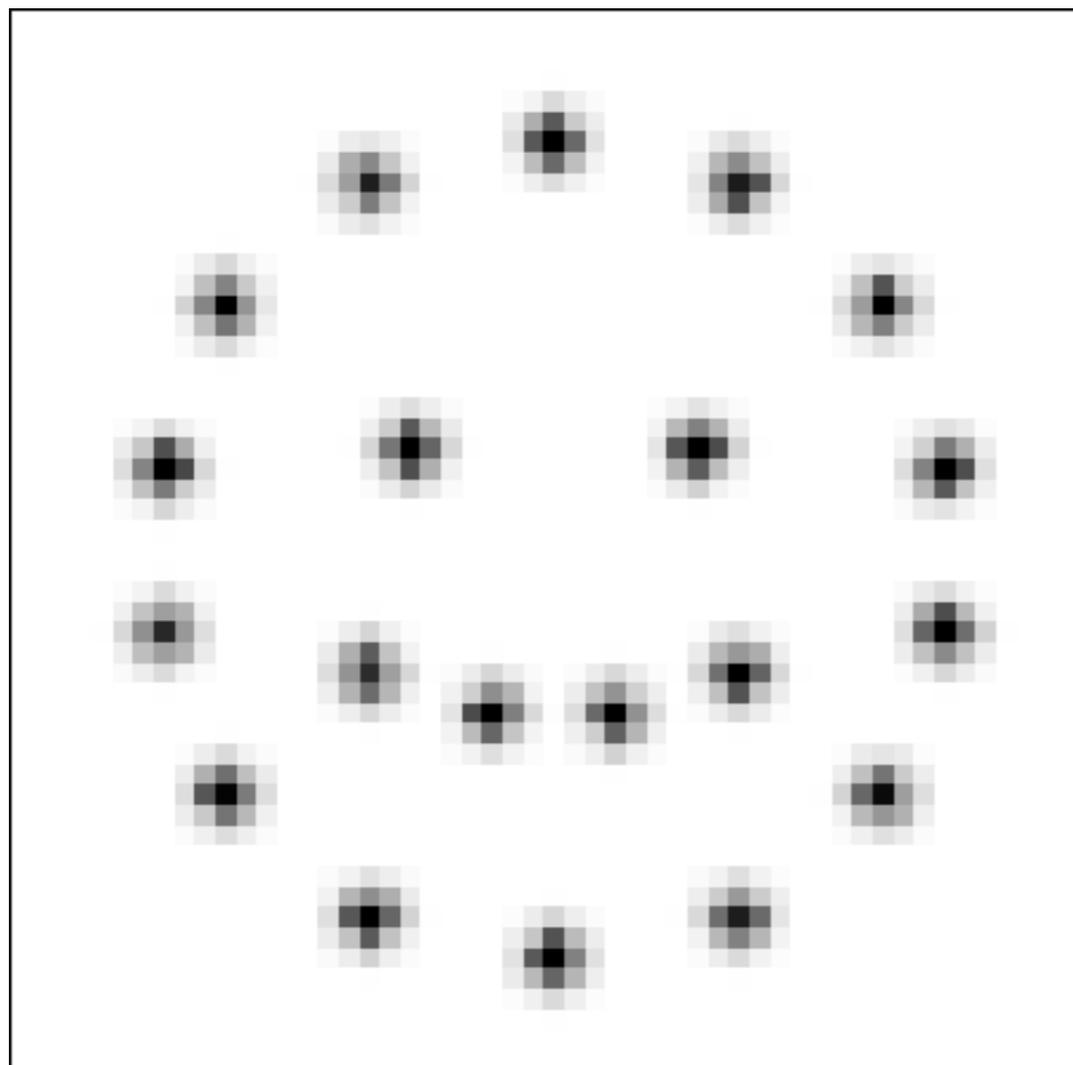
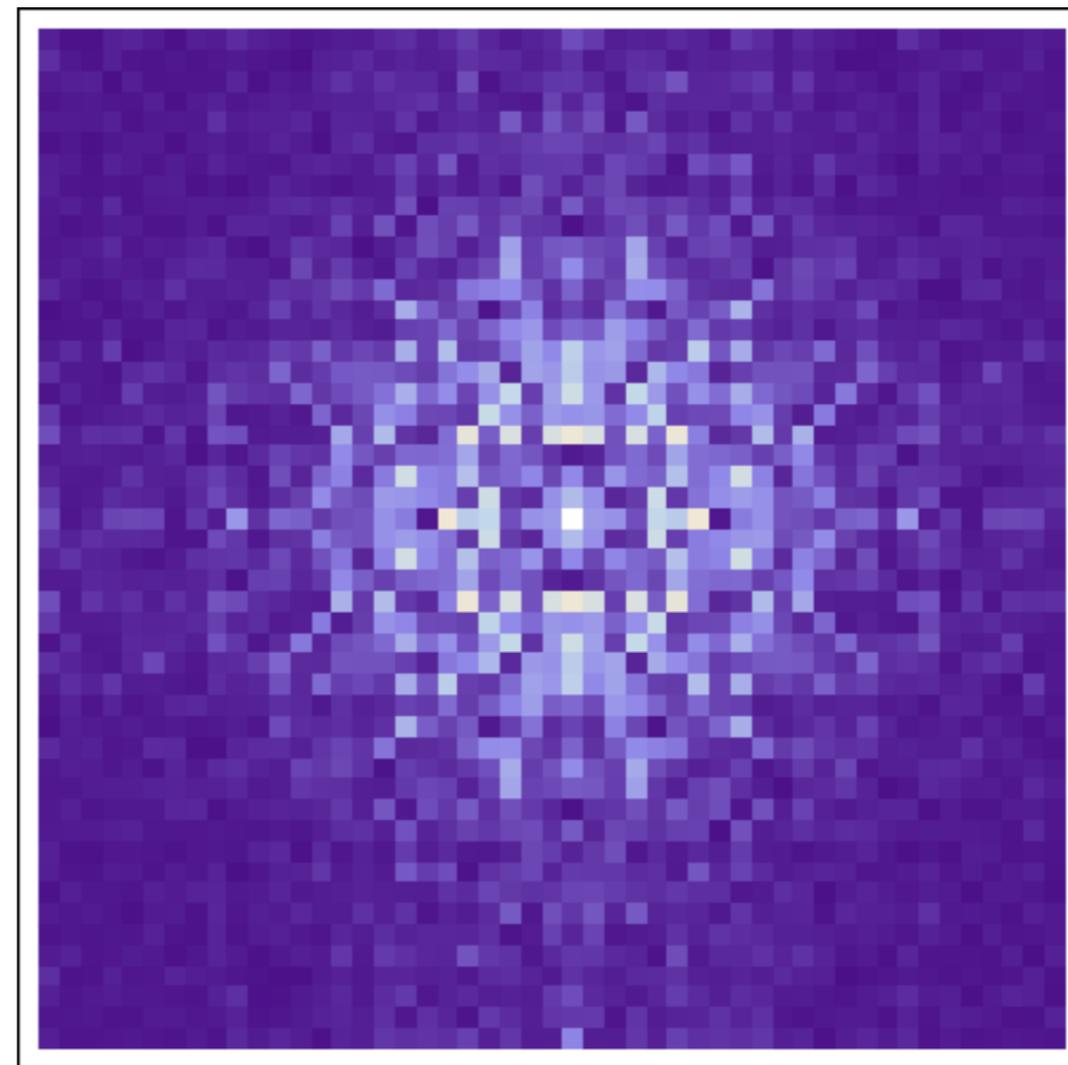
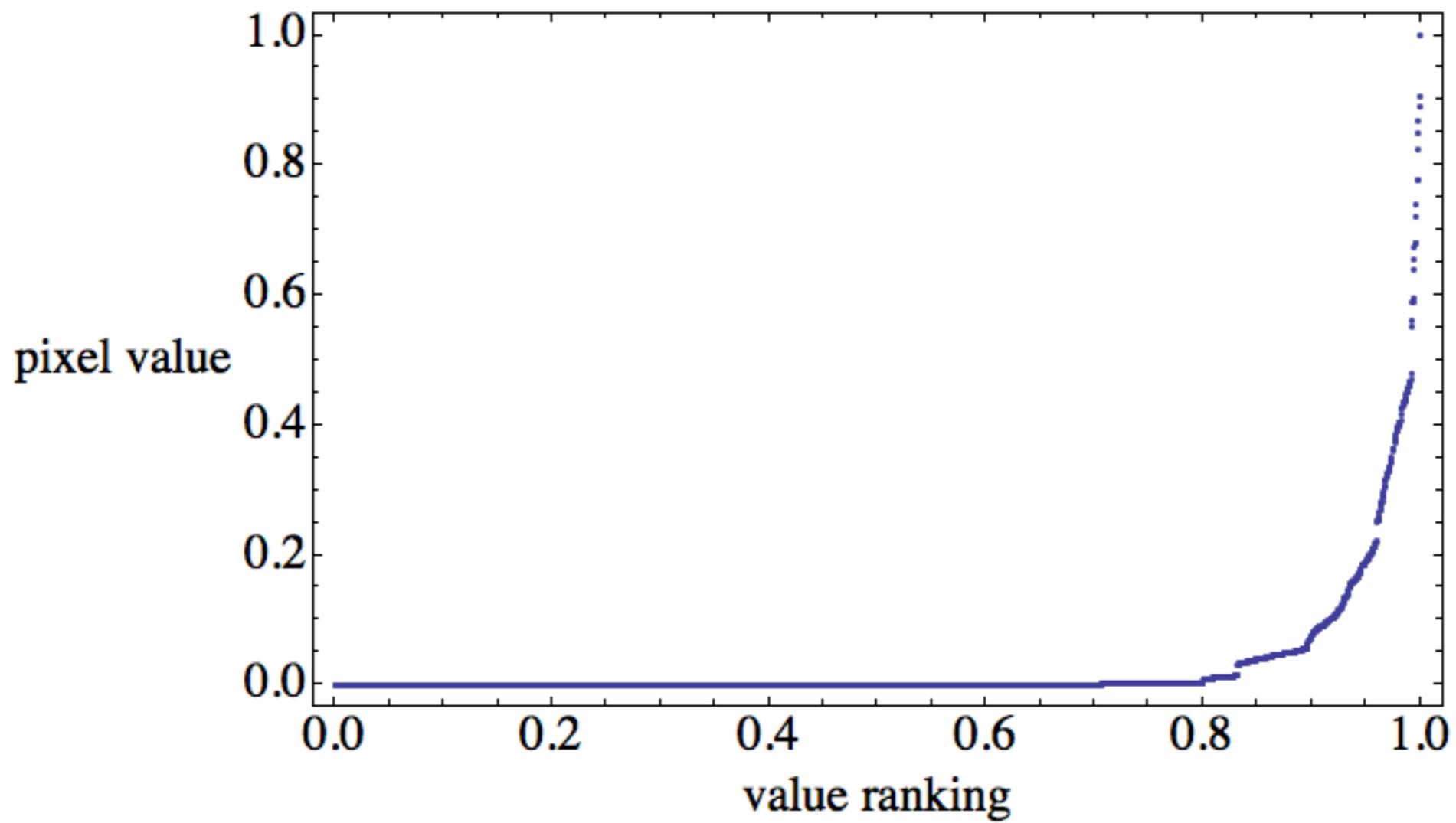


image (electron density)
in one unit cell



Fourier magnitudes
(diffraction data)



Forcing more than 50% of the pixels to be zero, when true, should give a unique reconstruction.

constraint projections

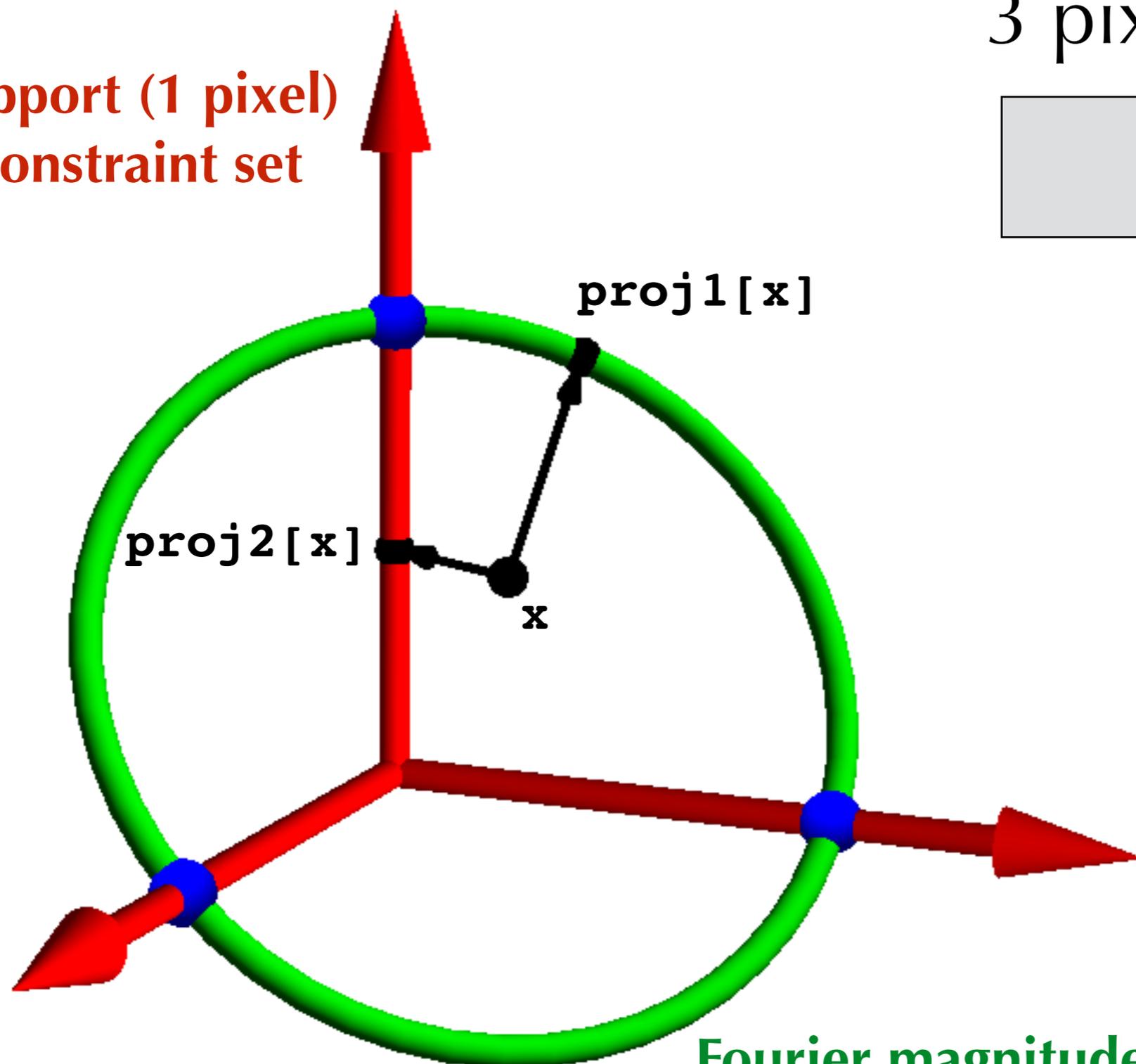
x : image (electron density)

proj1[x] : replace Fourier magnitudes of **x** with measured values, when available

proj2[x] : keep a fixed fraction of the largest pixels of **x**, set the rest to zero

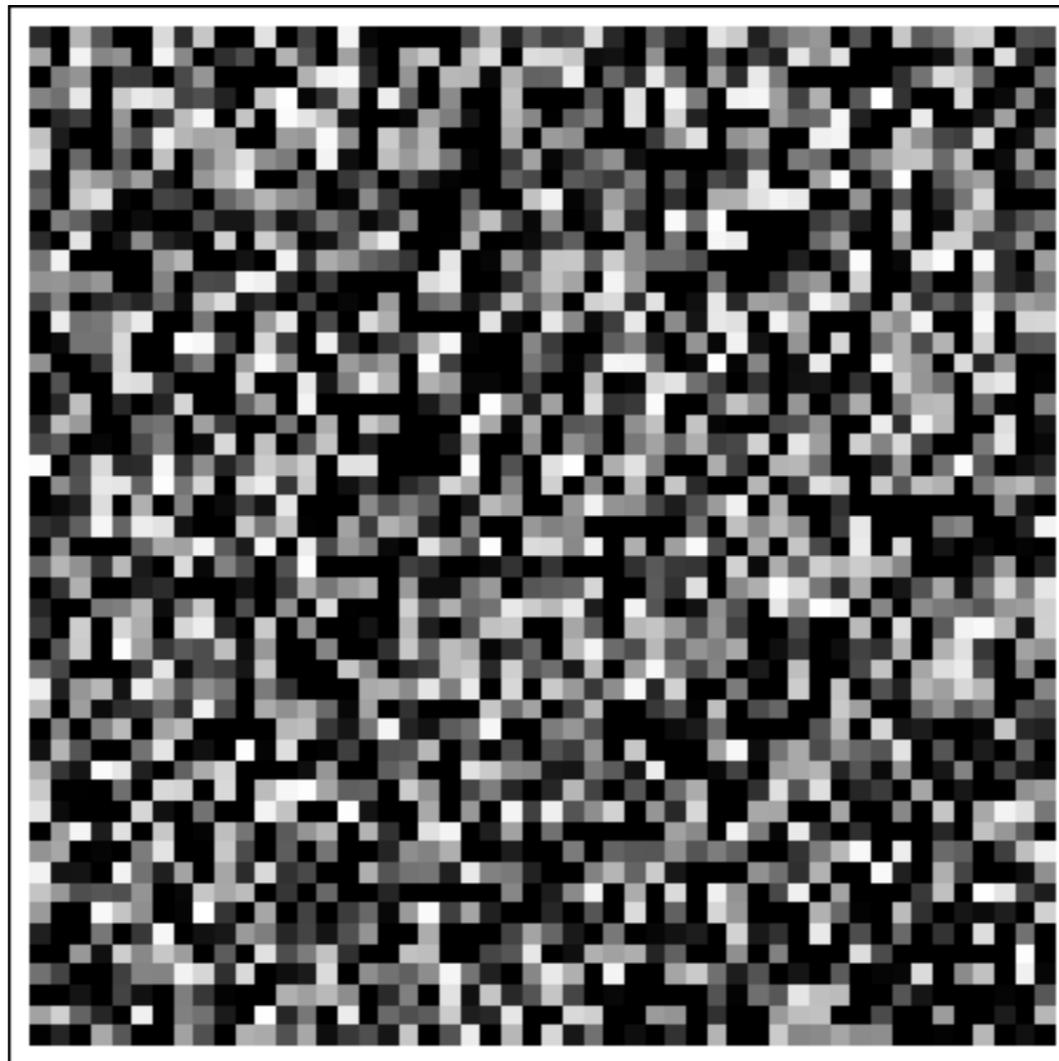
support (1 pixel)
constraint set

3 pixel image

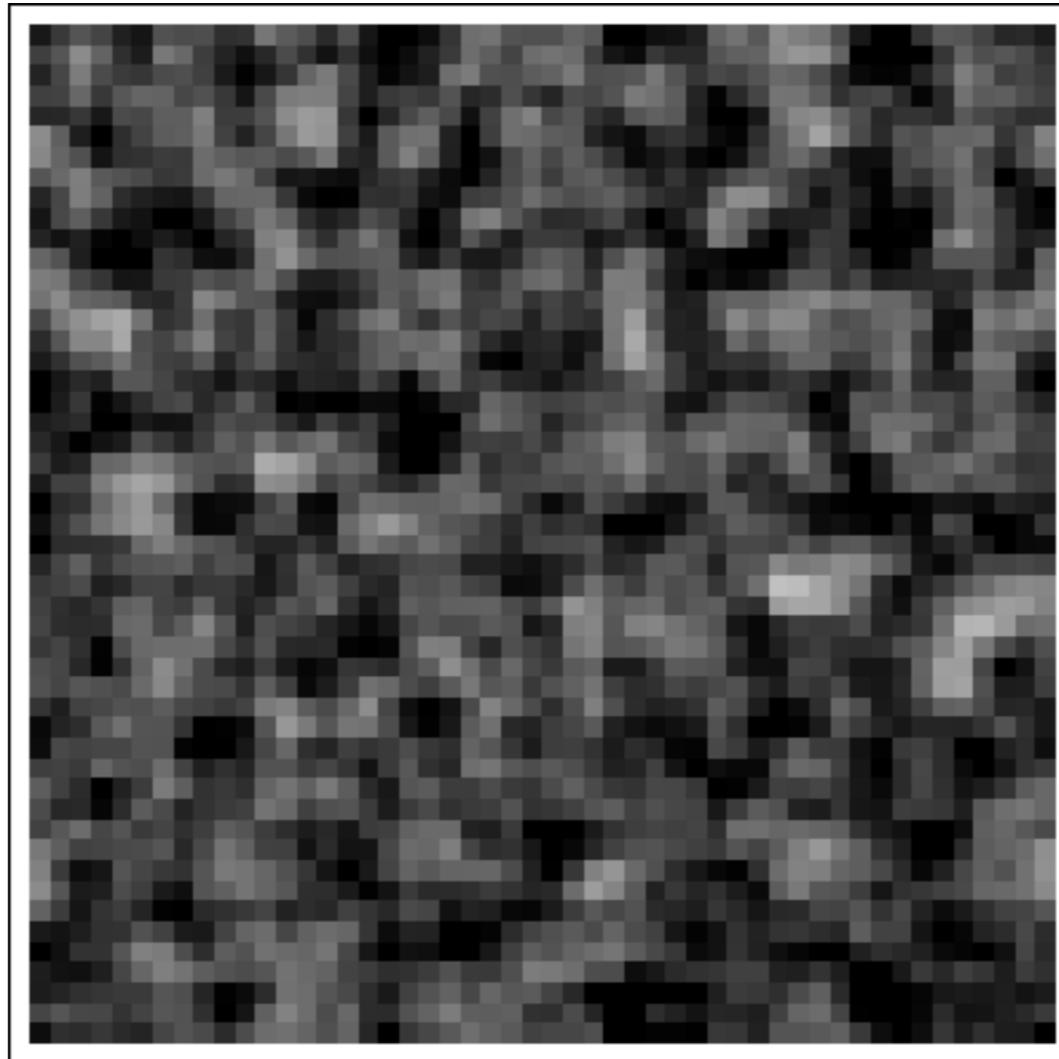


Fourier magnitude
constraint set

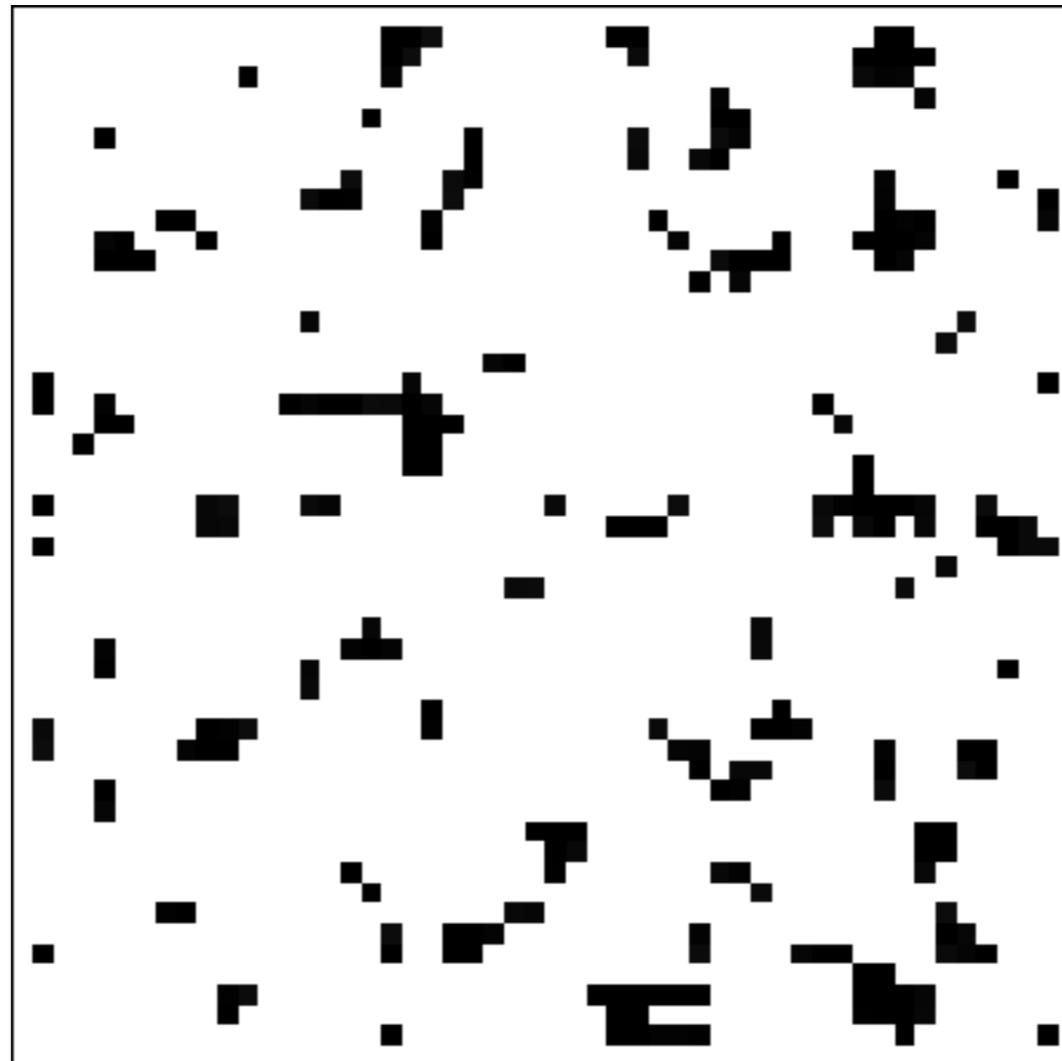
x = random



proj1[x]

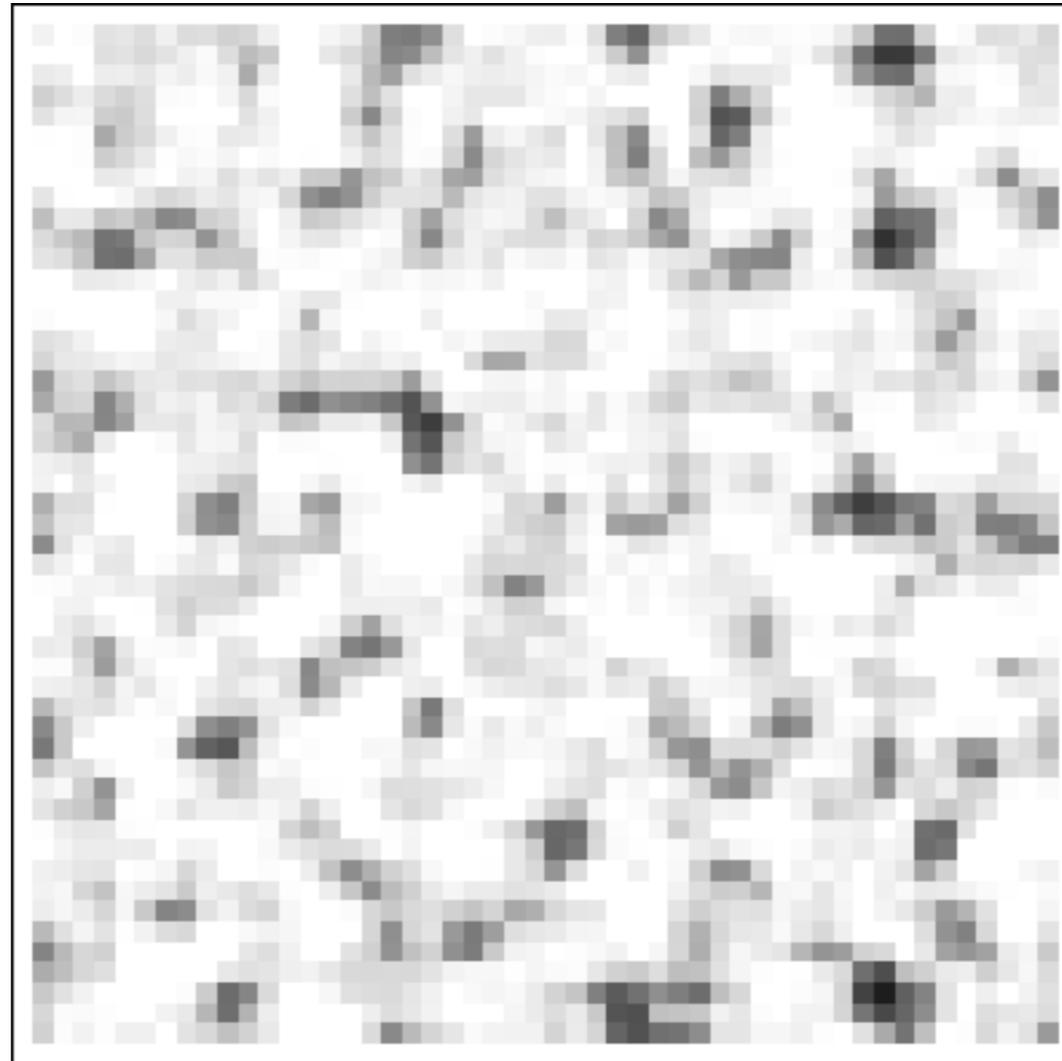


`proj2[proj1[x]]`



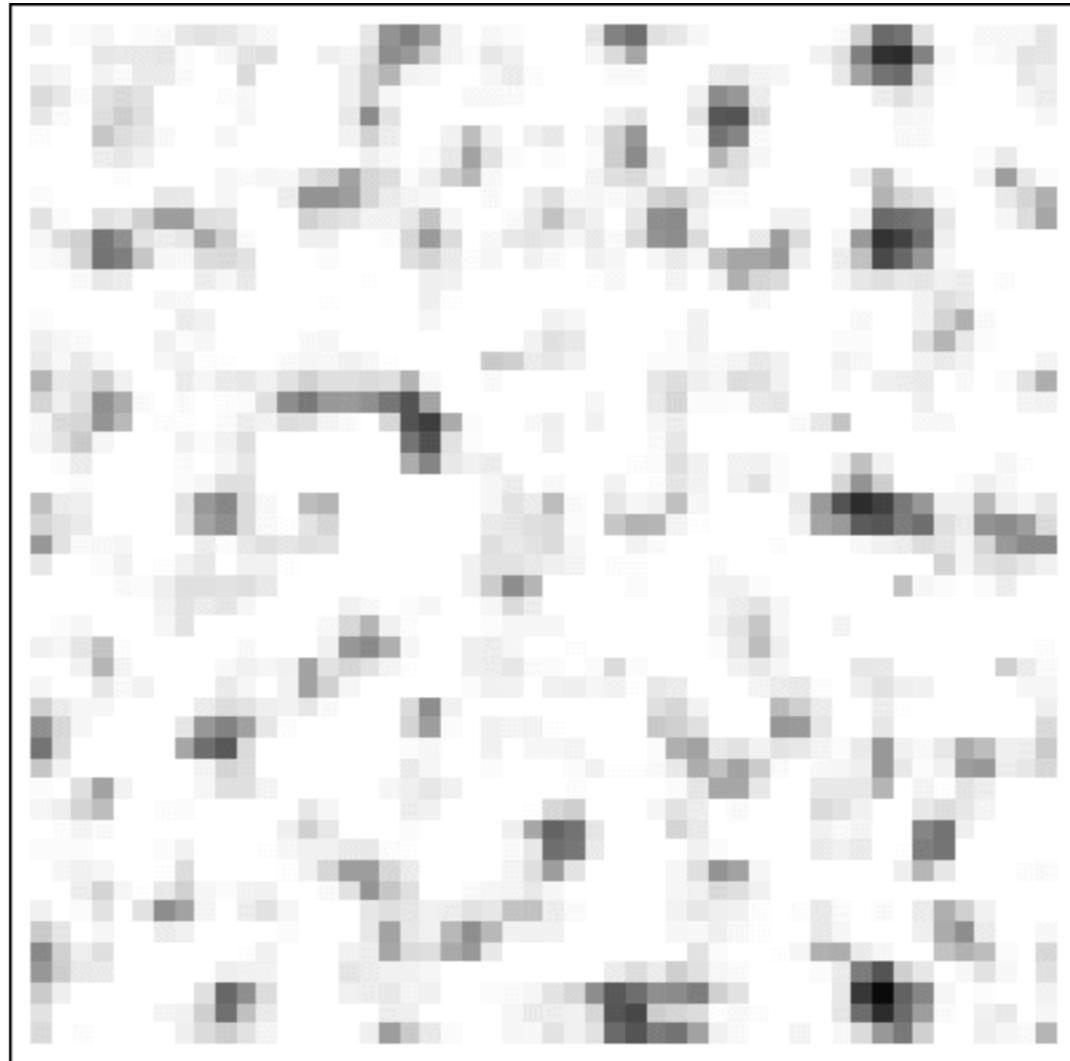
support fraction = 10%

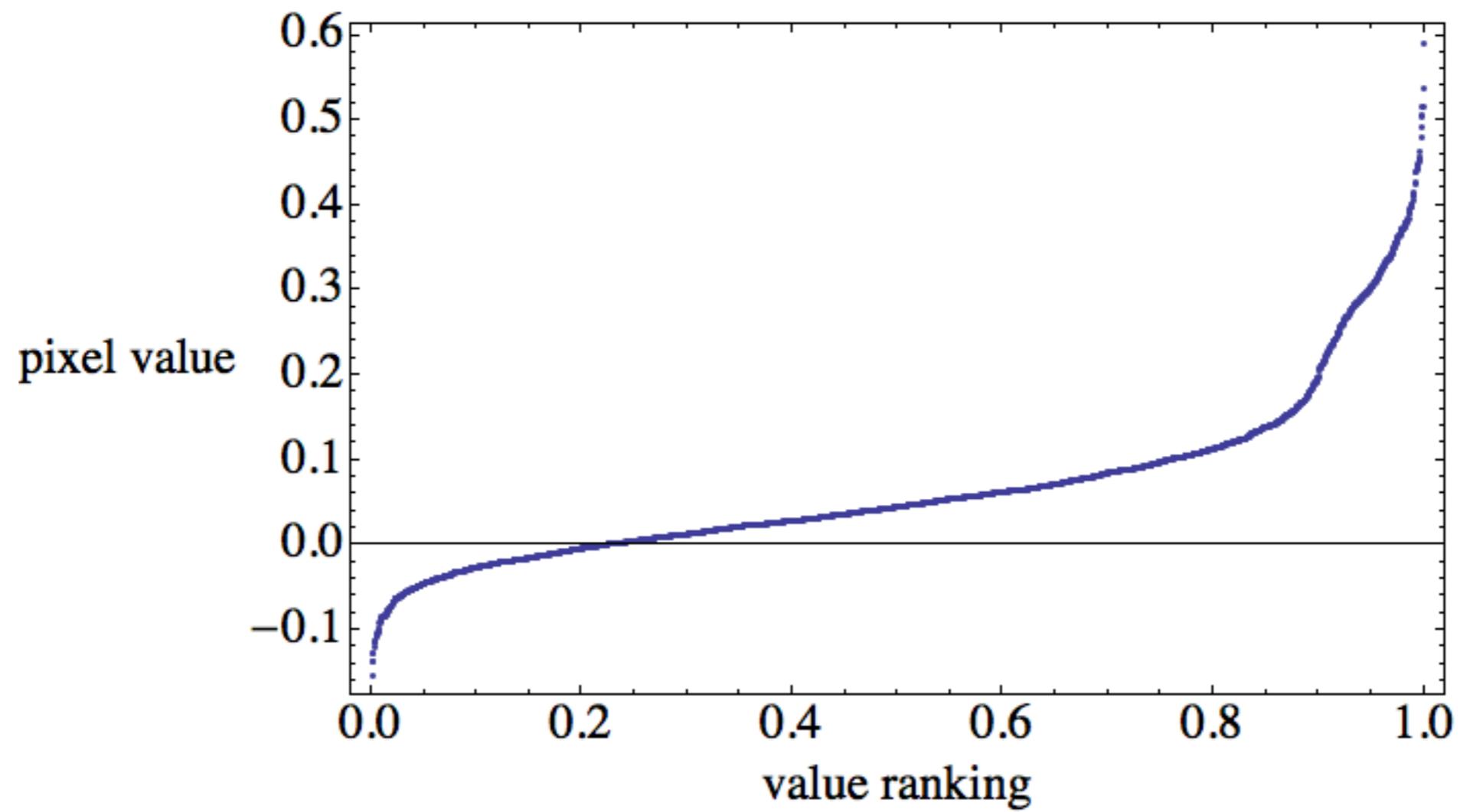
proj1 [proj2 [proj1 [x]]]



“alternating map”

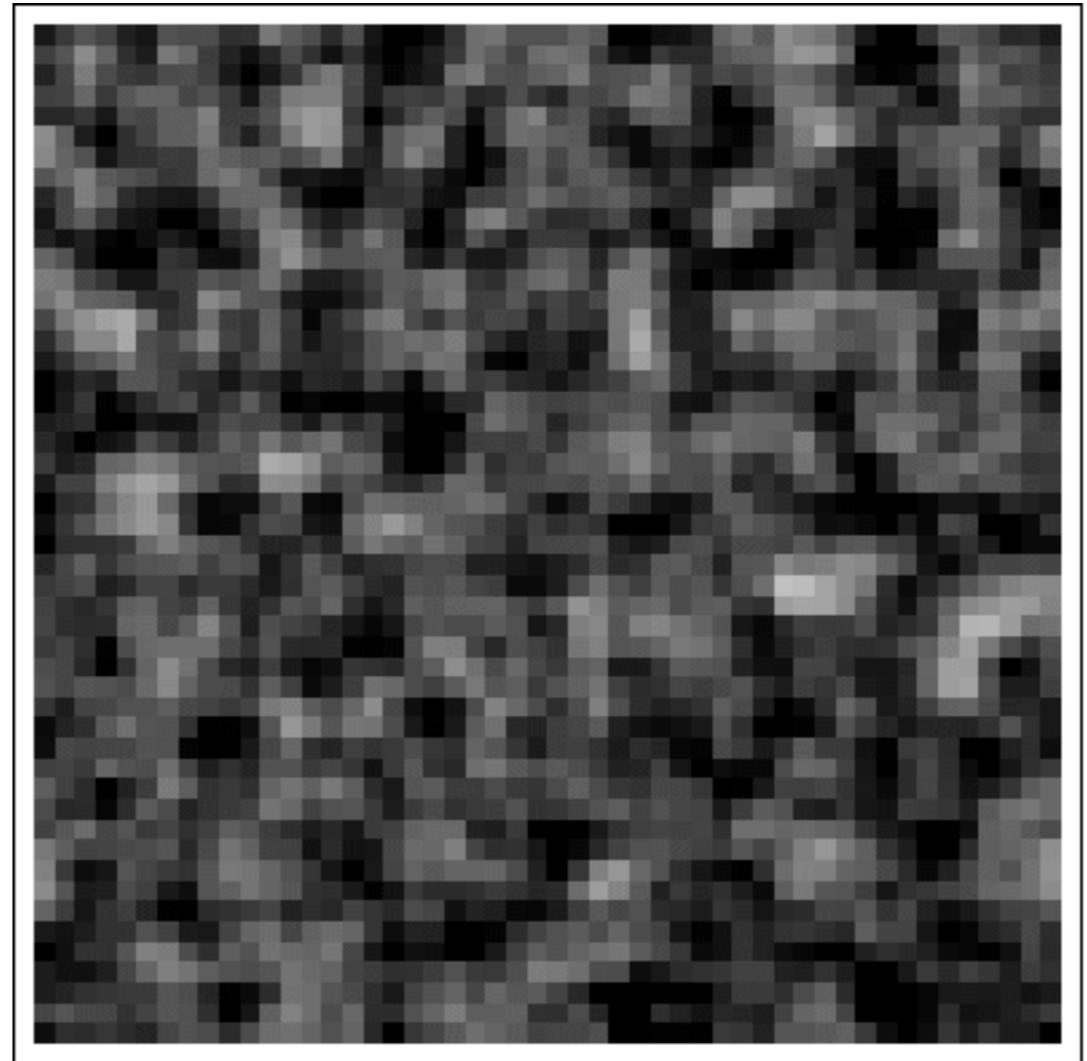
```
Do [  
  x = proj2[x];  
  x = proj1[x];  
  
  render[x];  
  
  , {20}]
```

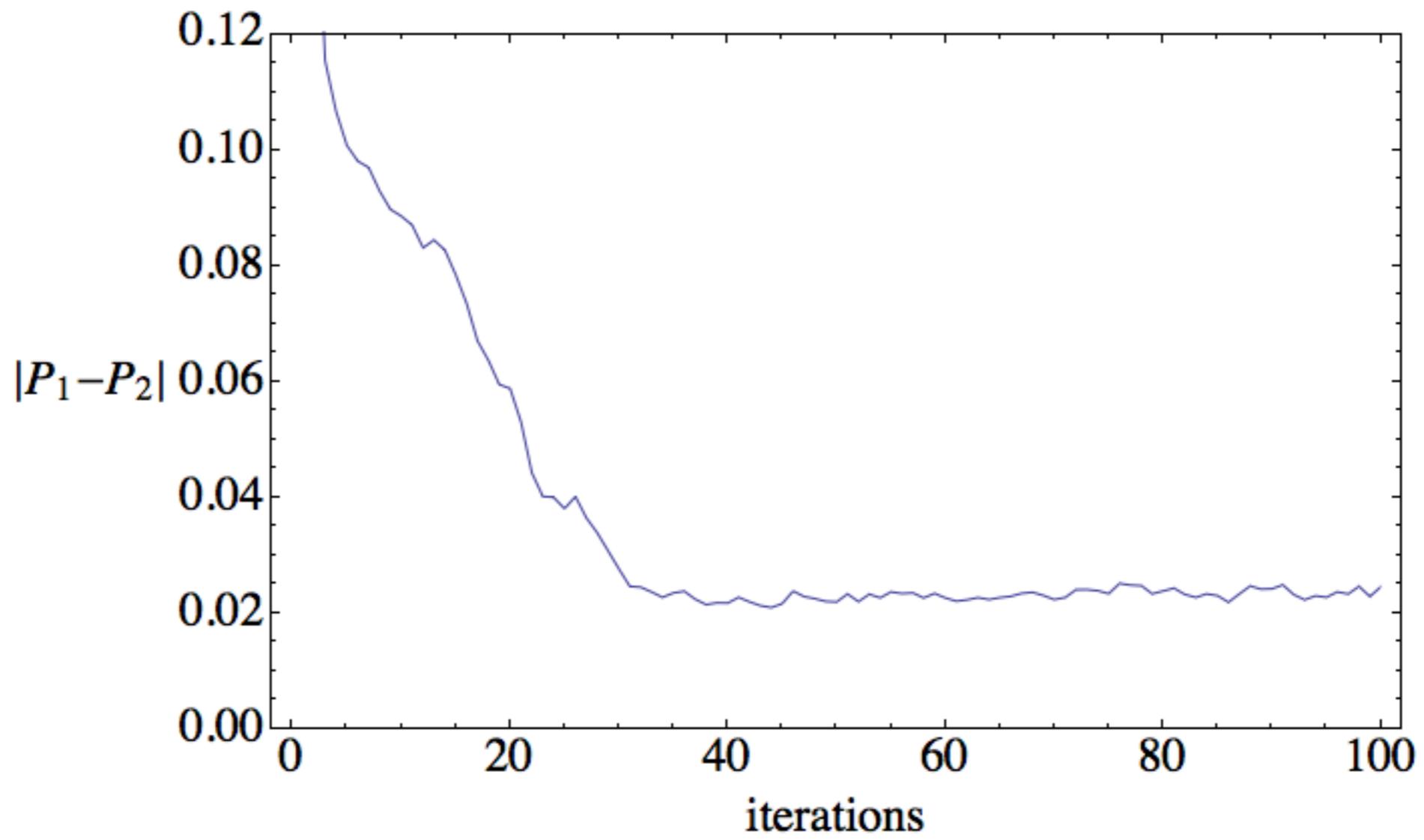


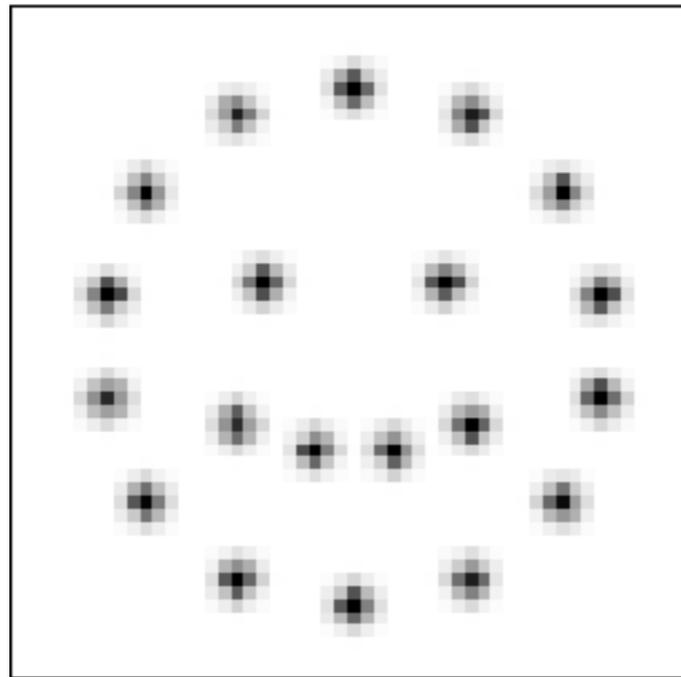


“difference map”

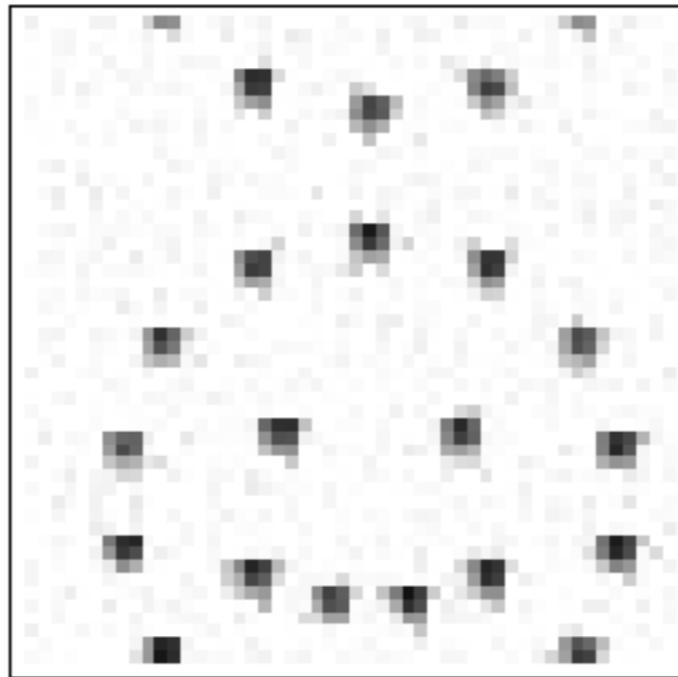
```
Do [  
  p1 = proj1[x];  
  p2 = proj2[2 p1 - x];  
  x += p2 - p1;  
  
  render[p1];  
  
  , {100}]
```



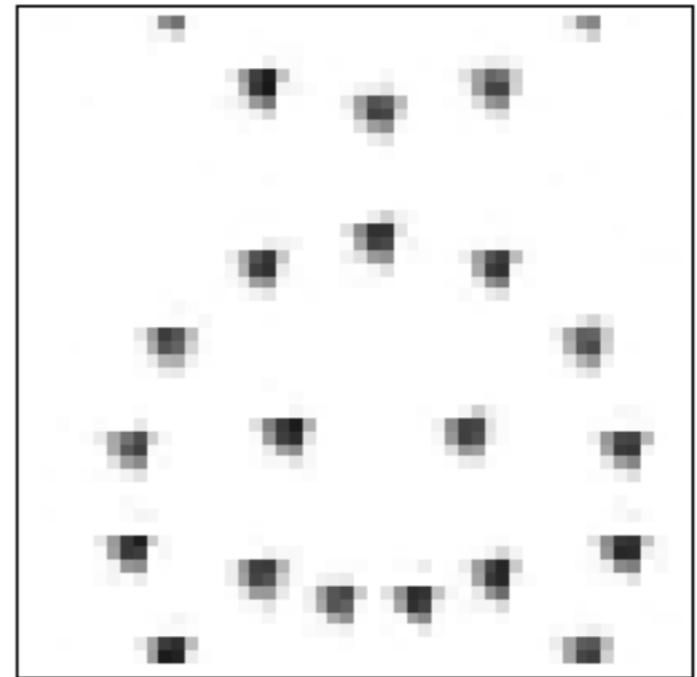




original



phase
reconstruction



after
averaging

difference map publications

Phase retrieval by iterated projections

Veit Elser

J. Opt. Soc. Am. A **20**, 40-55 (2003)

Solution of the crystallographic phase problem by iterated projections

Veit Elser

Acta Cryst. A **59**, 201-209 (2003)

Searching with iterated maps

Veit Elser, Ivan Rankenburg, and Pierre Thibault

Proc. Nat'l Acad. Sci. USA **104**, 418-423 (2007)

phase reconstruction of a decagonal quasicrystal

- integrated Bragg peak data: average structure
- weakest prior constraint: electron density support

data

High-temperature structural study of decagonal Al–Cu–Rh

Paweł Kuczera, Janusz Wolny and Walter Steurer

Acta Cryst. (2014). B70, 306–314

space group: $P10_5/mmc$

1460 unique reflections

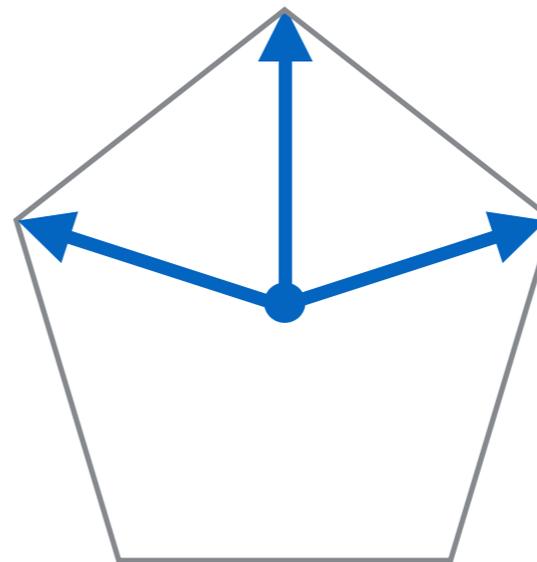
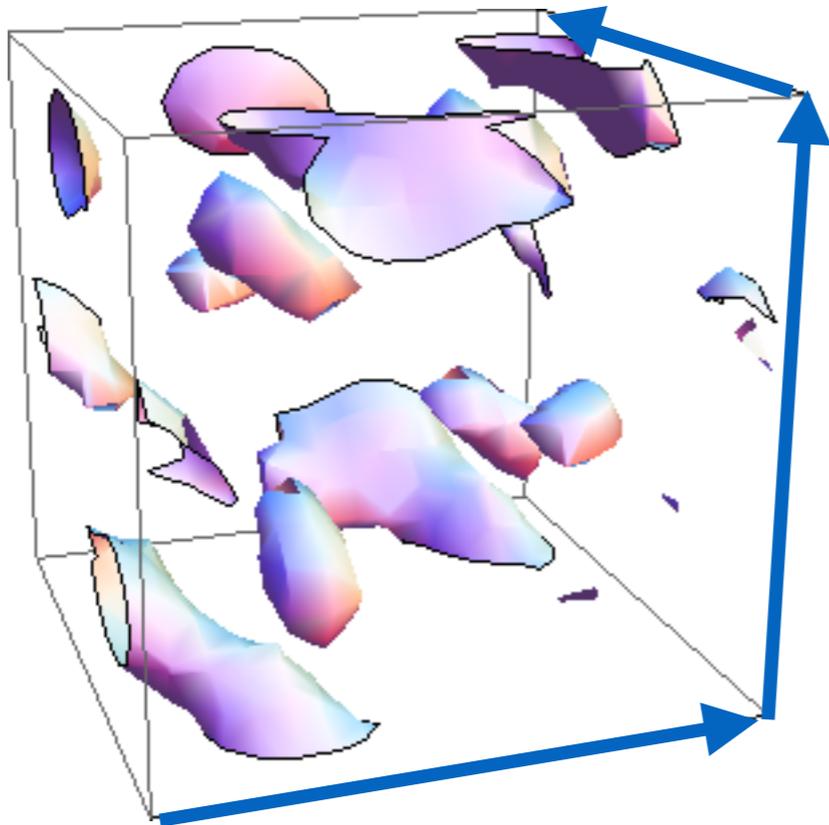
h1	h2	h3	h4	h5	F	sigF
0	0	0	0	2	948.905	47.4453
0	-1	-1	0	1	761.942	38.0971
0	0	0	0	4	692.956	34.6478
					• • •	

$$|h1|, |h2|, |h3|, |h4| < 8 \quad |h5| < 5$$

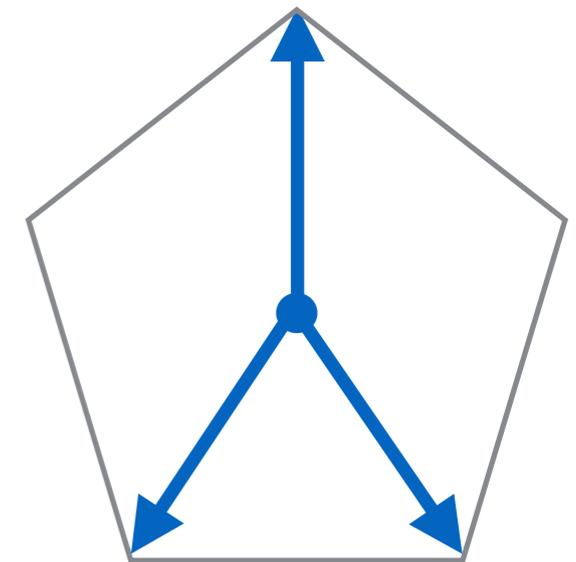
18 × 18 × 18 × 18 × 12 voxels

new challenges

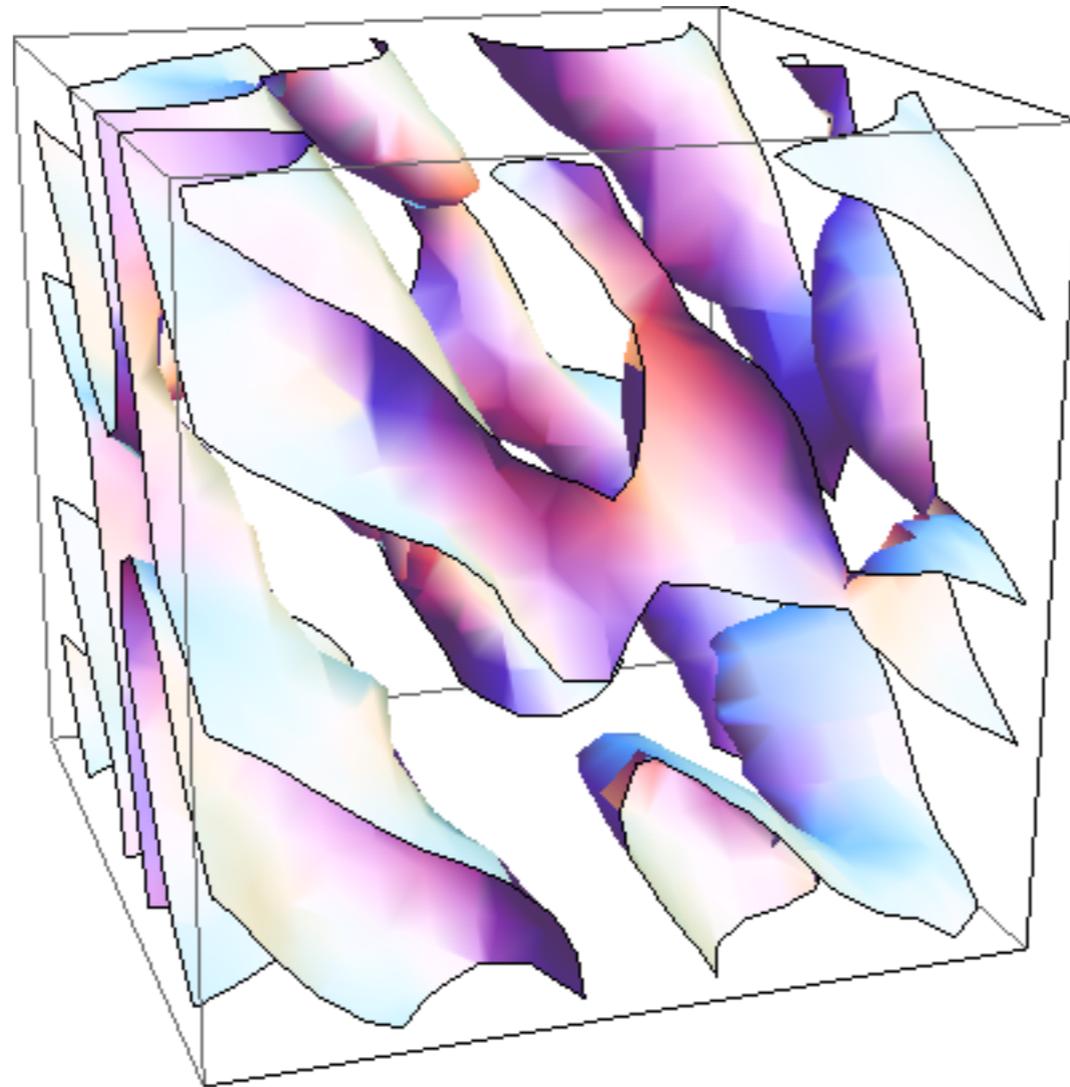
- **symmetry:** implement space group with symmetry orbits of Fourier transform
- **rendering:** project two of the five dimensions



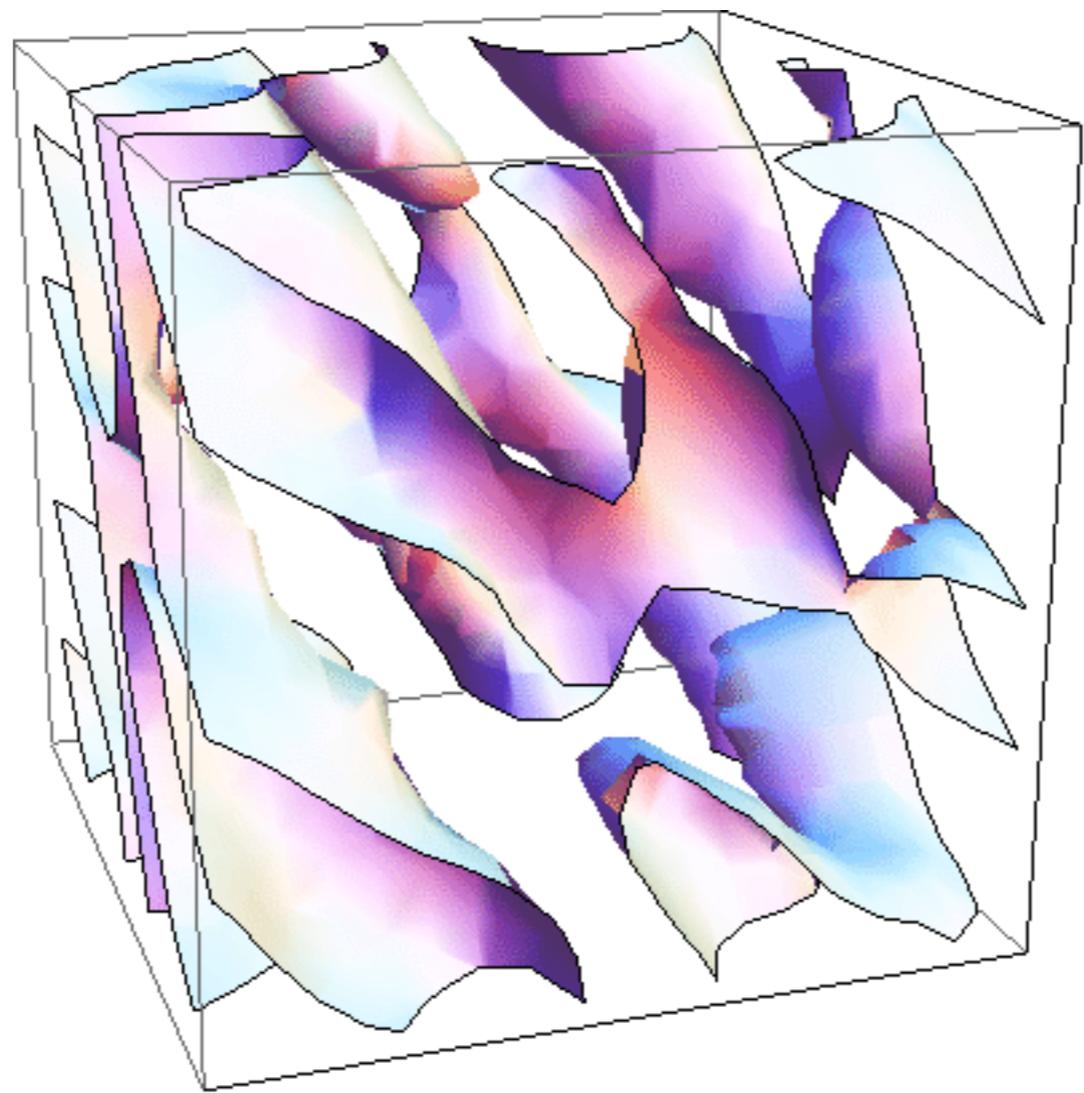
para

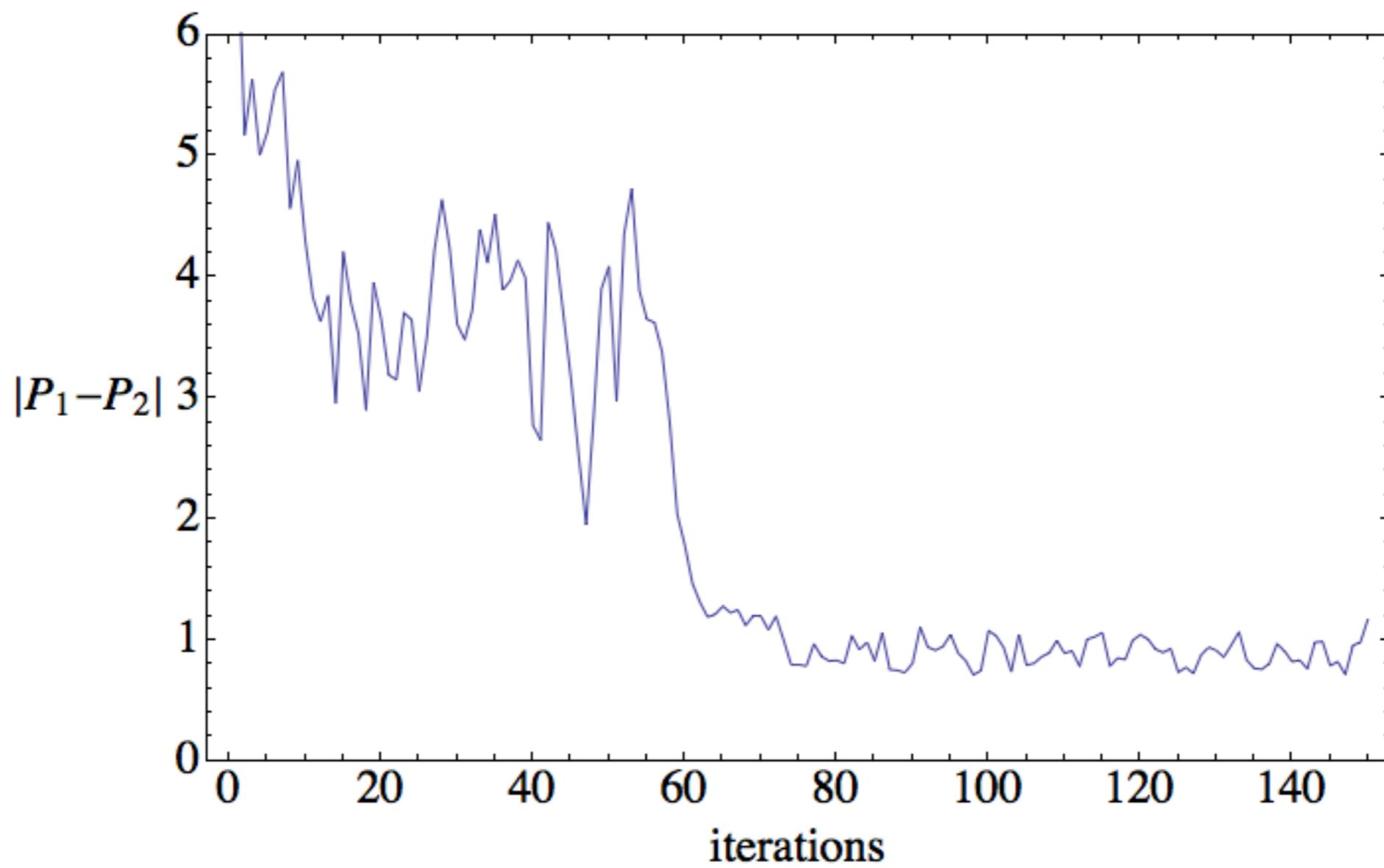


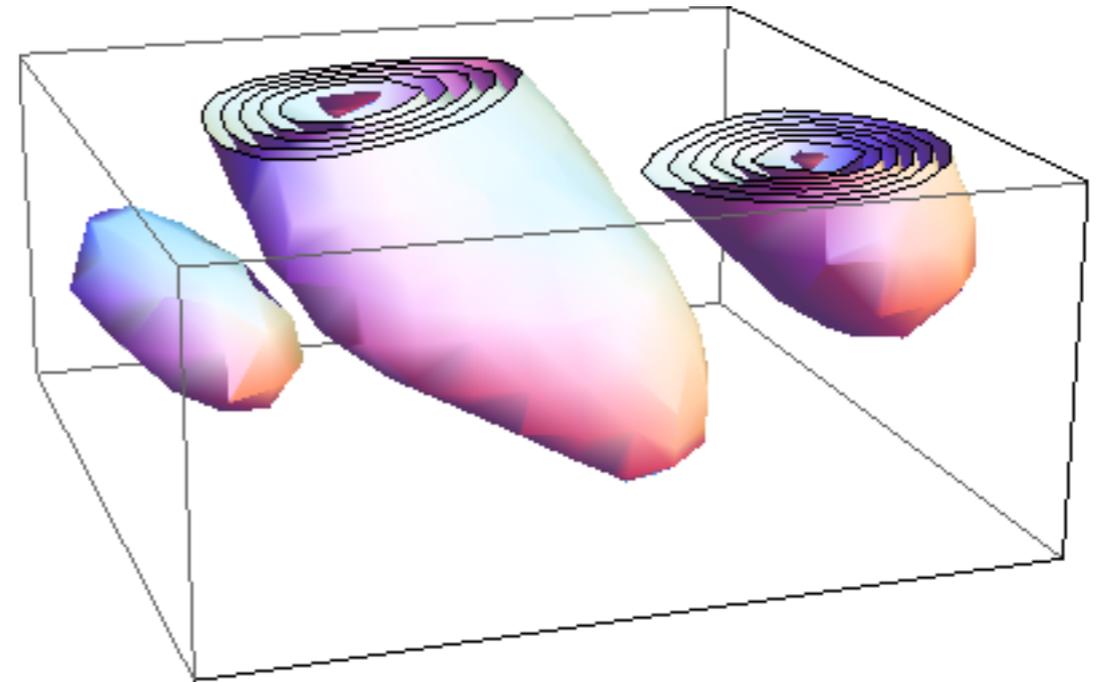
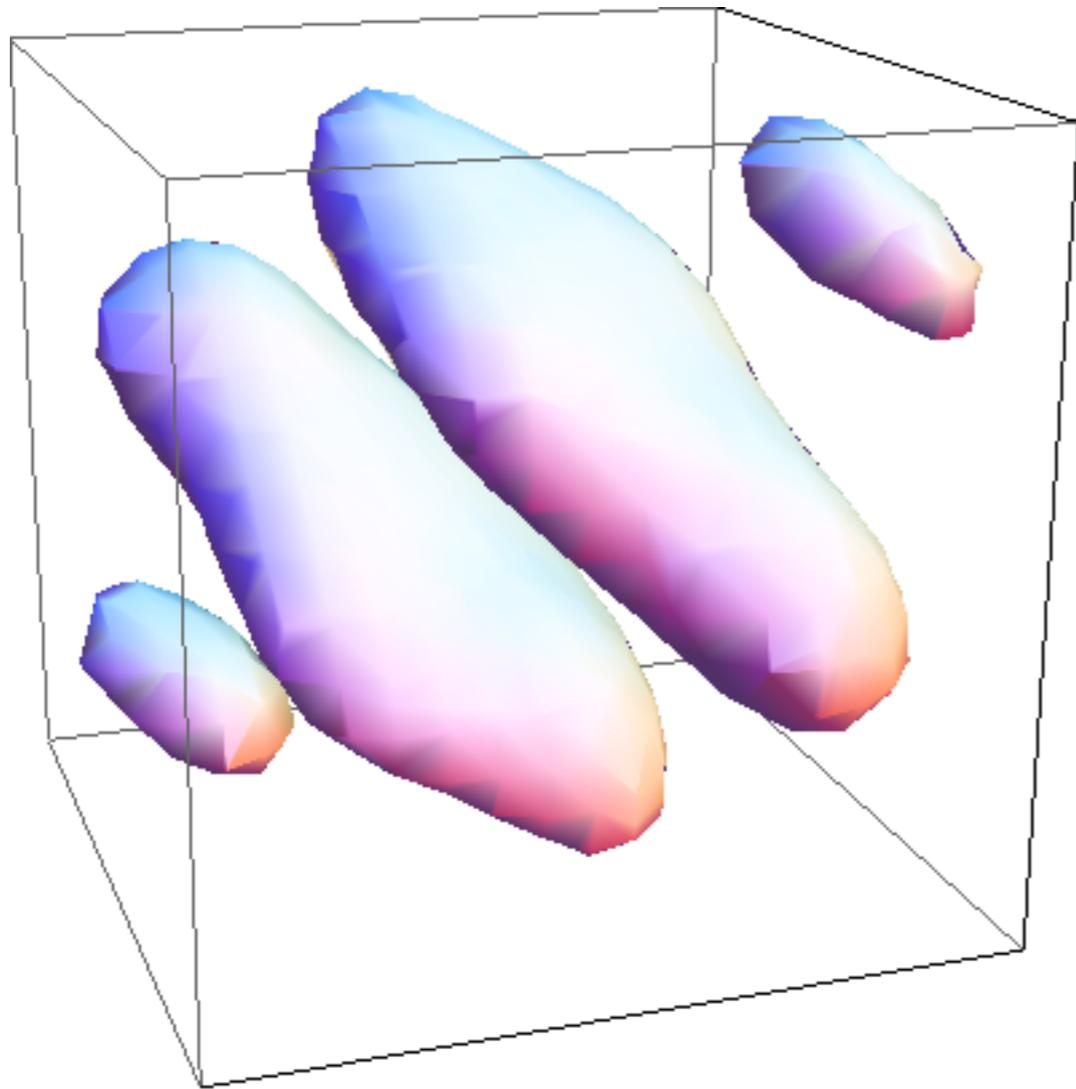
perp



support : 20%

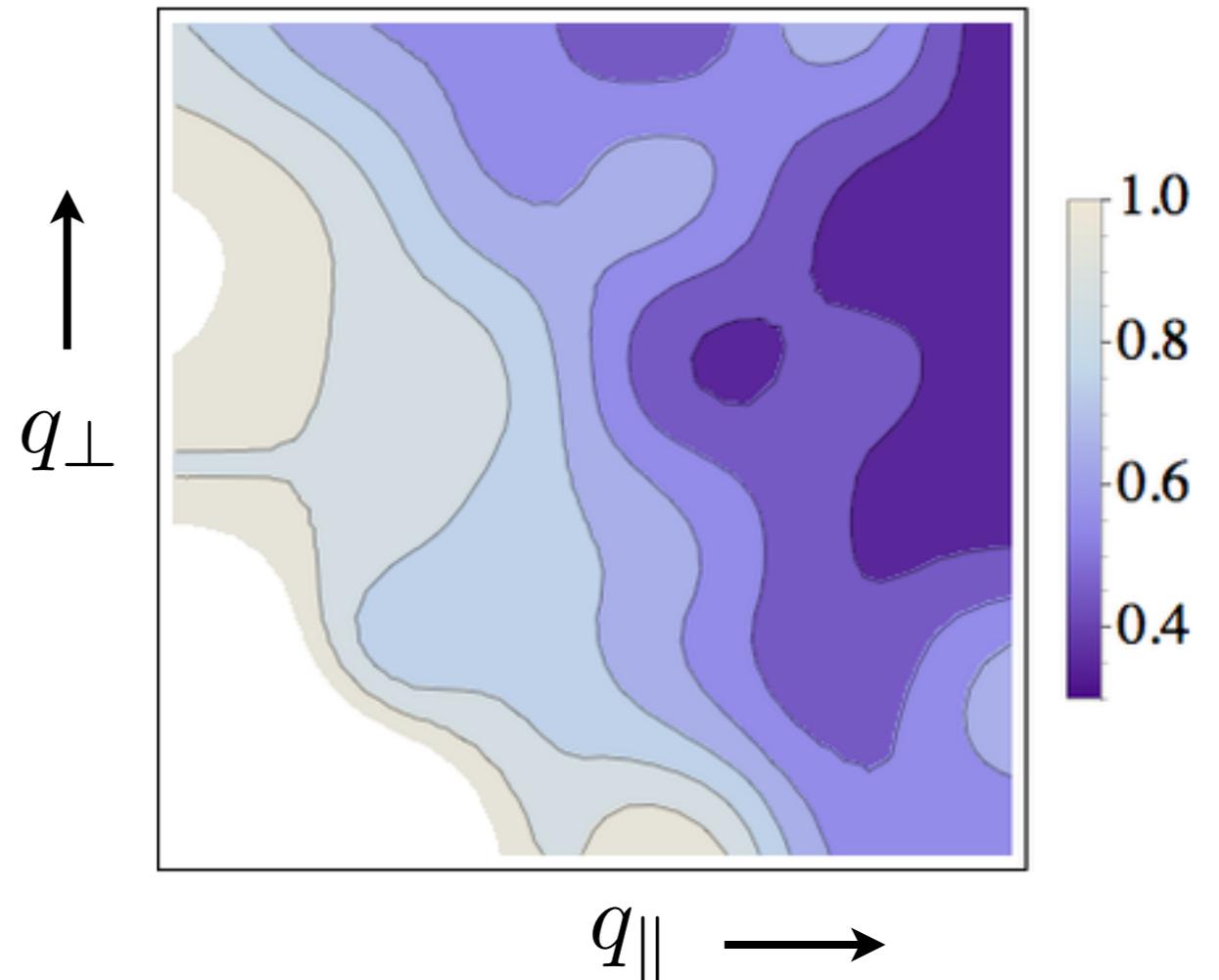




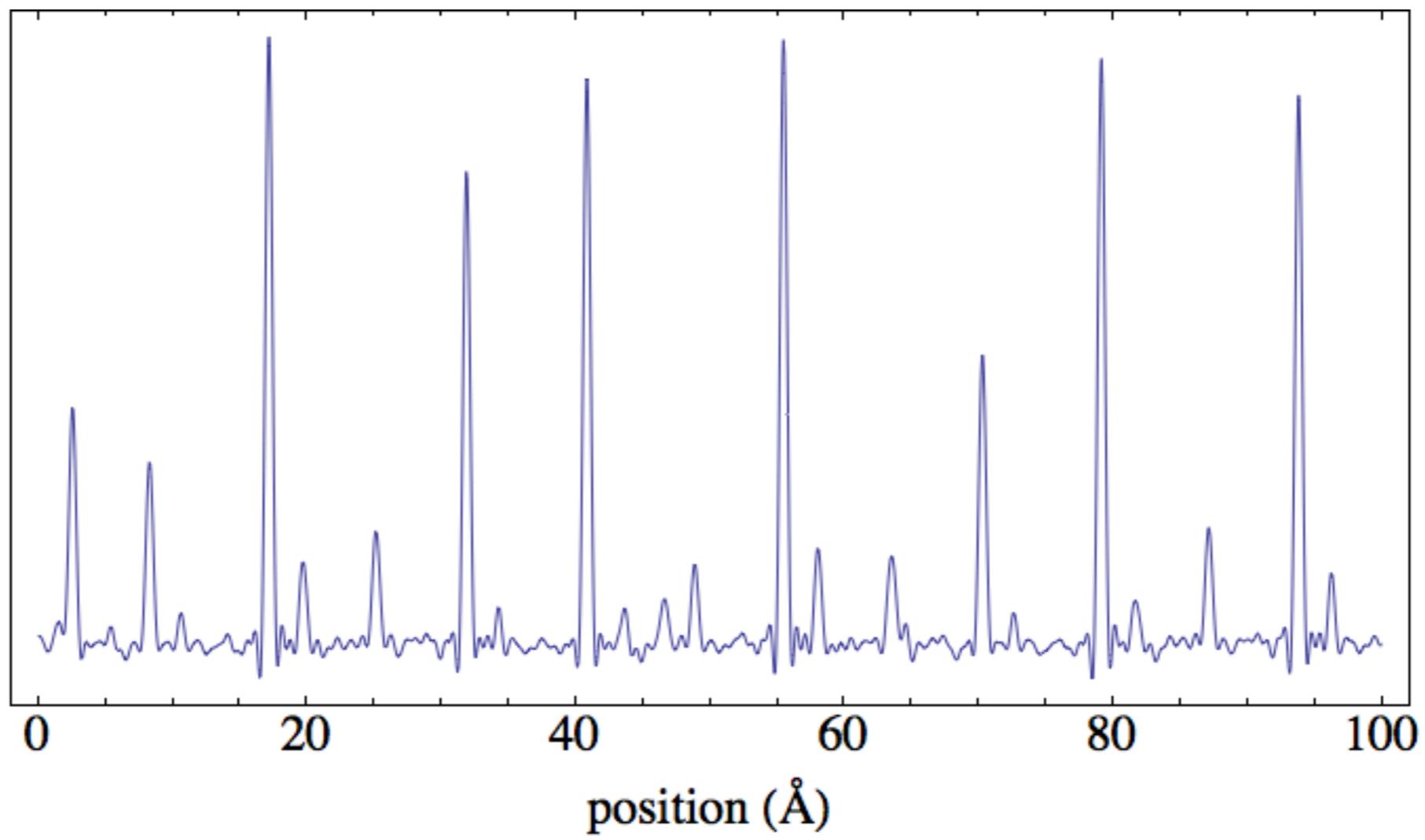


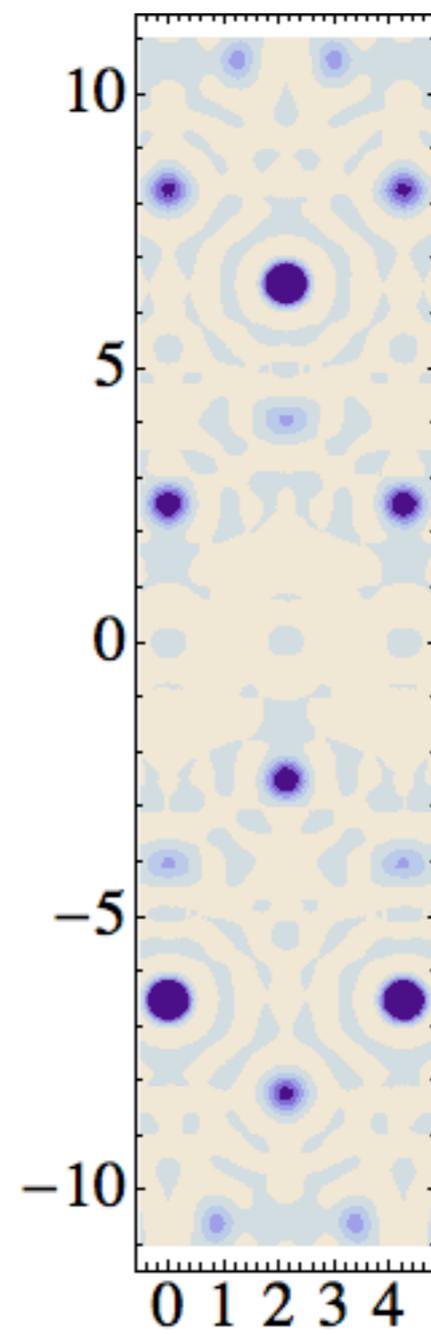
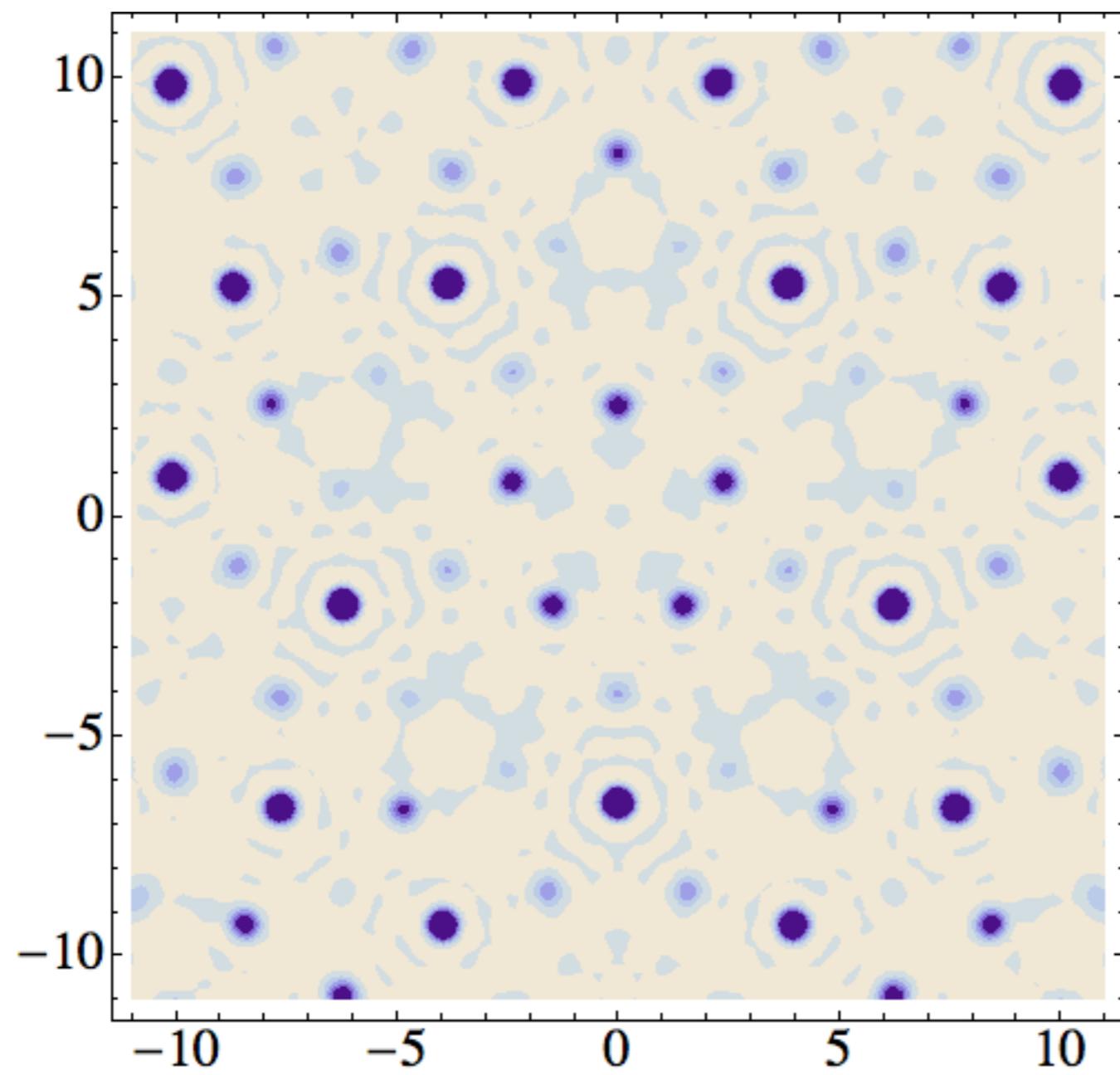
phase retrieval transfer function

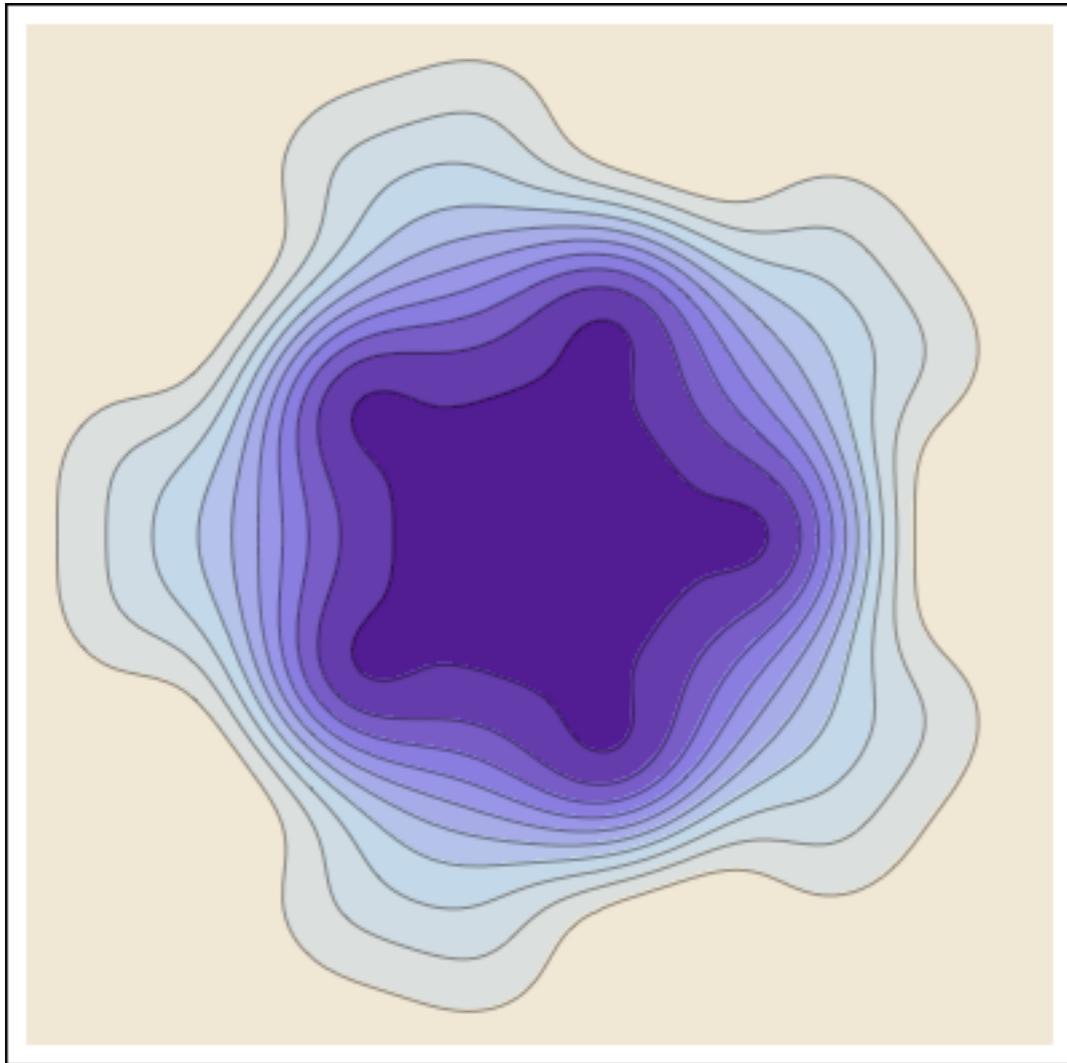
$$\langle e^{i\theta_{\mathbf{q}}} \rangle = \frac{|\langle F_{\mathbf{q}} \rangle|}{|F_{\mathbf{q}}|}$$



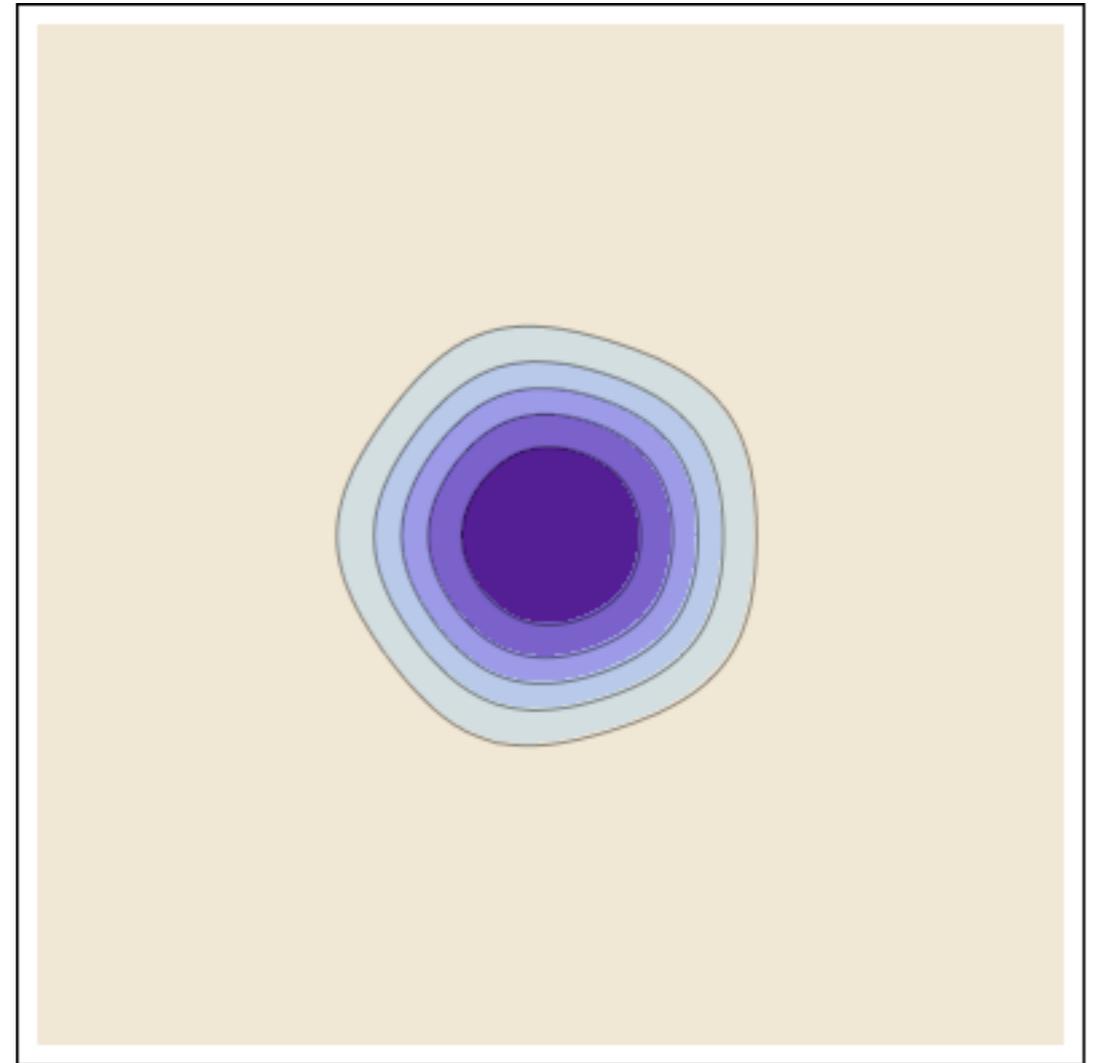
$$h_5 = 0$$





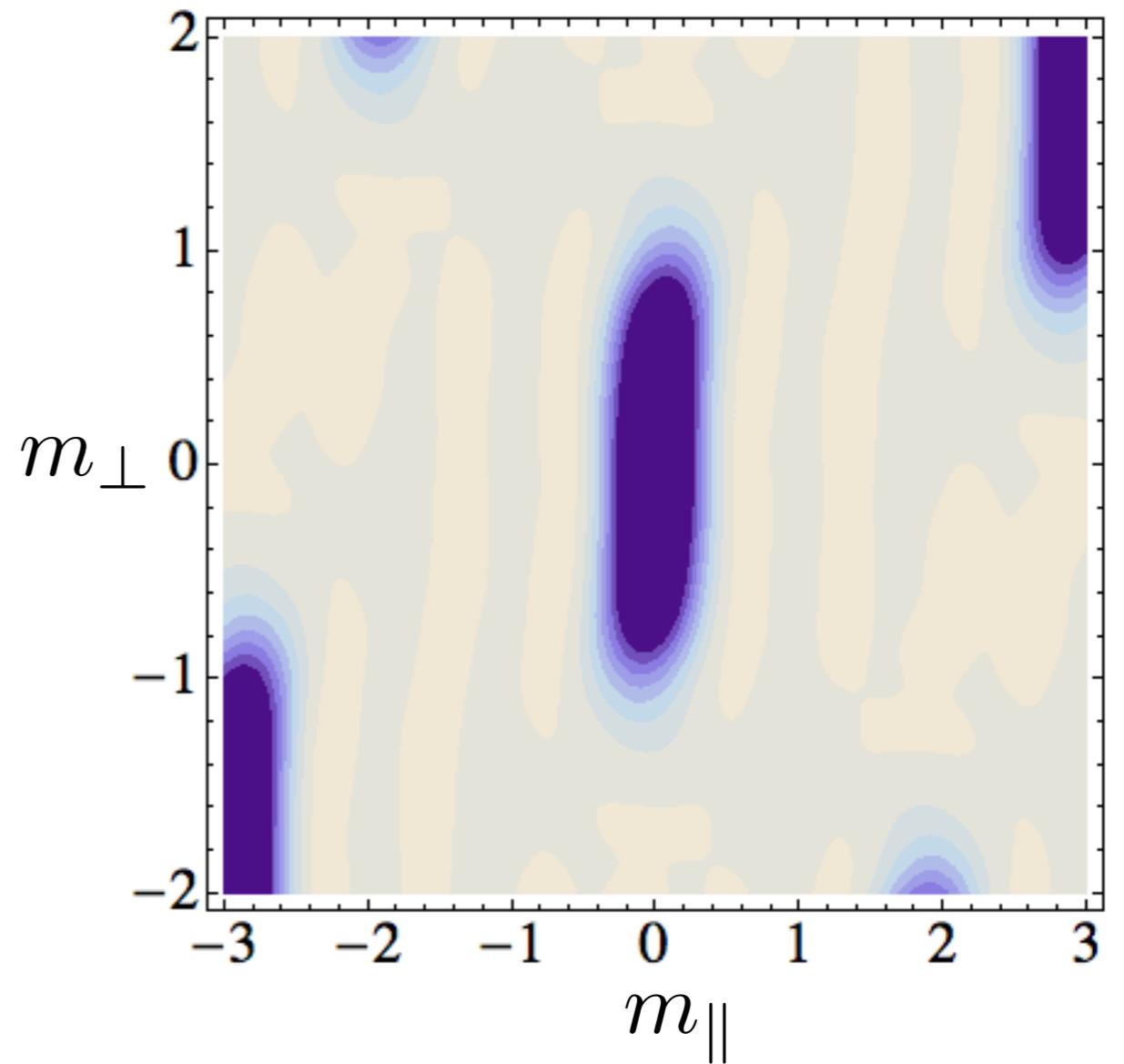
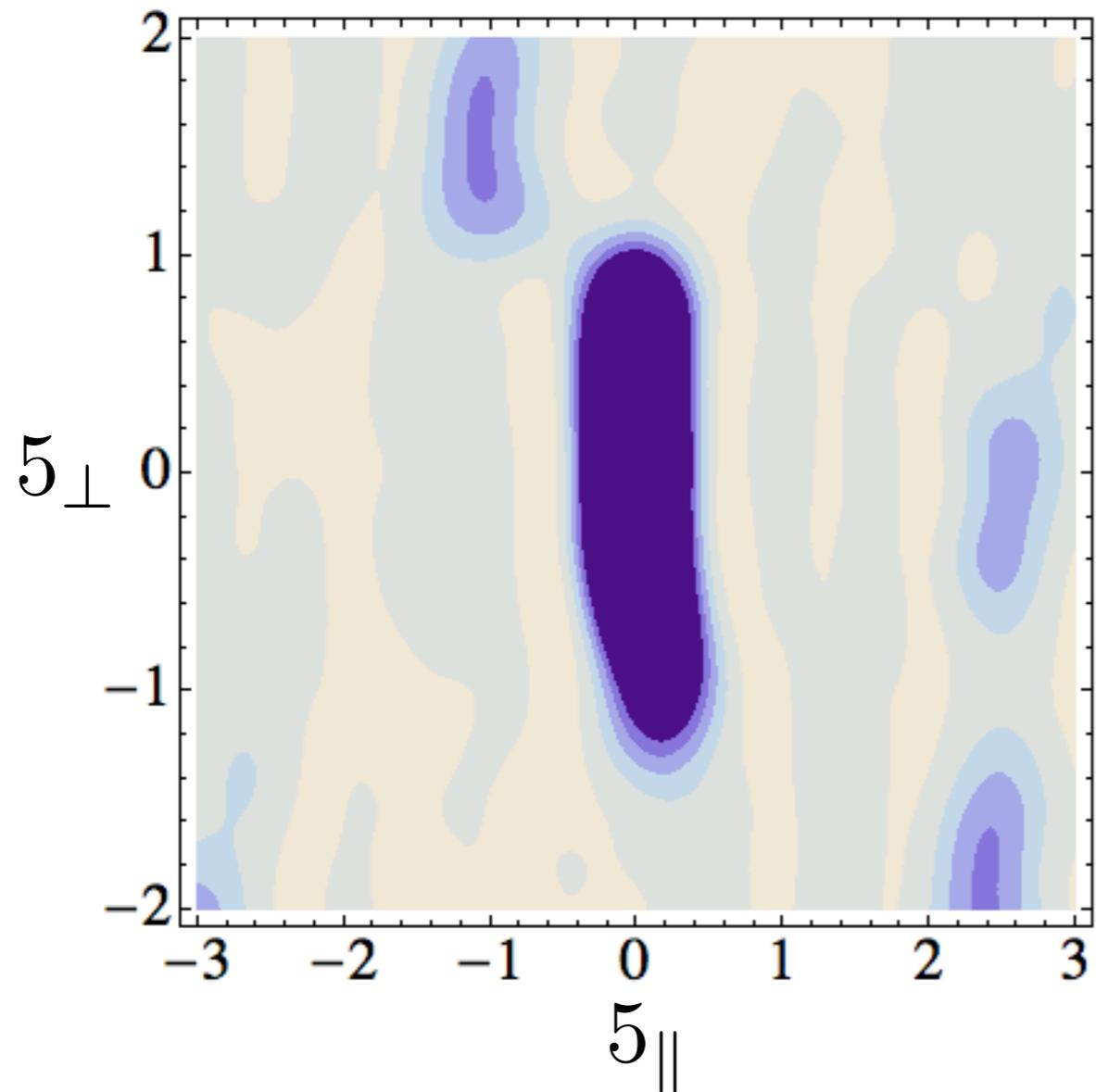


$[2/5, 2/5, 2/5, 2/5, 0]$



$[1/5, 1/5, 1/5, 1/5, 1/4]$

phason jumps



summary

- Direct methods are indispensable for the interpretation of crystallographic data.
- Unbiased reconstructions use the weakest possible prior constraints.
- The electron density support constraint allows for the non-spherical shapes of “atomic surfaces” in quasicrystals.
- The difference map iteration scheme is well suited for the two-constraint problem in phase retrieval.

FIN

Remerciements:

Données: Paweł Kuczera, Walter Steurer

Groupes d'espace: Ron Lifshitz

Présentation et logiciels:

<http://uuuuuu.lassp.cornell.edu>