Numerical methods for the Ginzburg–Landau problem

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Nico Schlömer Wim Vanroose

Universiteit Antwerpen

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The phenomenon of superconductivity

Superconductivity occurs in certain materials (usually) **very low temperatures**.

Characteristics:

- Zero (0) electrical resistance,

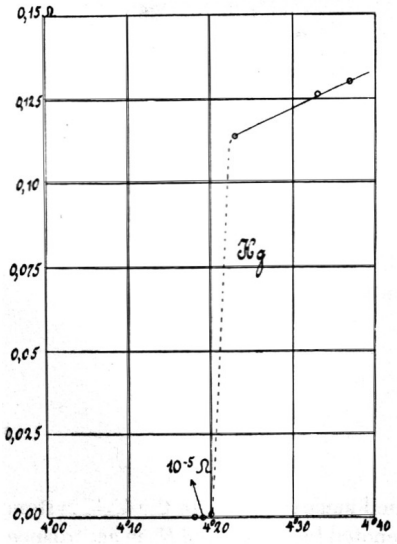
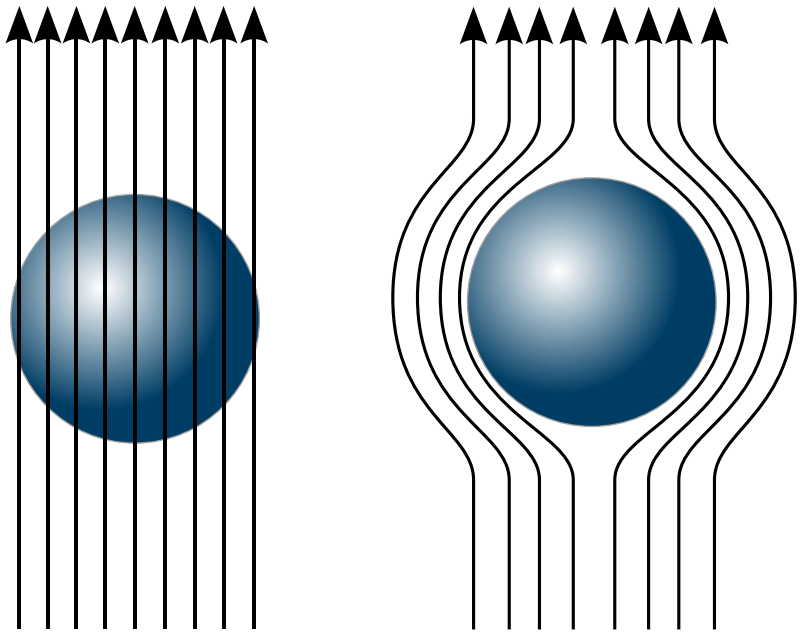


Figure: Extract from Kamerlingh Onnes' historical paper (**1911**).

The Meißner effect

- expulsion of the surrounding magnetic field (Meißner-effect).



(a) $T > T_c$. (b) $T < T_c$.

The Meißner effect (cont.)

- expulsion of the surrounding magnetic field (Meißner-effect).

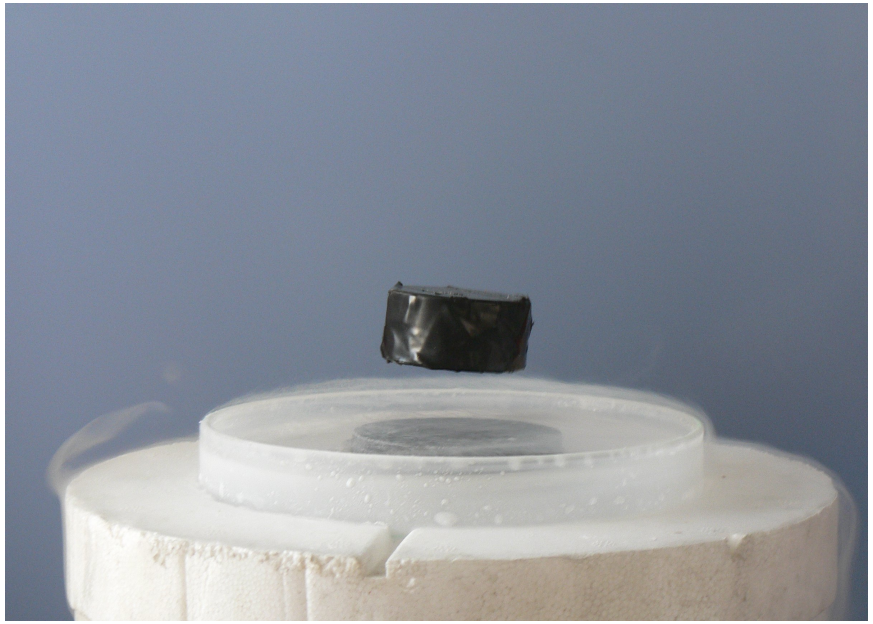


Figure: The Meißner effect “live”.

The intermediate state

There are **three** distinct material states:

- normal conductivity
- mixed state
- superconductivity

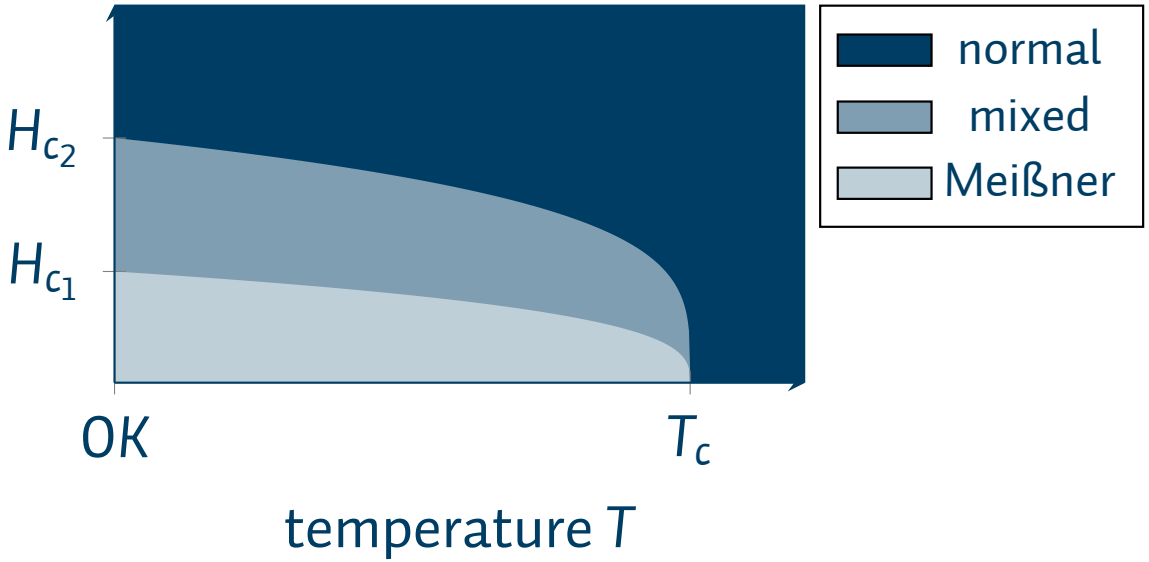
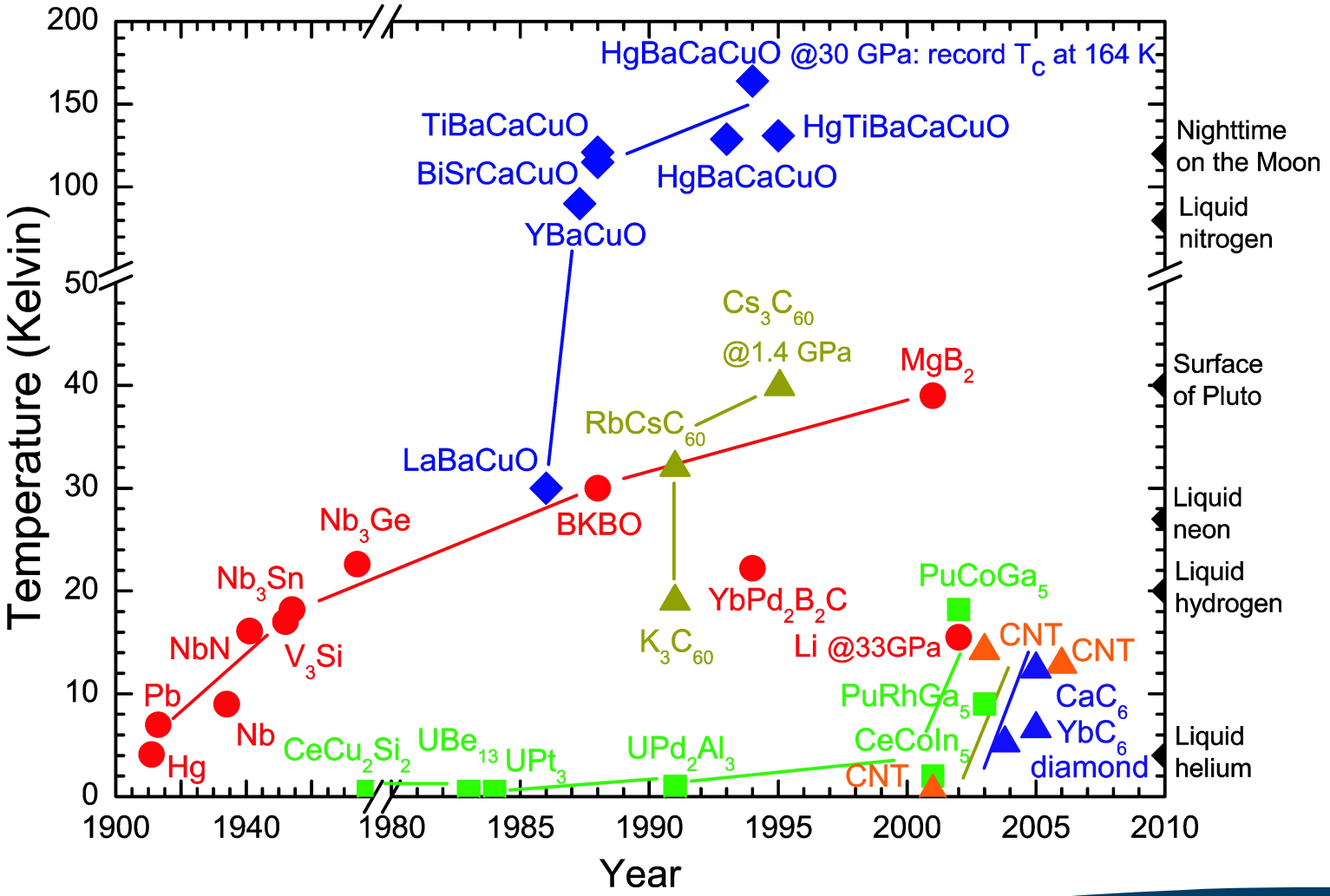


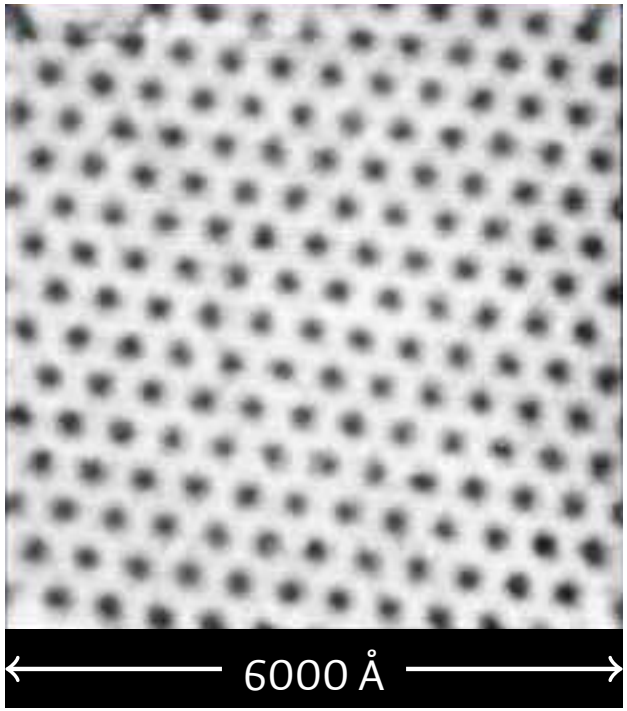
Figure: The states of a type-II superconductor in an H-T diagram.

Superconductor timeline



The intermediate state

Characterized by an incomplete Meißner effect, formation of **vortices**.



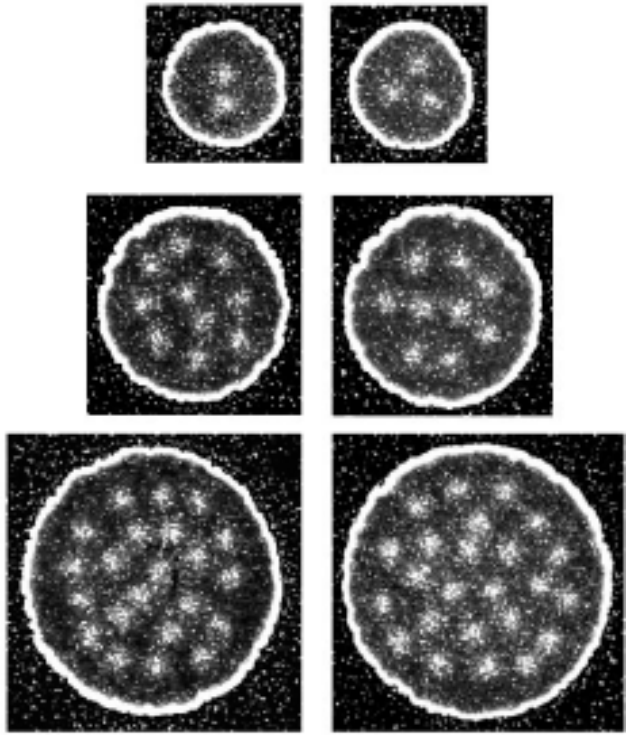


Figure: Left: [Triangular (Abrikosov) pattern]. Right: Symmetric sample.

Mathematical description

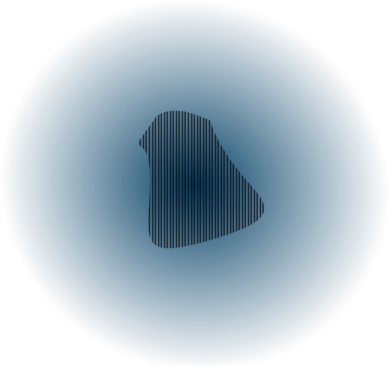
A superconductor state is characterized by

- the supercurrent density $\rho(\mathbf{x}, t) \in C(\Omega_1)$,

$$\rho = |\psi|^2$$

- the magnetic (vector) field $\mathbf{B}(\mathbf{x}, t) \in (C(\mathbb{R}^n))^n$

$$\mathbf{B} = \nabla \times \mathbf{A}$$



Ginzburg-Landau: free energy

$$G(\psi, \mathbf{A}) - G(0, \mathbf{A}) = \int_{\mathbb{R}^3} \left[\frac{1}{2} \left| -\mathrm{i}\nabla\psi - \mathbf{A}\psi \right|^2 + \frac{1}{4} \left(1 - |\psi|^2 \right)^2 \right.$$
$$\left. + \kappa^2 (\nabla \times \mathbf{A})^2 - 2\kappa^2 (\nabla \times \mathbf{A}) \cdot \mathbf{H}_0 \right] \mathrm{d}\mathbf{x},$$

$\psi : \Omega \to \mathbb{C}$ . . . order parameter
$\mathbf{A} : \mathbb{R}^3 \to \mathbb{R}^3$ . . . magnetic vector potential

The Ginzburg-Landau equations

Euler-Lagrange $\Longrightarrow$

$$\begin{cases} (-\mathrm{i}\nabla - \mathbf{A})^2 \psi = \psi \left(1 - |\psi|^2\right) & \text{on } \Omega_1 \\ -\nabla \times (\nabla \times \mathbf{A}) = \dfrac{1}{\kappa^2} \left(\dfrac{1}{2\mathrm{i}} \left(\overline{\psi} \nabla \psi - \psi \nabla \overline{\psi}\right) - |\psi|^2 \mathbf{A} \right) & \text{on } \mathbb{R}^n \\ \mathbf{n} \left(-\mathrm{i}\nabla - \mathbf{A}\right) \psi|_\Gamma = 0, & \text{on } \Gamma \\ \lim\limits_{\mathbf{x} \to \infty} \nabla \times \mathbf{A} = \mathbf{H}_0. \end{cases}$$

Extreme type-II superconductors

...simplification

$$\kappa \gg 1.$$

$$\begin{cases} (-\mathrm{i}\nabla - \mathbf{A})^2 \psi = \psi \left(1 - |\psi|^2\right) & \text{on } \Omega_1 \\ -\nabla \times (\nabla \times \mathbf{A}) = 0 & \text{on } \mathbb{R}^3 \\ \mathbf{n}\,(-\mathrm{i}\nabla - \mathbf{A})\,\psi|_\Gamma = 0, & \text{on } \Gamma \\ \lim\limits_{\mathbf{x}\to\infty} \nabla \times \mathbf{A} = \mathbf{H}_0. \end{cases}$$

Extreme type-II superconductors

$$\left\{ \begin{array}{l} -\nabla \times (\nabla \times \mathbf{A}) = 0 \\ \lim\limits_{\mathbf{x}\to\infty} \nabla \times \mathbf{A} = \mathbf{H}_0. \end{array} \right\} \qquad \Longrightarrow \mathbf{A}(H_0)$$

Extreme type-II Ginzburg-Landau equations

$$\begin{cases} (-\mathrm{i}\nabla - \mathbf{A}(H_0))^2 \psi = \psi \left(1 - |\psi|^2\right) & \text{on } \Omega_1 \\ \mathbf{n}\,(-\mathrm{i}\nabla - \mathbf{A}(H_0))\,\psi|_\Gamma = 0, & \text{on } \Gamma \end{cases}$$

Example solutions

Extreme type-II Ginzburg-Landau equations

$$\begin{cases} (-\mathrm{i}\nabla - \mathbf{A}(H_0))^2\,\psi - \psi\,(1 - |\psi|^2) = 0 & \text{on } \Omega_1 \\ \mathbf{n}\,(-\mathrm{i}\nabla - \mathbf{A}(H_0))\,\psi|_\Gamma = 0 & \text{on } \Gamma \end{cases} \qquad (\mathcal{GL})$$

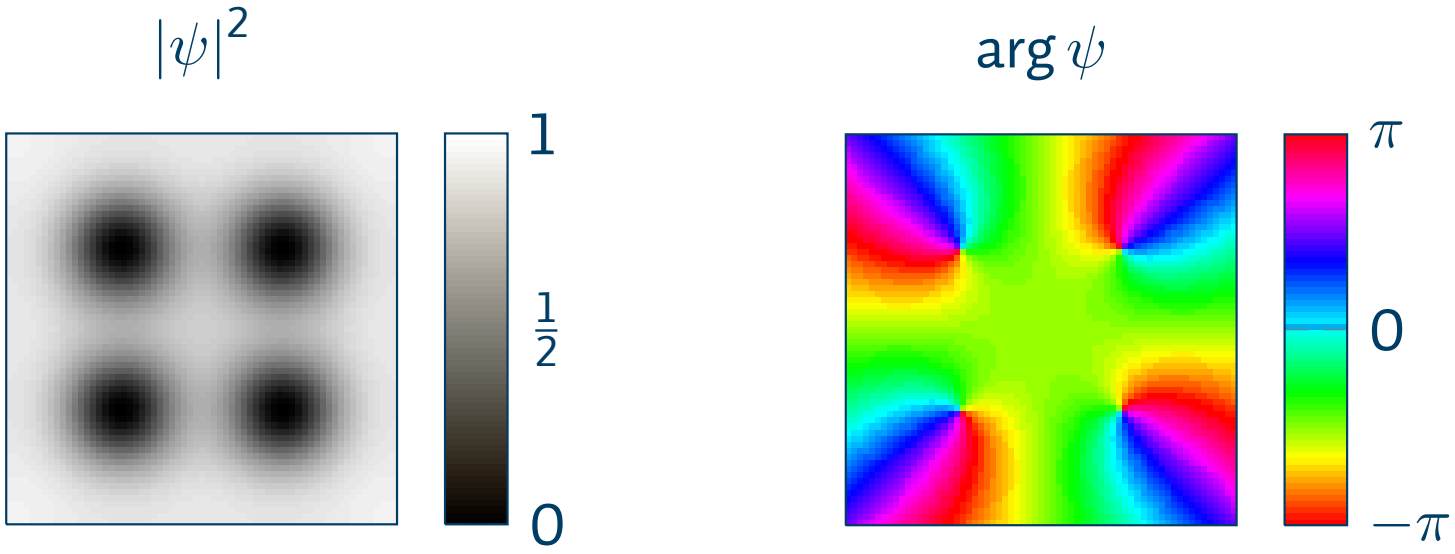


Figure: Solution of $(\mathcal{GL})$, square-shaped domain, $H_0 = 0.4$.

Selected references

Qiang Du, Max D. Gunzburger, and Janet S. Peterson.
Analysis and approximation of the Ginzburg–Landau model of superconductivity.
SIAM Rev., 34:54–81, March 1992.

H.G. Kaper and M.K. Kwong.
Vortex configurations in type-II superconducting films.
Journal of Computational Physics, 119(1):120–131, June 1995.

J. Müller
Superconducting rings show hints of half-quantum vortices.
Physics Today, 64(3), March 2011.

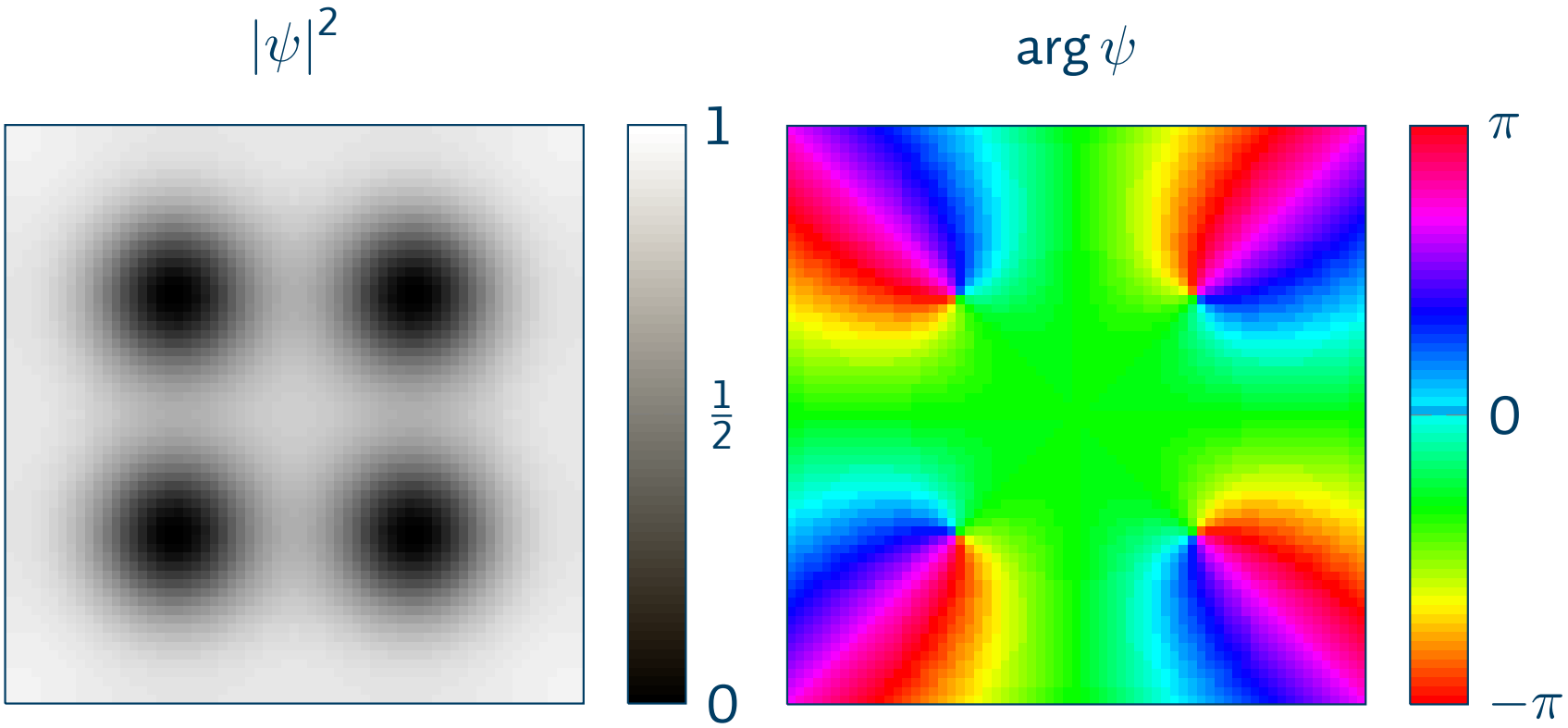
Funny properties I

Gauge invariance!

Extreme type-II Ginzburg-Landau equations

$$\begin{cases} \left(-\mathrm{i}\nabla - \mathbf{A}(H_0)\right)^2 \psi - \psi\left(1 - |\psi|^2\right) = 0 & \text{on } \Omega_1 \\ \mathbf{n}\left(-\mathrm{i}\nabla - \mathbf{A}(H_0)\right)\psi|_\Gamma = 0 & \text{on } \Gamma \end{cases} \qquad (\mathcal{GL})$$

More solutions



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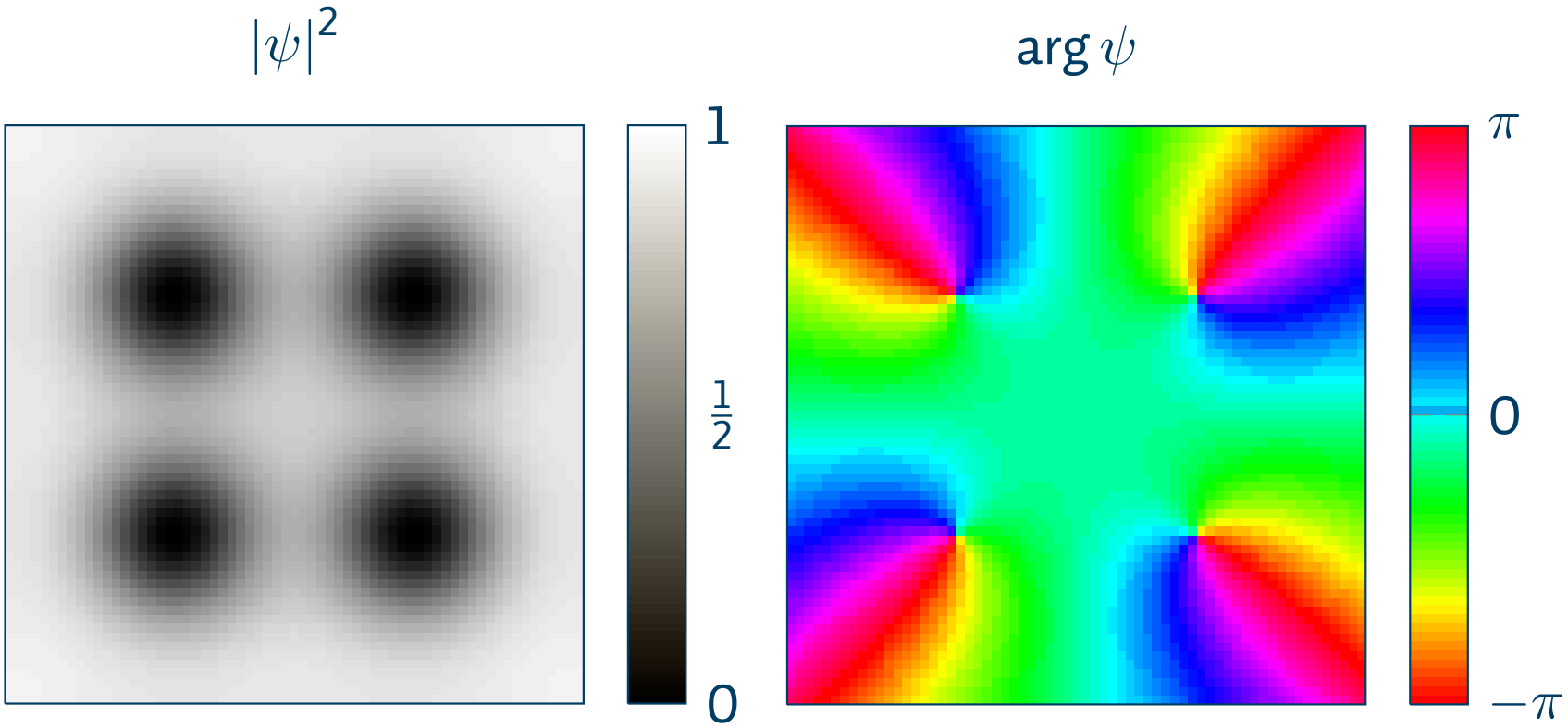

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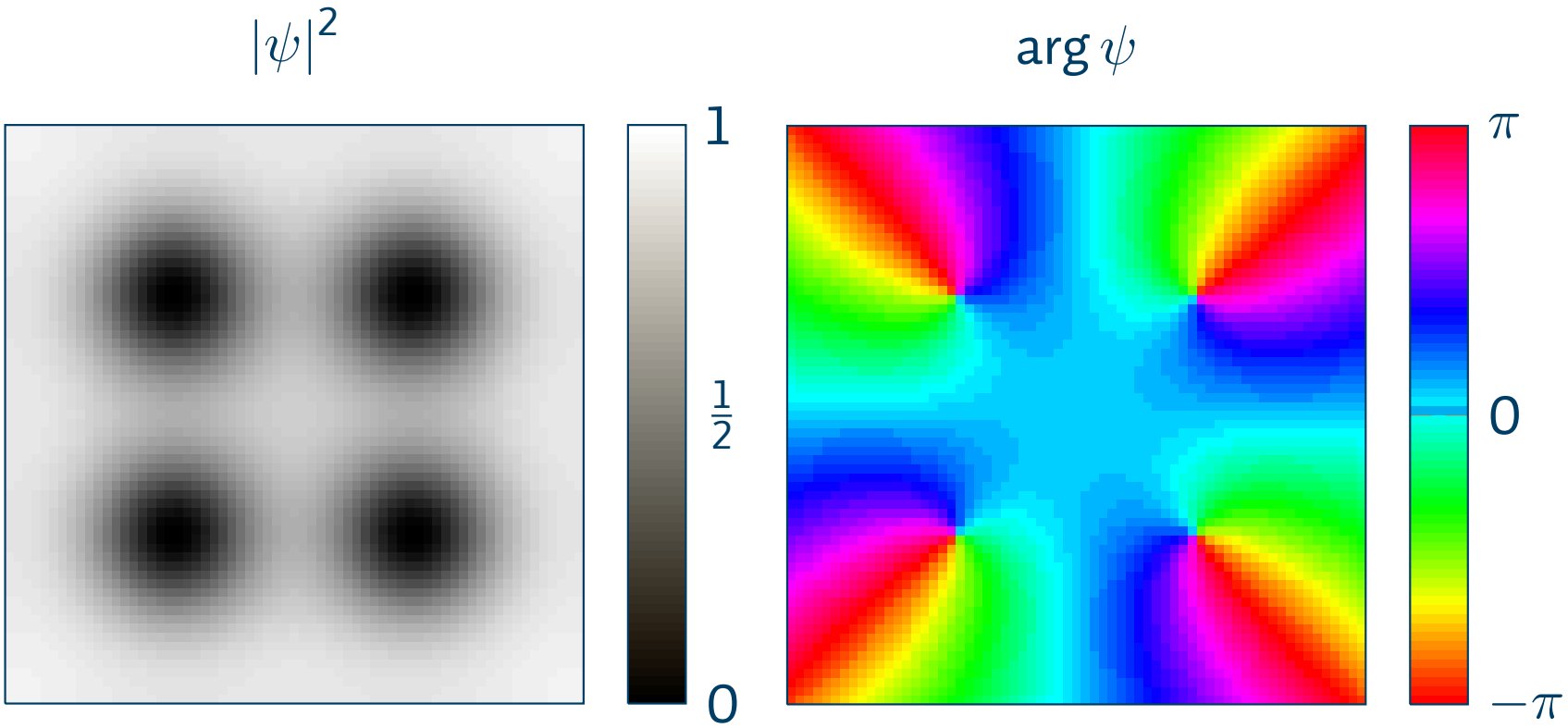

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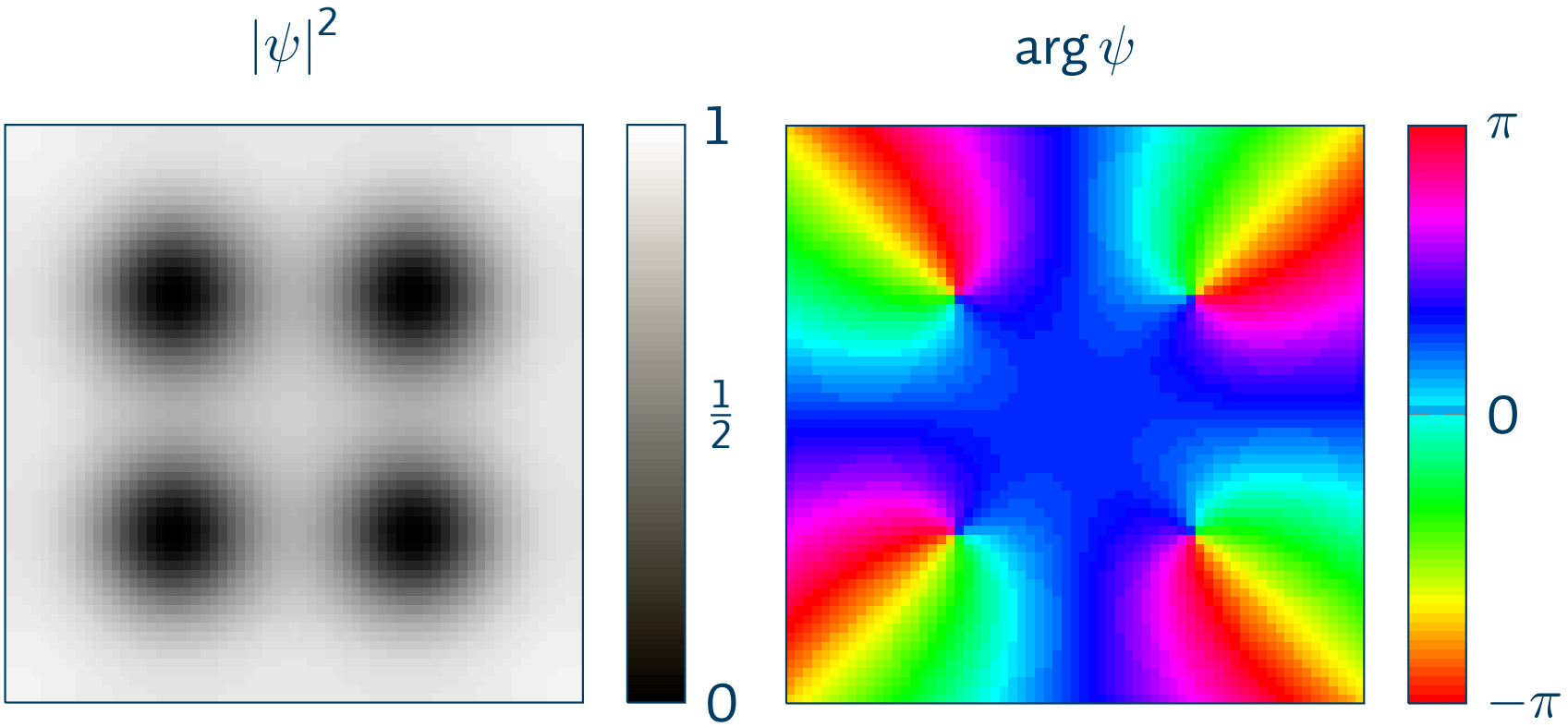

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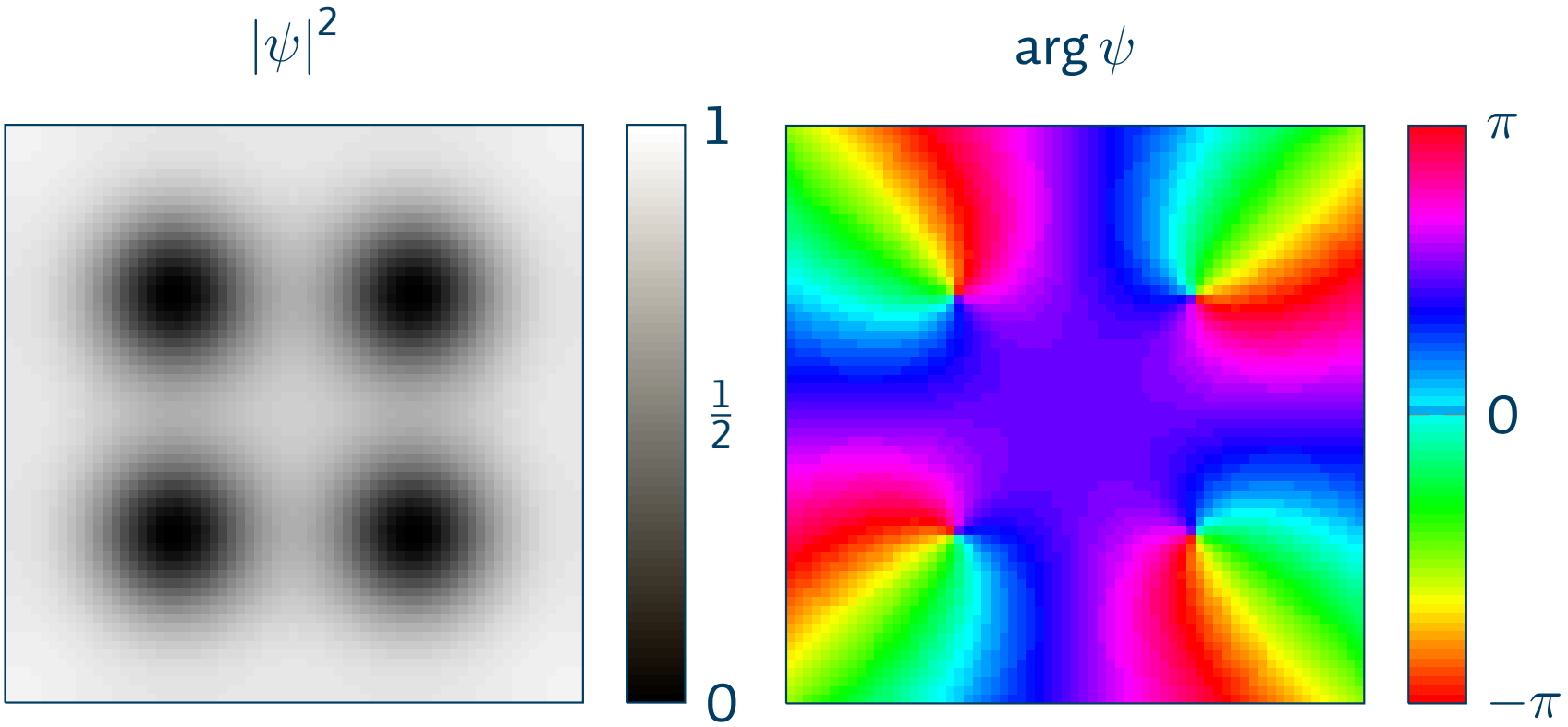

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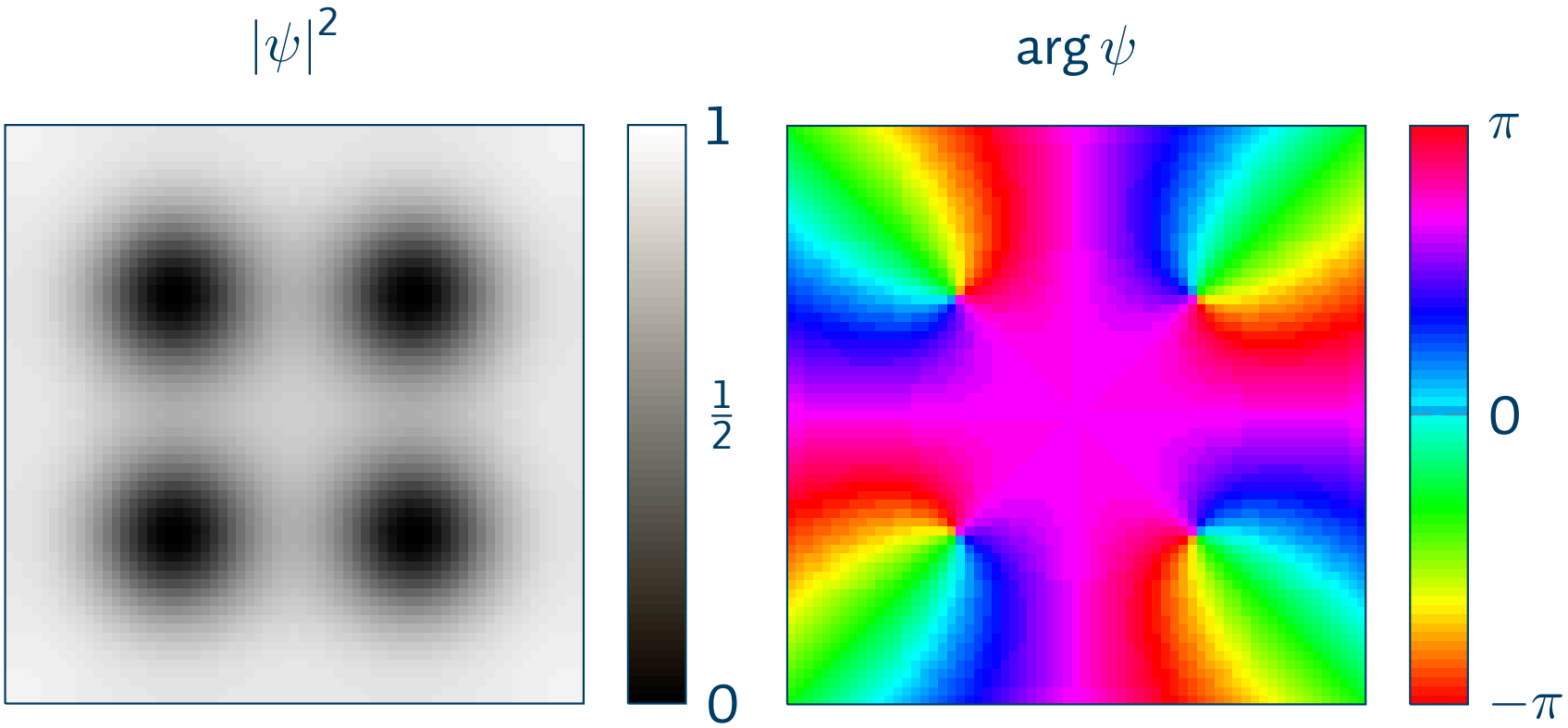

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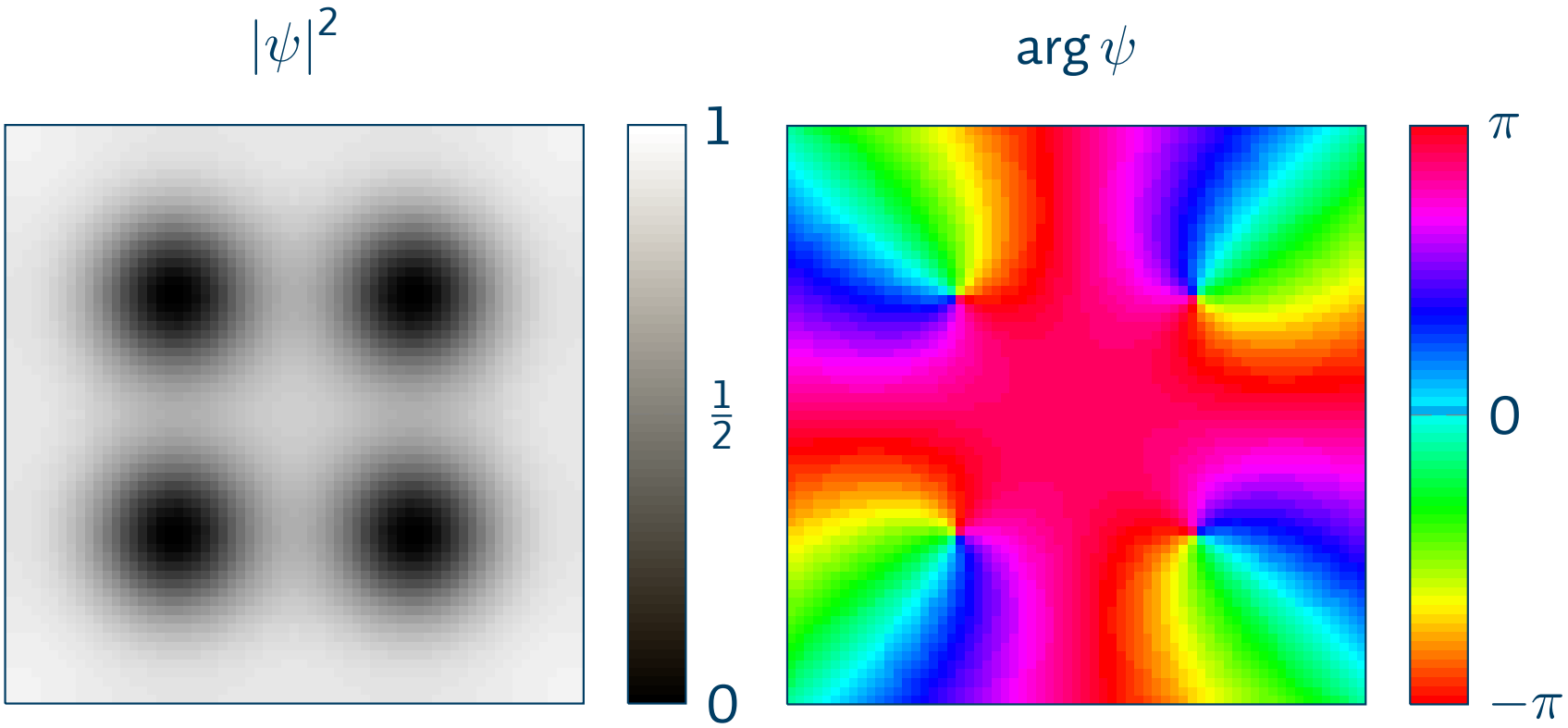

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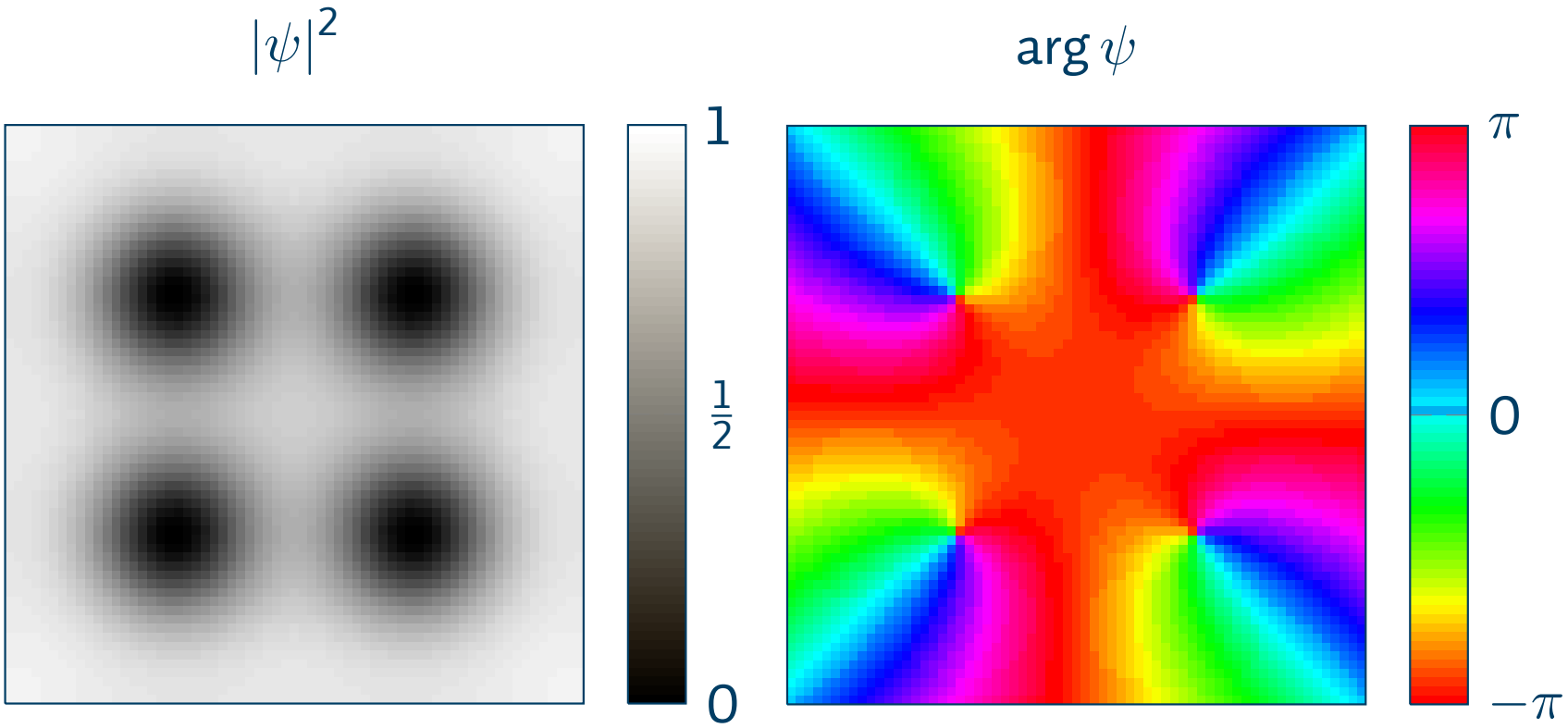

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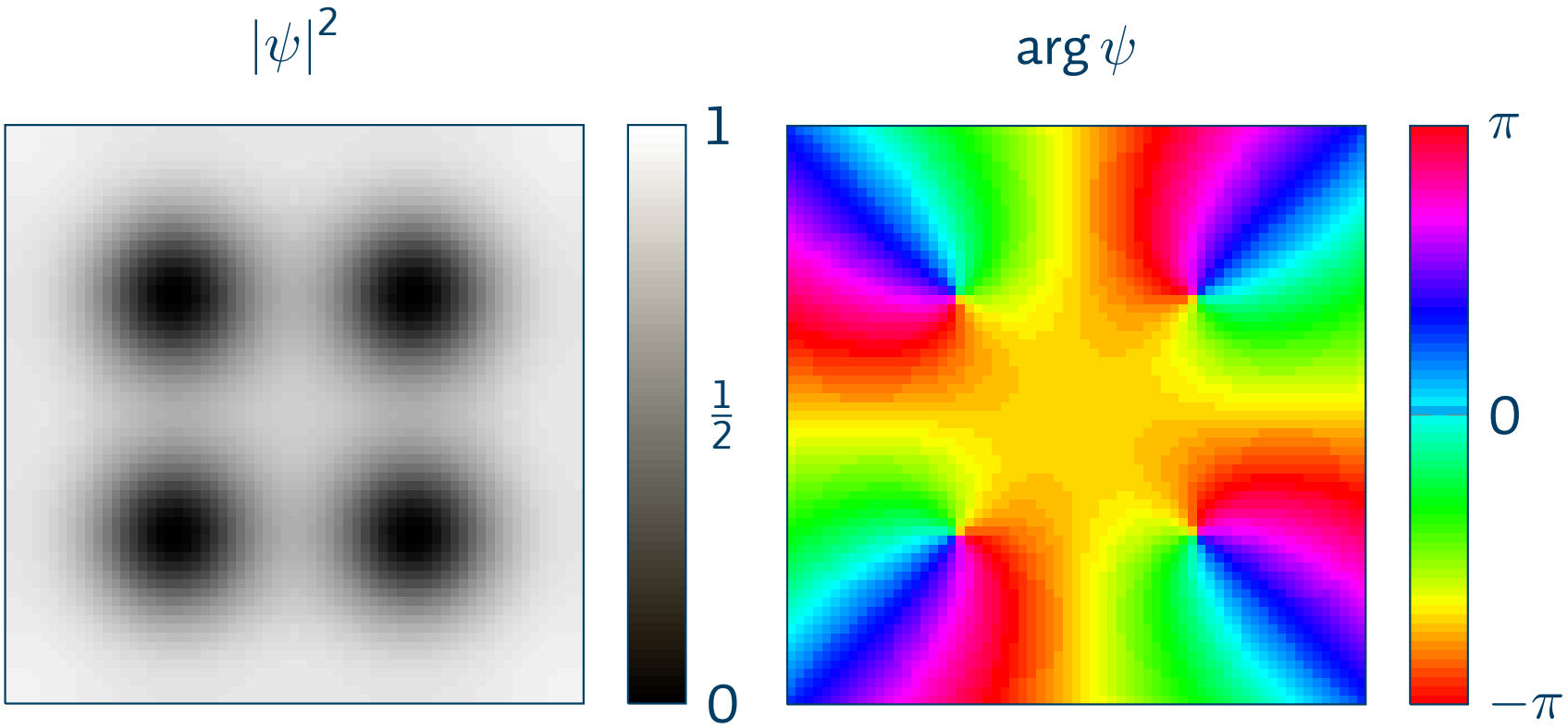

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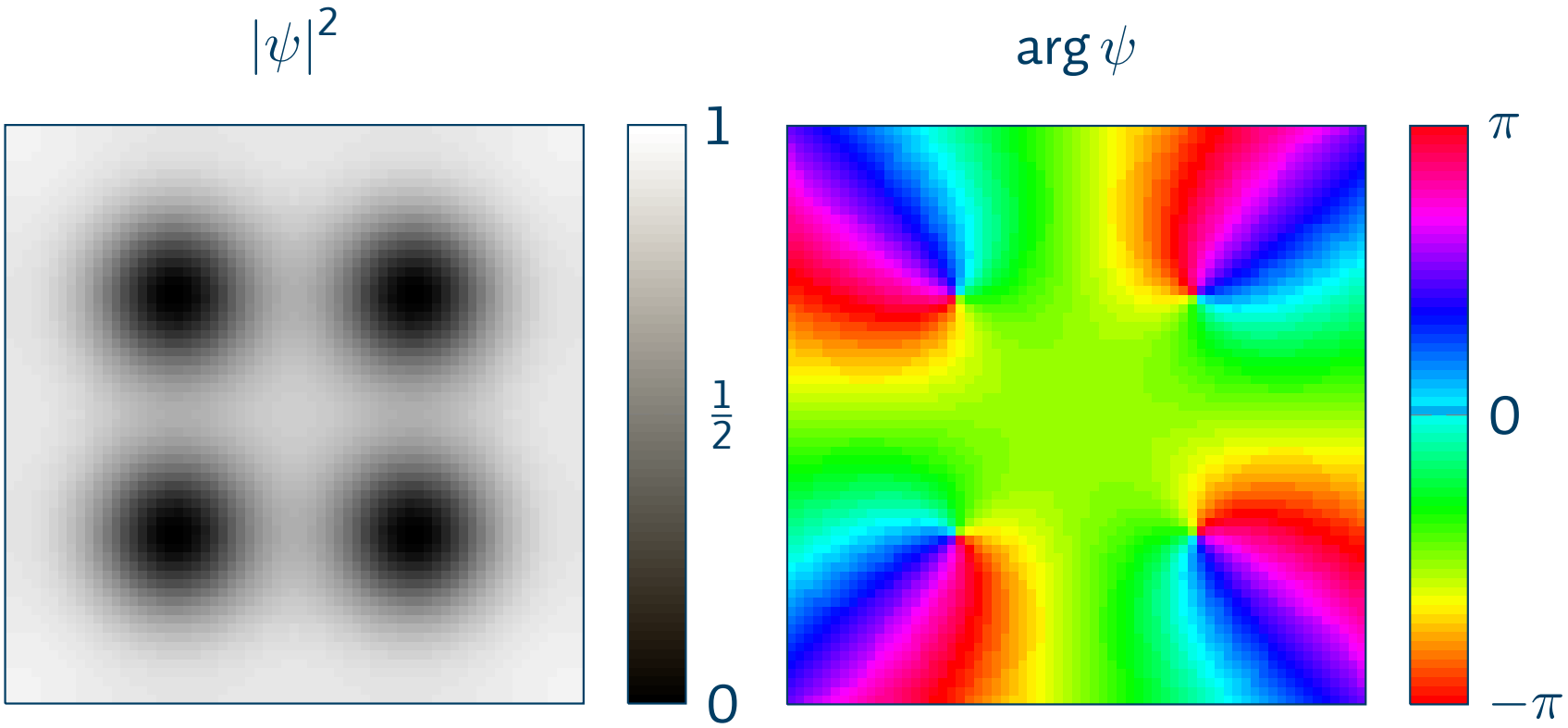

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Gauge invariance

The equations ($\mathcal{GL}$) have the property that

$$F(\chi, \mathbf{A}) = \alpha F(\psi_2, \mathbf{A}_2)$$

with

$$\psi_2 = \psi \exp(\mathrm{i}\chi)$$
$$\mathbf{A}_2 = \mathbf{A} + \boldsymbol{\nabla}\chi$$

for **any** $\chi \in C^1_{\mathbb{R}}(\Omega_2)$, i.e., **gauging** doesn't play a role.

Gauge invariant discretizations

Problem

When plain discretizing ($\mathcal{GL}$) with standard finite differences, this gauge invariance is ***not preserved****.*

How to deal with this? Answer: Variable transformation.

$$U_x(x) := \exp\left\{-\mathrm{i}\int_{\mu_0}^{\mu} A_\mu(\xi)\,\mathrm{d}\xi\right\},$$

U_y, U_z analogously,

(for Cartesian grids).

Gauge invariant discretizations (cont.)

Ginzburg–Landau eqns.

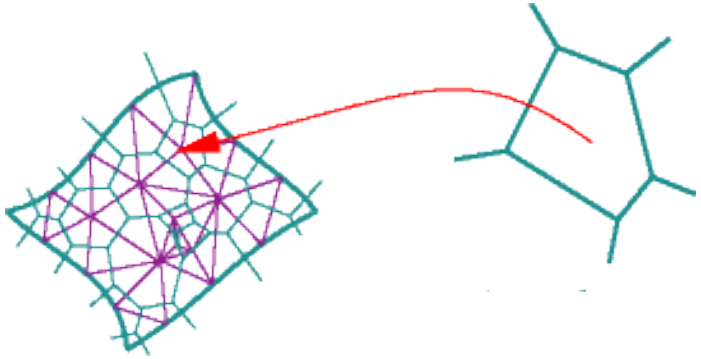
$$0 = \sum_{\mu \in \{x,y,z\}} \overline{U}_\mu \frac{\partial^2}{\partial^2 \mu} (U_\mu \psi) - \psi \left(1 - |\psi|^2\right) \quad \text{on } \Omega$$

$$0 = -\mathrm{i} \overline{U}_\mu \frac{\partial}{\partial \mu} (U_\mu \psi) \quad \forall \mu \in \{x, y, z\} \quad \text{on } \partial\Omega$$

for Cartesian grids.

Finite volumes

$$0 = \int_{\Omega_r} F(\psi) = \int_{\Omega_r} (-\mathrm{i}\nabla - \mathbf{A})^2 \psi - \int_{\Omega_r} \psi \left(1 - \psi\overline{\psi}\right)$$



$$0 = \int_{\Omega_r} F(\psi) = \underbrace{\int_{\Omega_r} (-\mathrm{i}\nabla - \mathbf{A})^2 \psi}_{\text{similar to Laplacian}} - \underbrace{|\Omega_r| \psi_k \left(1 - \psi_k \overline{\psi}_k\right)}_{\text{mass lumping}}$$

GI: numerical consequences

From gauge invariance follows:

Problem

For each solution $(\psi_0, \mathbf{A}_0)$*, there is a space* S *such that*

$$J_{(\psi_0, \mathbf{A}_0)}(\psi, \mathbf{A}) = 0$$

for each $(\psi, \mathbf{A}) \in S$*.*

Consequence: In each solution, J is **rank-deficient** by dim S!

Newton iteration for original problem

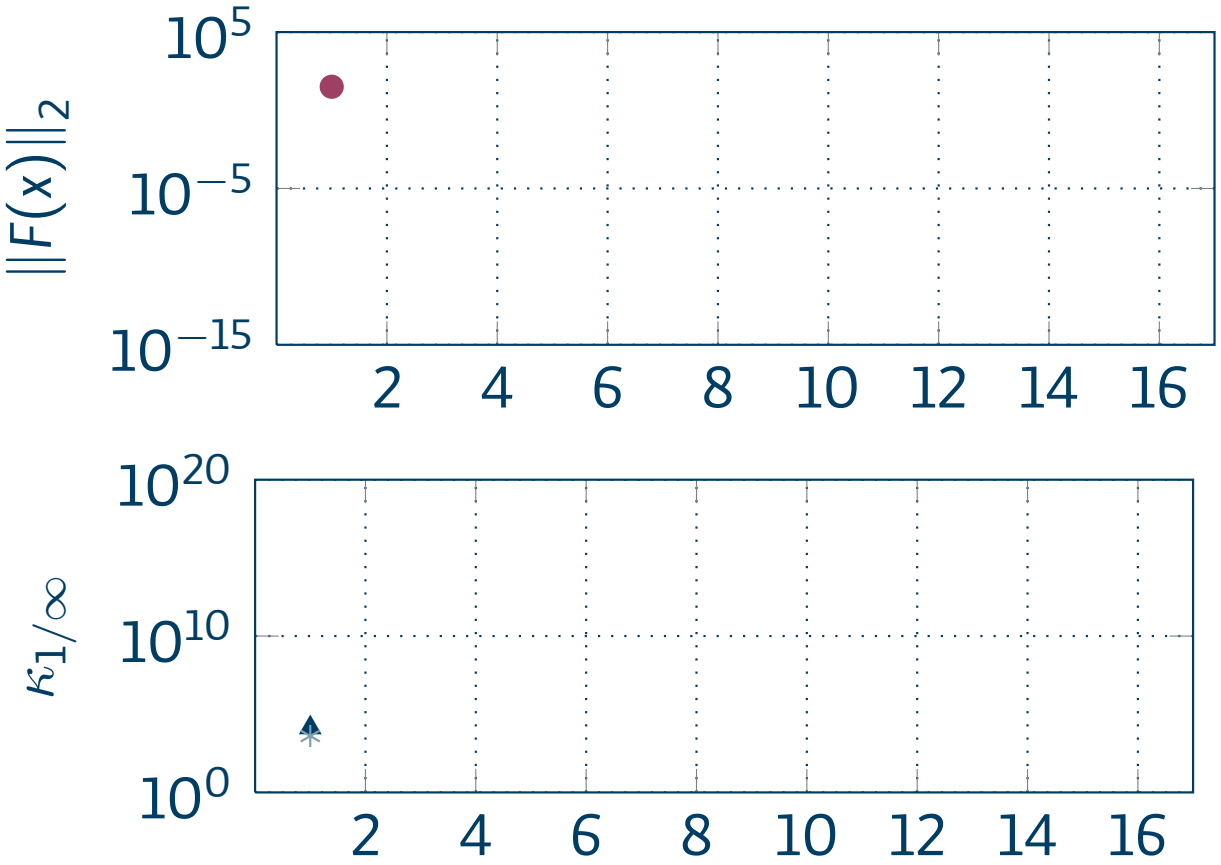


Figure: Typical behavior of the Newton residual (here: with *LU* solves for the linear equation system).

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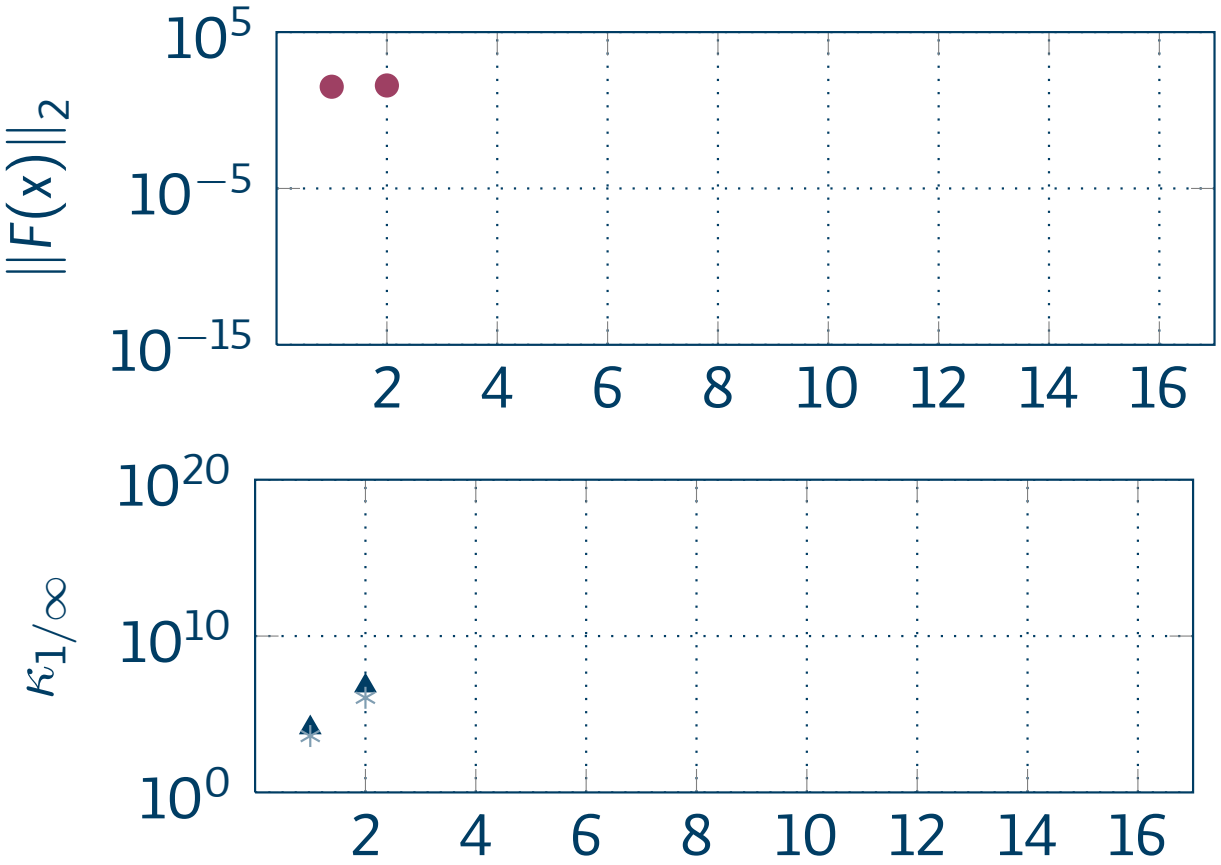

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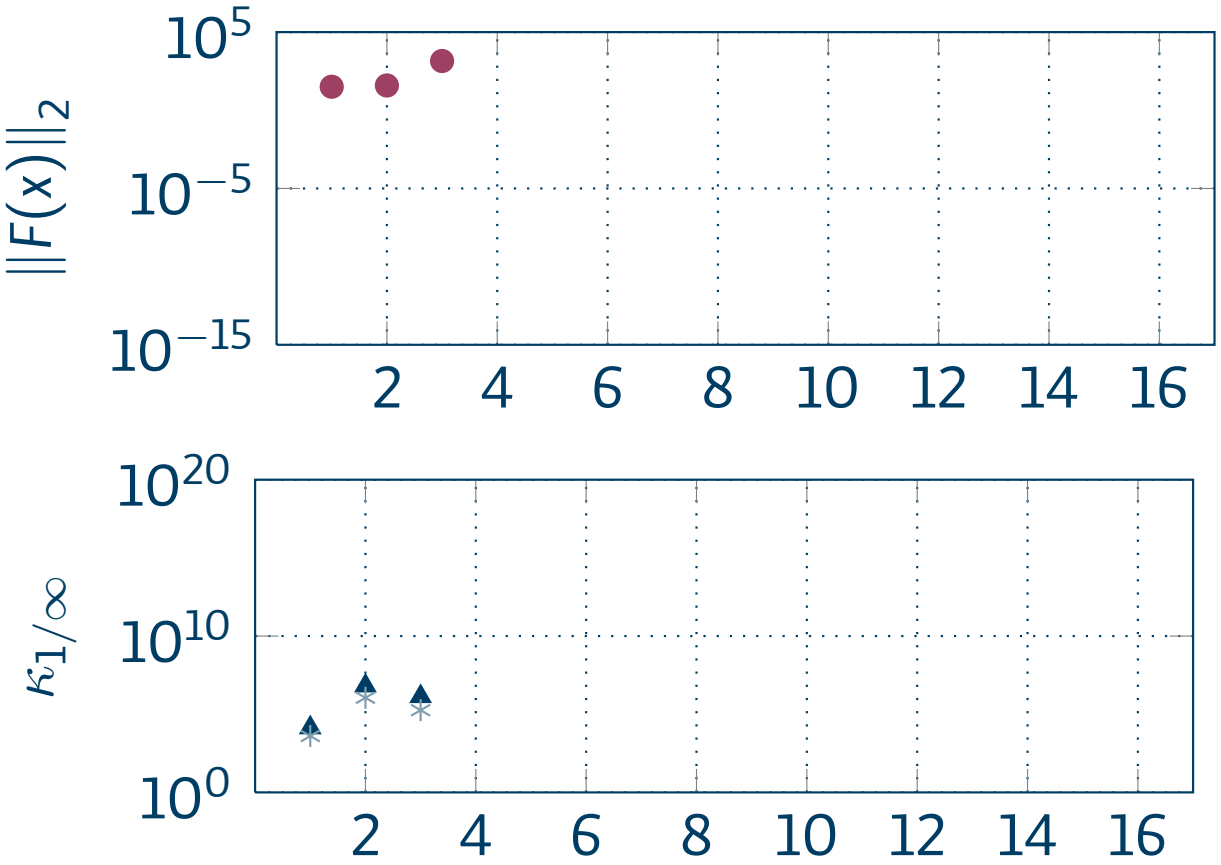

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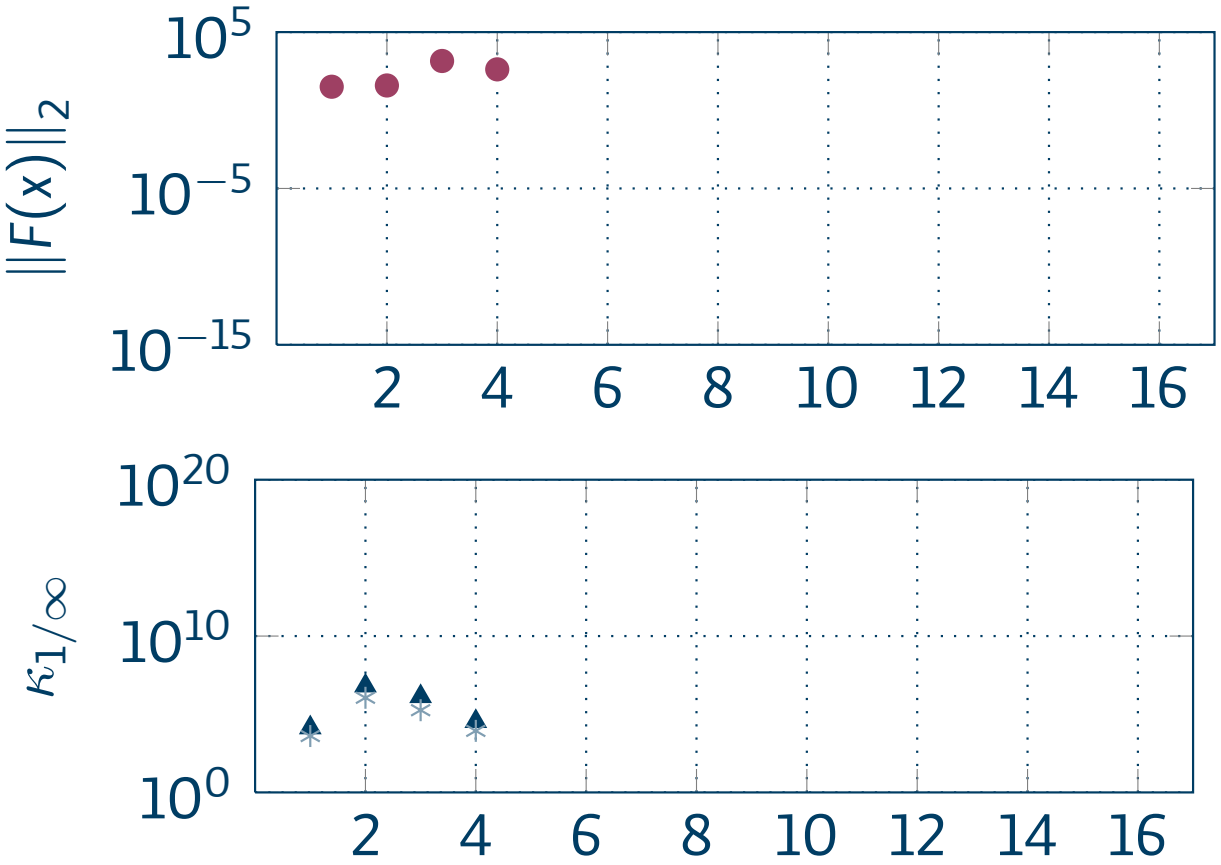

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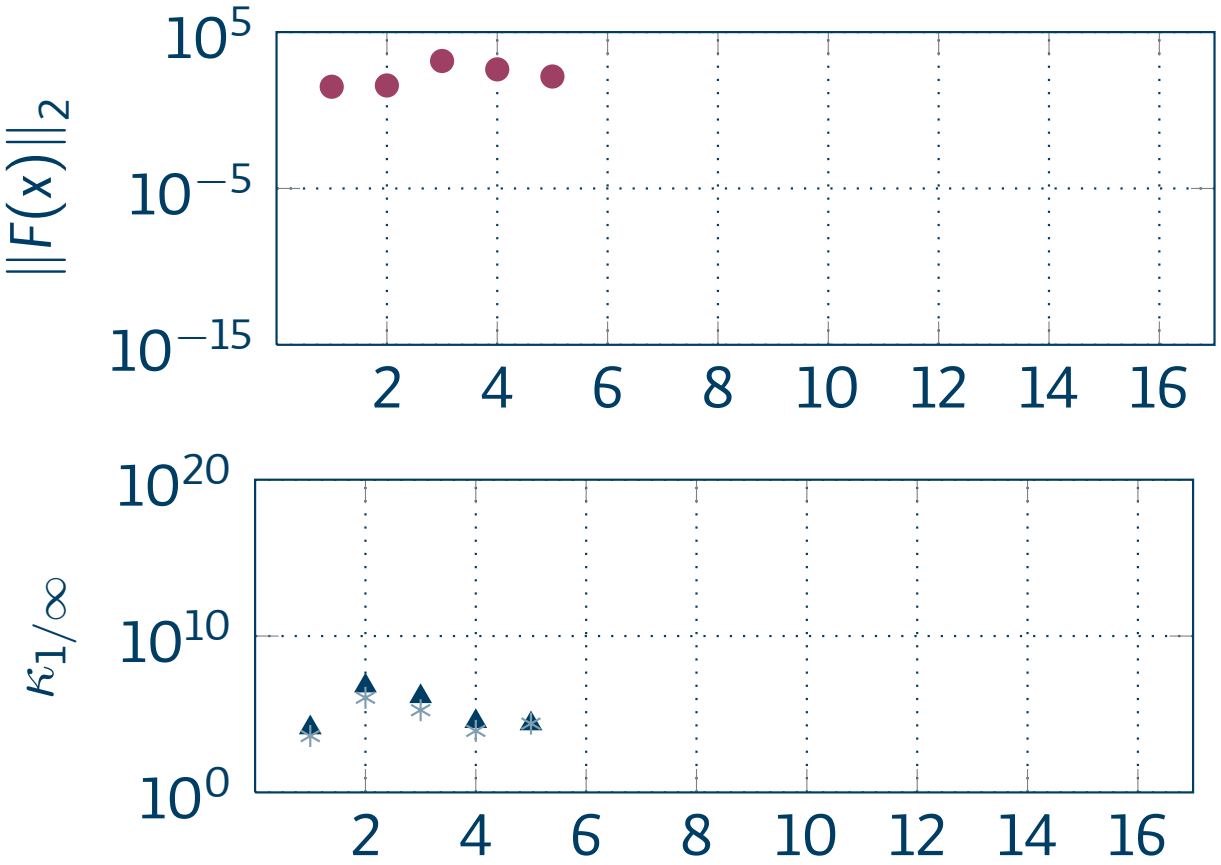

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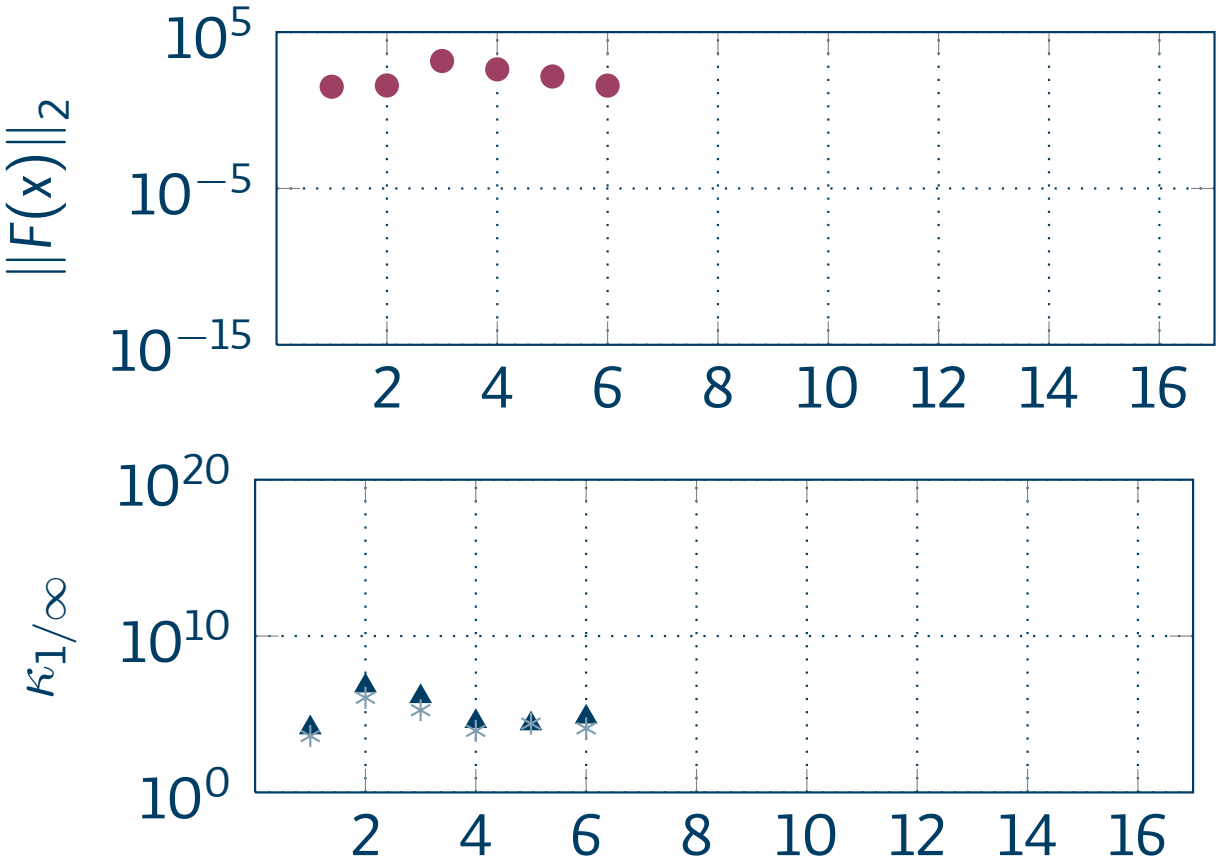

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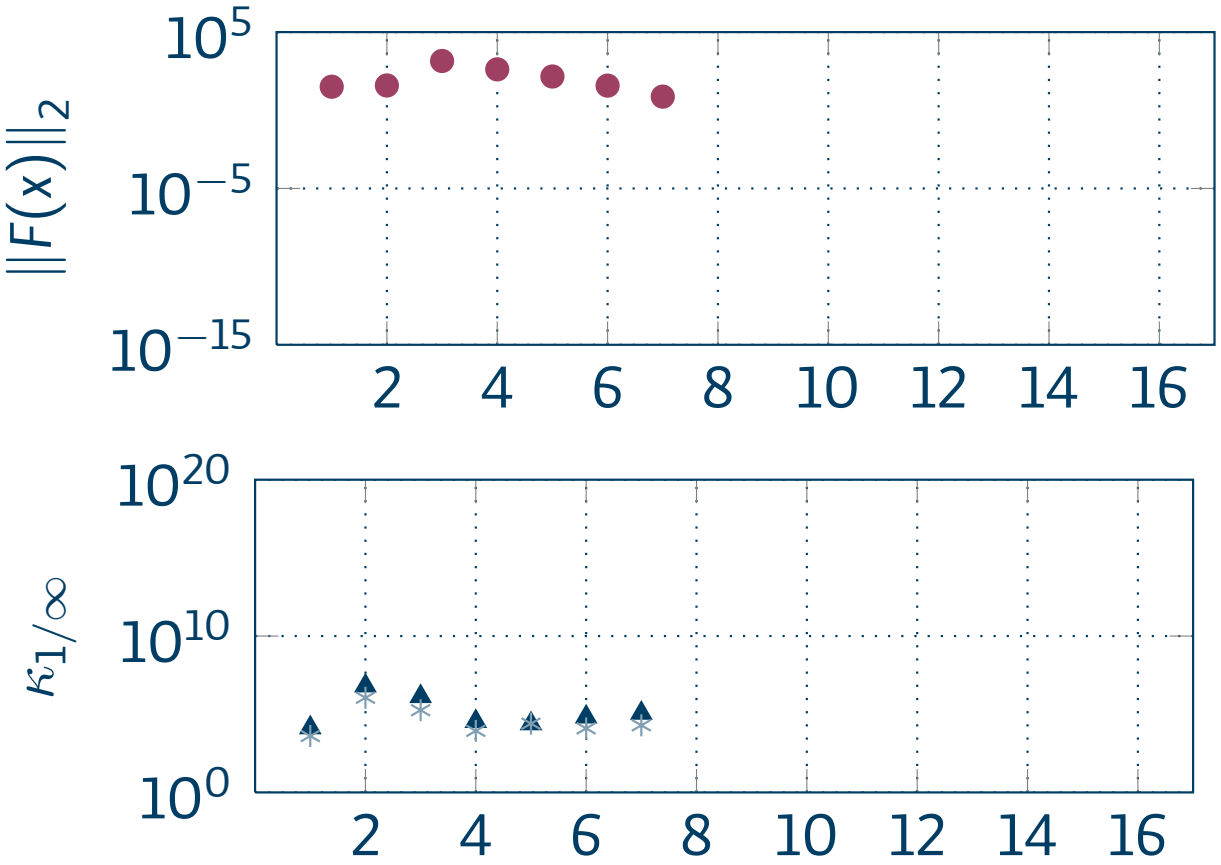

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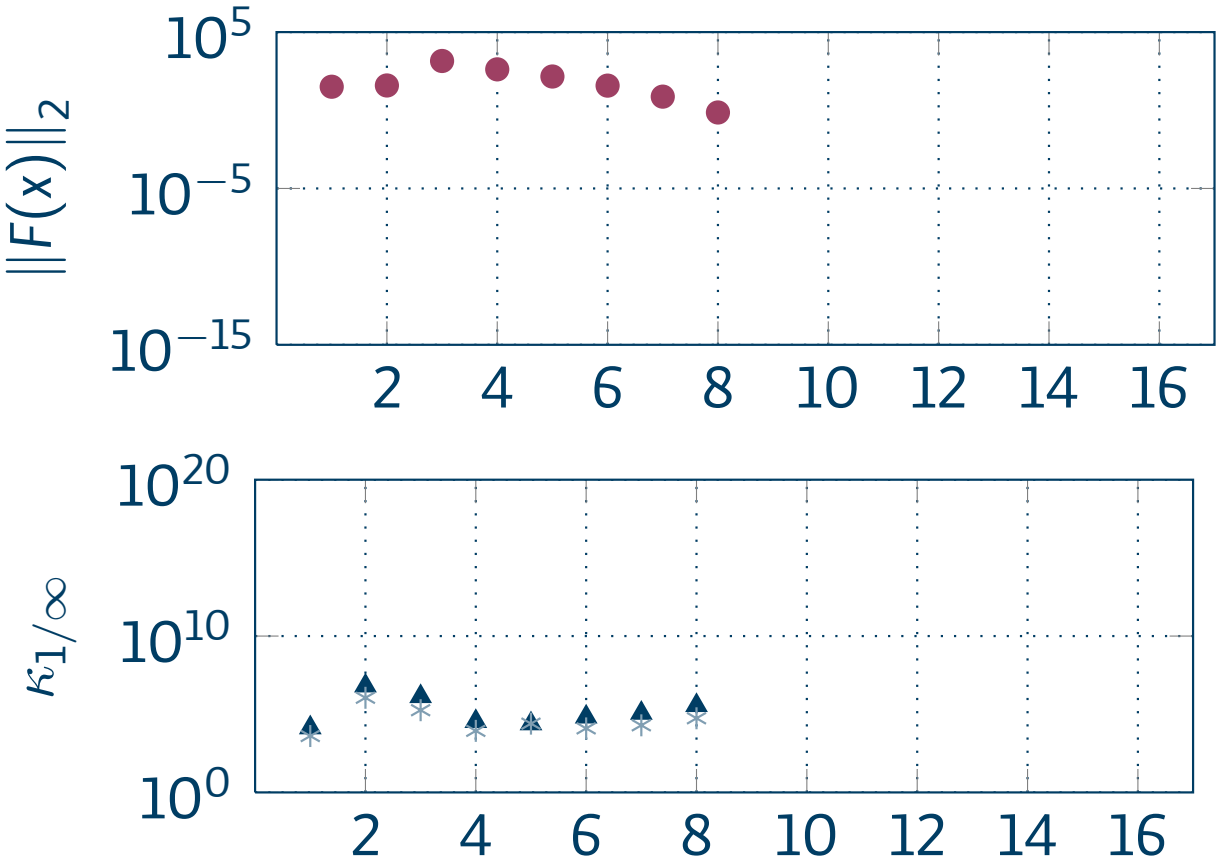

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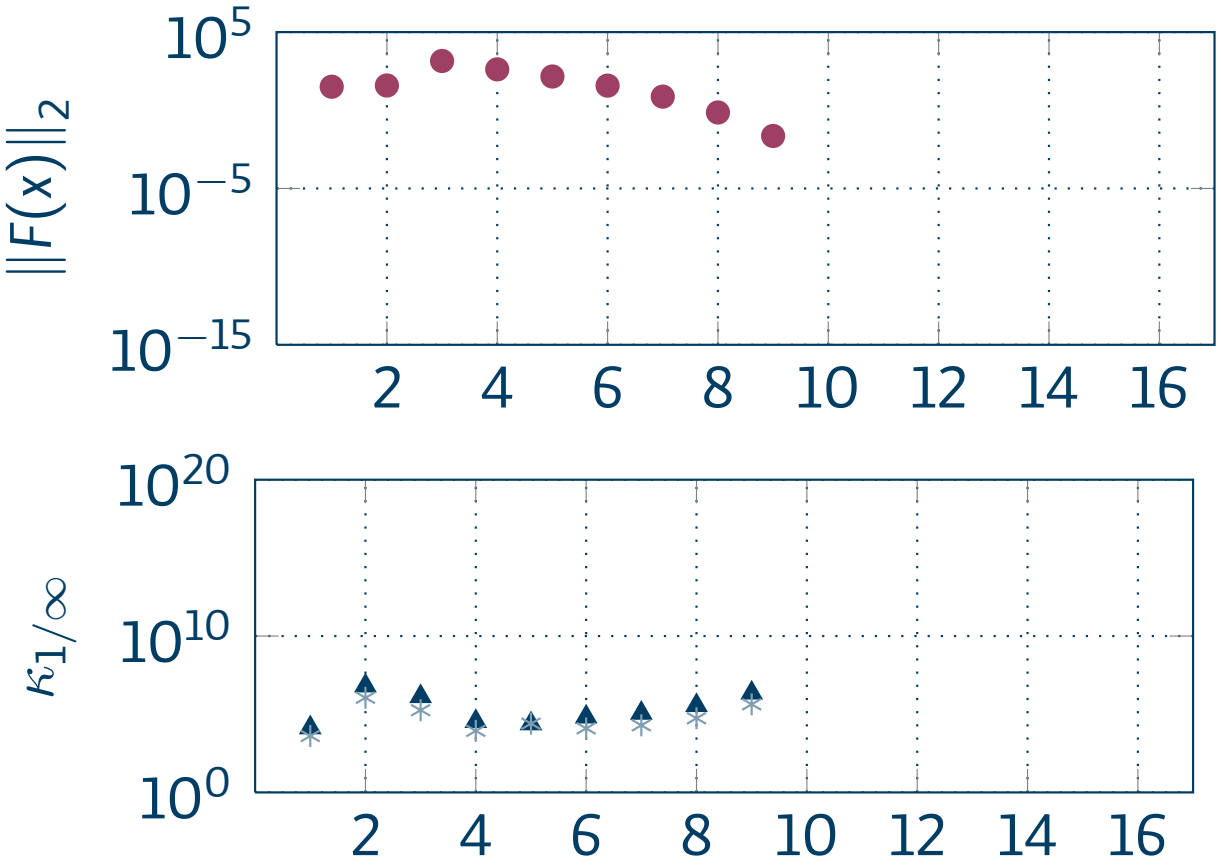

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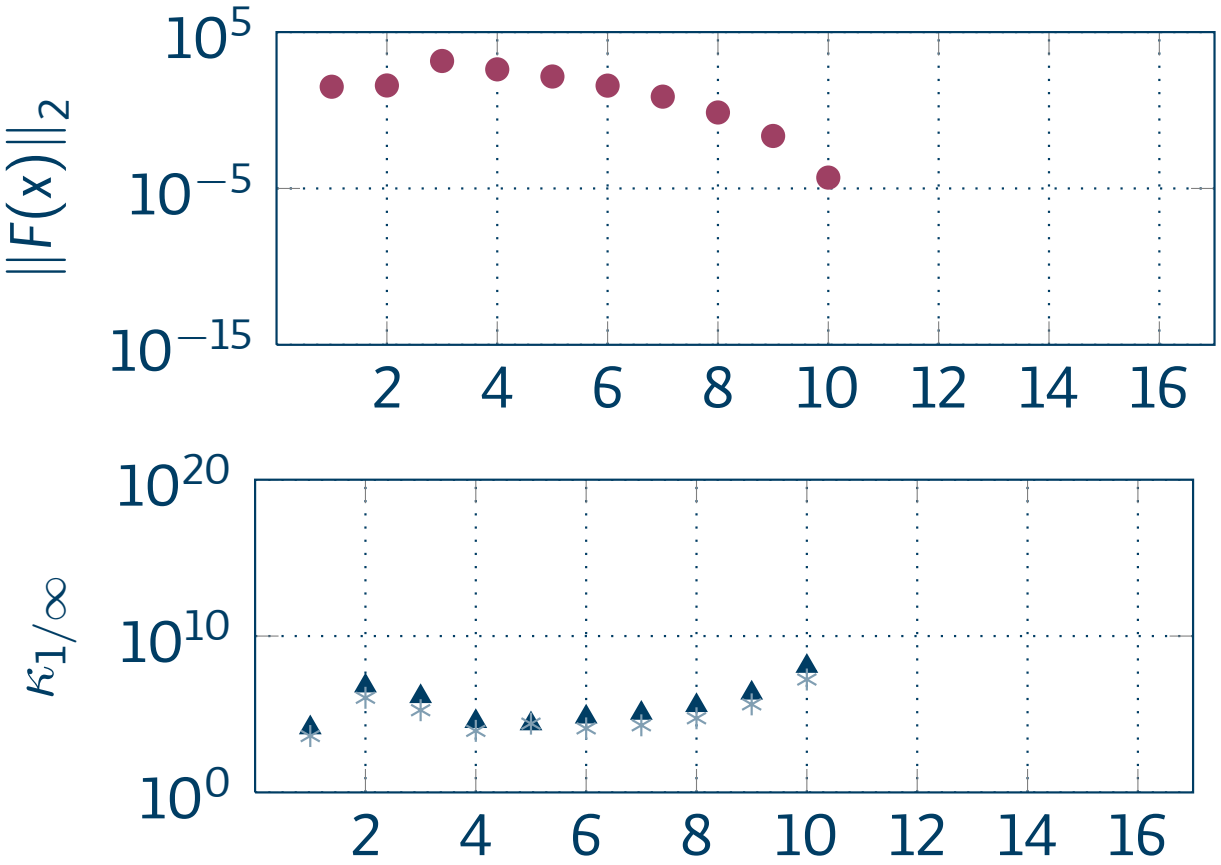

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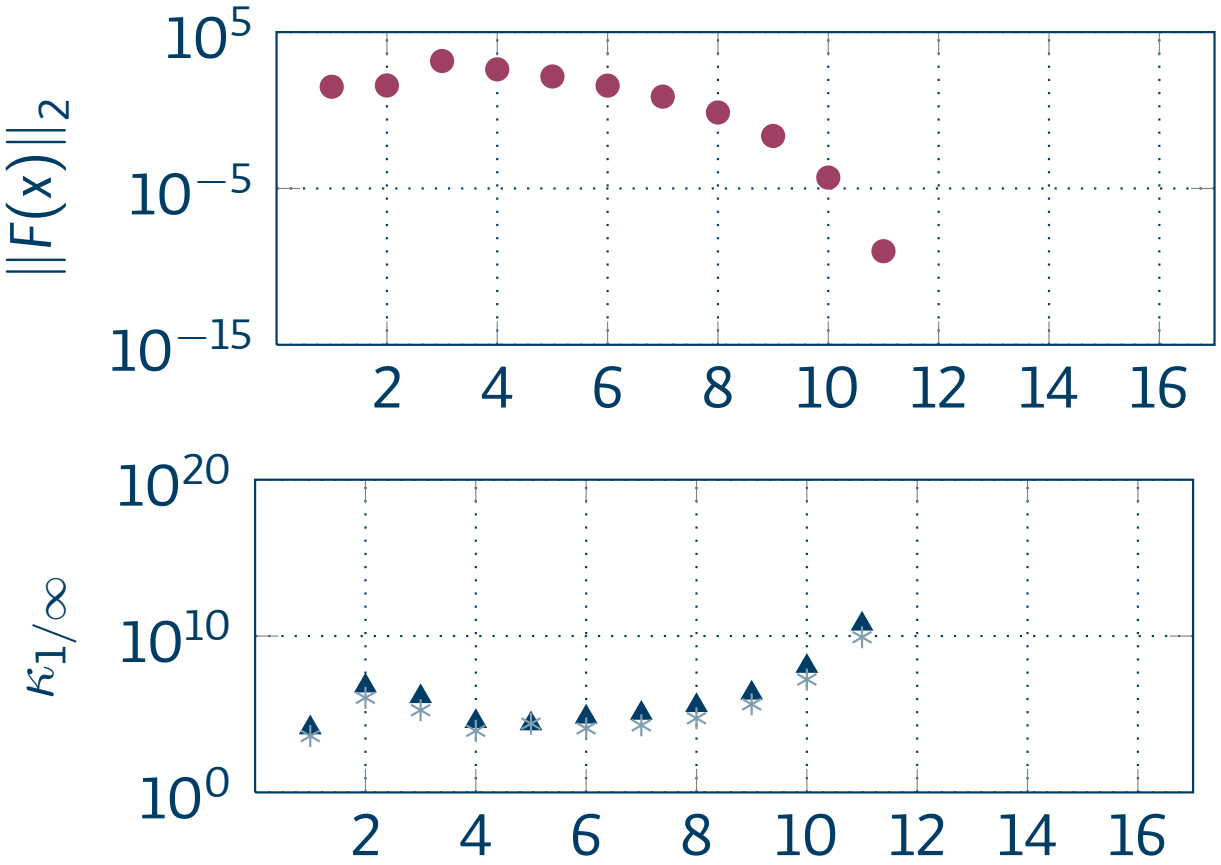

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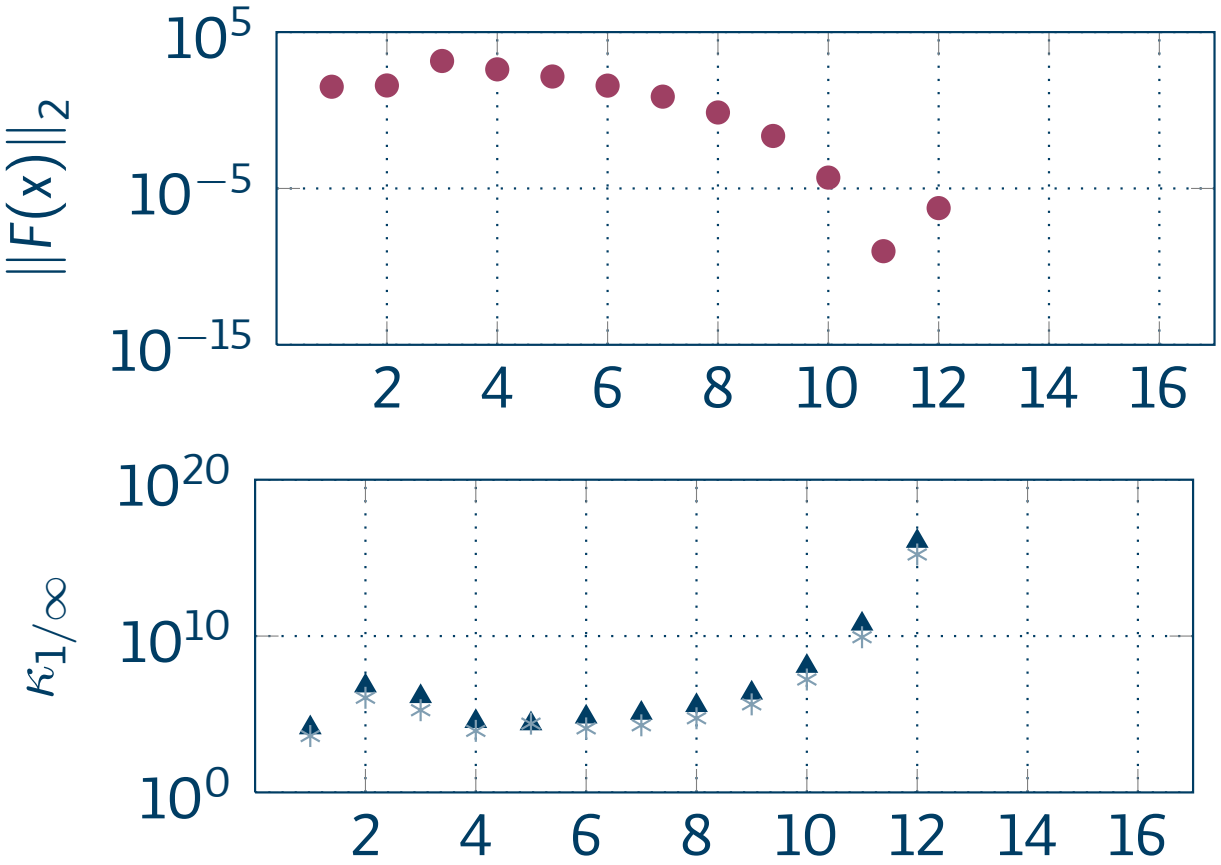

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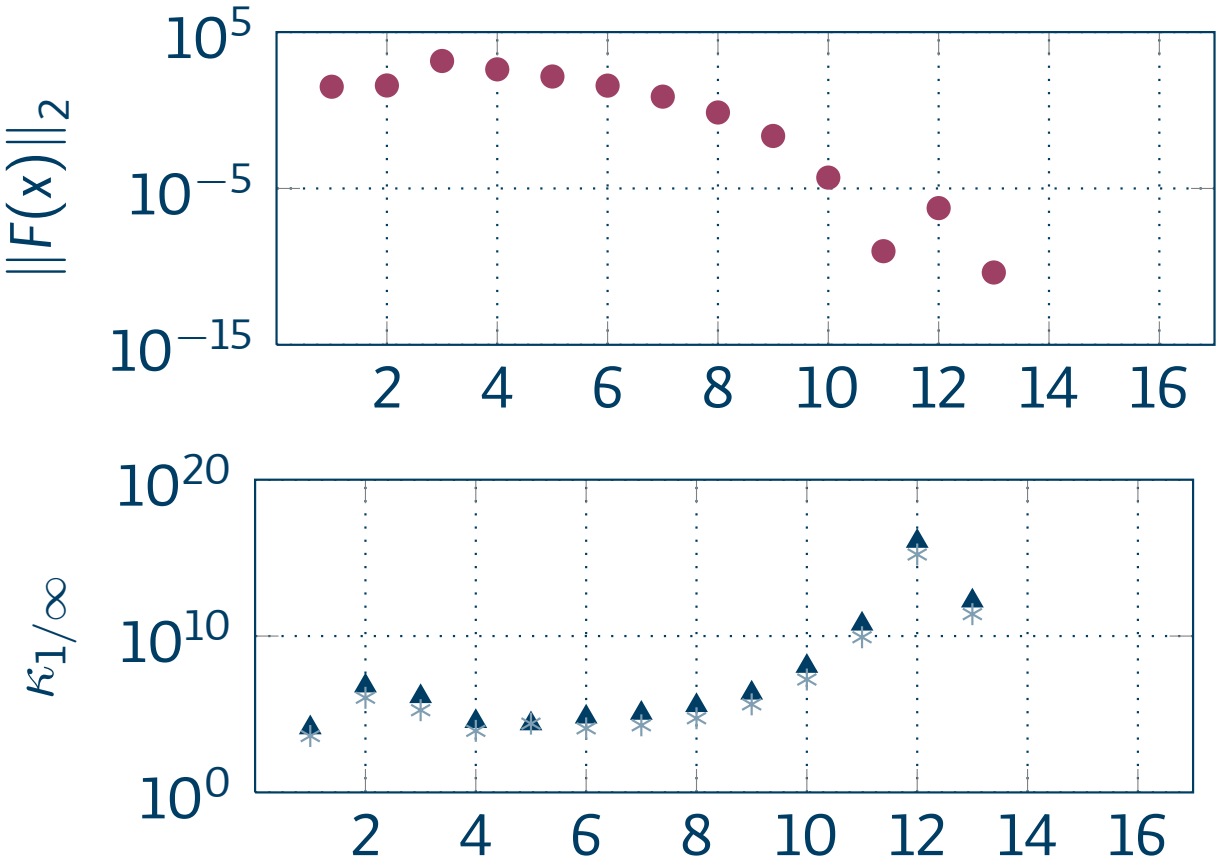

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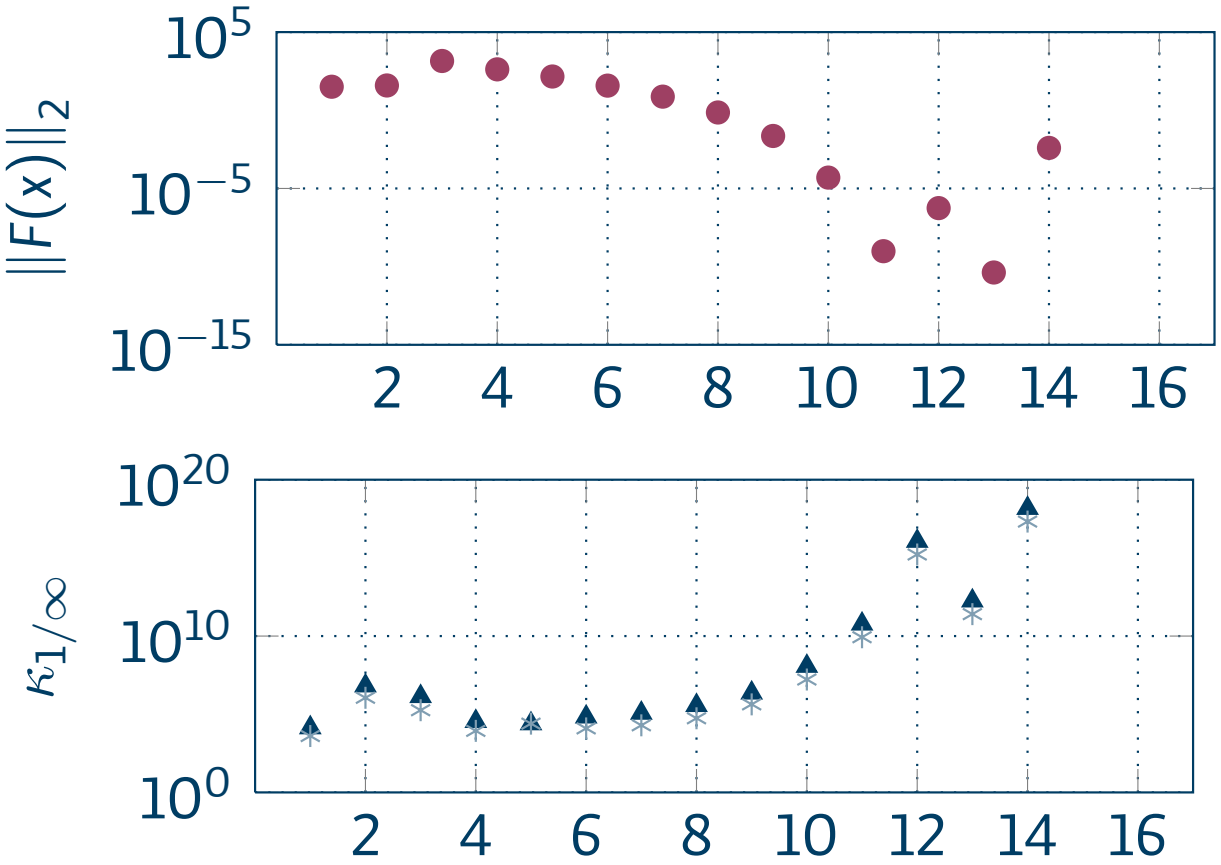

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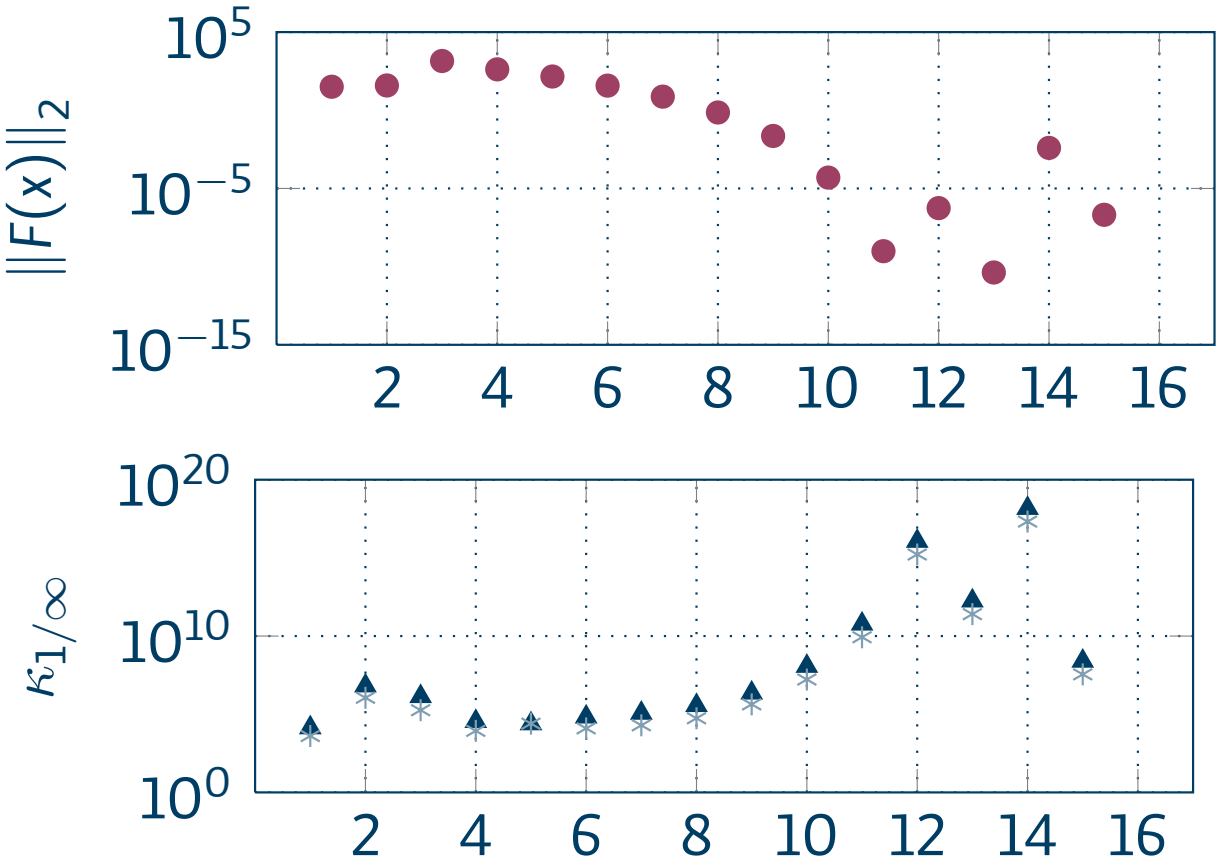

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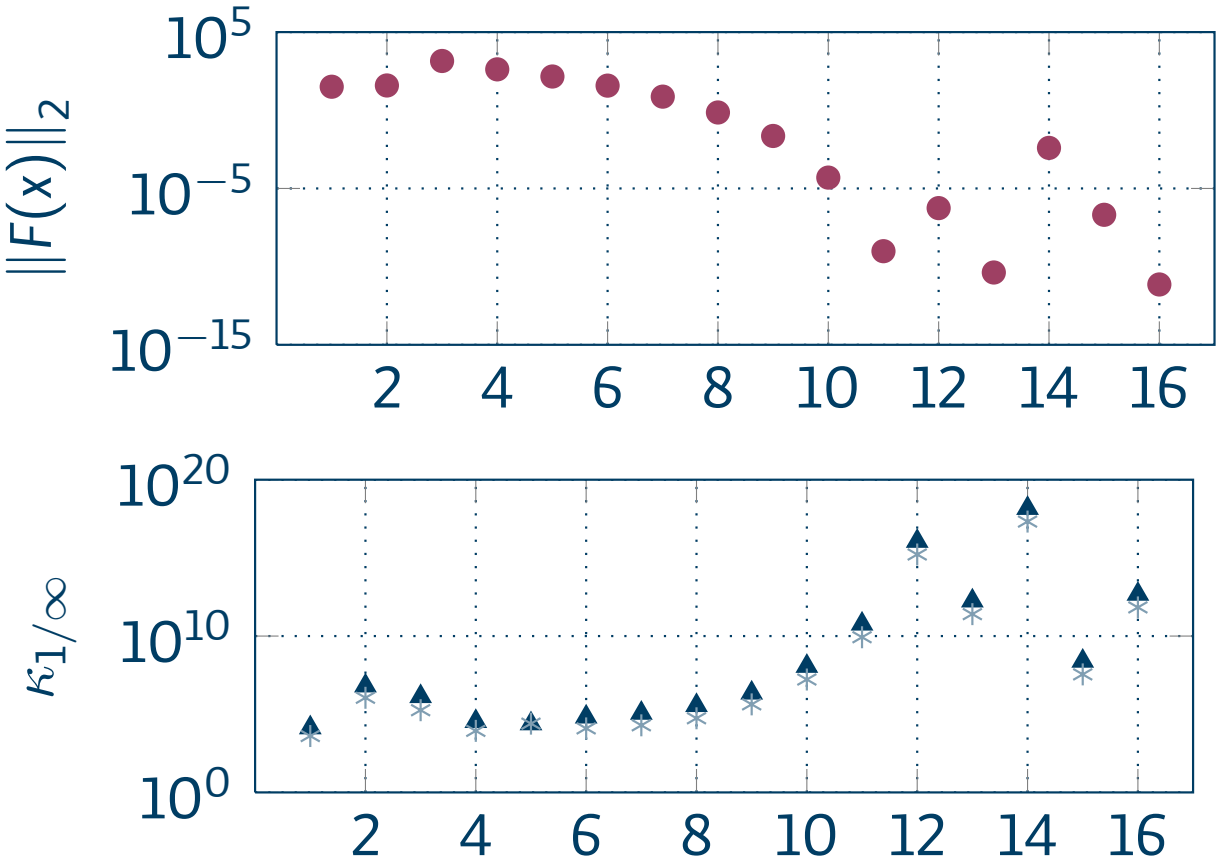

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General approach: phase conditions

Alan R. Champneys, Björn Sandstede
Numerical computation of coherent structures, 2007.

- $F(x)$ equivariant under the action of a finite-dimensional **Lie-group** G on $\mathcal{X}$ so that

$$gF(u) = F(gu) \quad \forall g \in G, u \in \mathcal{X}.$$

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- $F(x)$ equivariant under the action of a finite-dimensional **Lie-group** G on $\mathcal{X}$ so that

$$gF(u) = F(gu) \quad \forall g \in G, u \in \mathcal{X}.$$

- If F'_{u^*} has eigenvalue 0 with algebraic and geometric multiplicity m, choose **phase condition** of the form

$$\Phi : \mathcal{X} \to \mathbb{R}^m$$

where

$$\operatorname{alg} G \to \mathbb{R}^m, \quad \xi \mapsto \Phi \xi u^*$$

is invertible.

Pinning down χ

For $(\psi, \mathbf{A})_{k+1}$, one could for example demand that

$$\chi = \underset{\chi}{\operatorname{argmin}} \left\| \psi_{n+1} - \psi_n \right\|_2^2 .$$

Necessary condition:

$$\begin{aligned} 0 &= \frac{\mathrm{d}}{\mathrm{d}\chi_n} \left\| \psi_{n+1} - \psi_n \right\|_2^2 \\ &= \dots \\ &= 2\Re \left\{ -\mathrm{i} \left\langle \psi_{n+1}, \psi_n \right\rangle \right\} , \end{aligned}$$

Bordering: Algebraic framework

Theorem (Keller)

Let $A \in \mathbb{K}^{n\times n}$ *with* $\dim \mathcal{N}(A) = 1$. *Then* $\widetilde{A} = \begin{pmatrix} A & c \\ b^T & d \end{pmatrix}$ *is nonsingular if*

- $c \notin \mathcal{R}(A) = \mathcal{N}(A^T)^\perp$, *and*
- $b \notin \mathcal{R}(A^T) = \mathcal{N}(A)^\perp$.

...extension (S., Vanroose)

Let $L : X \to Y$ linear with $\dim \mathcal{N}(L) = k$. Then $\widetilde{L}\widetilde{x} := \begin{pmatrix} Lx + b\xi \\ f(x) + d\xi \end{pmatrix}$ has $\dim \mathcal{N}(\widetilde{L}) < \dim \mathcal{N}(L)$ iff

- $b \notin \mathcal{R}(L)$, and
- $\exists v \in \ker L$ with $f(v) \neq 0$.

Newton with bordered Jacobian

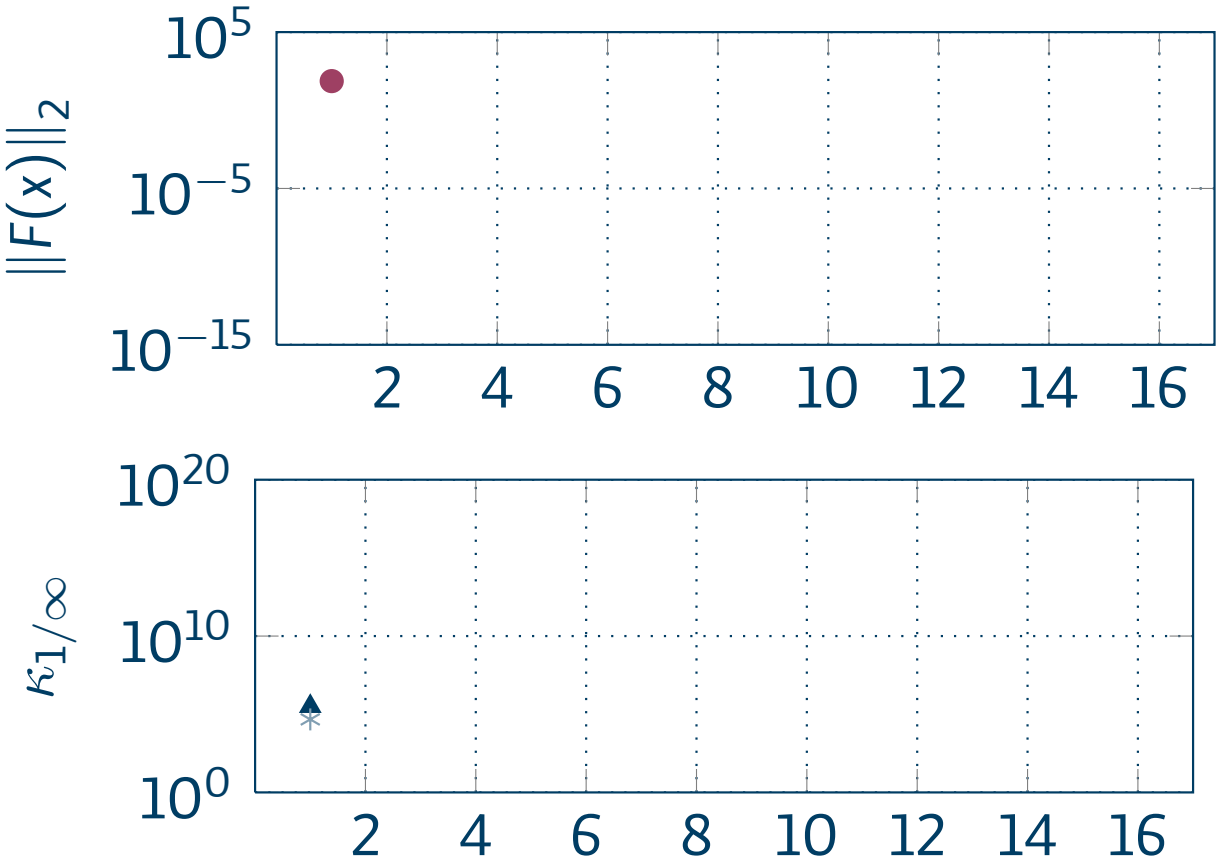
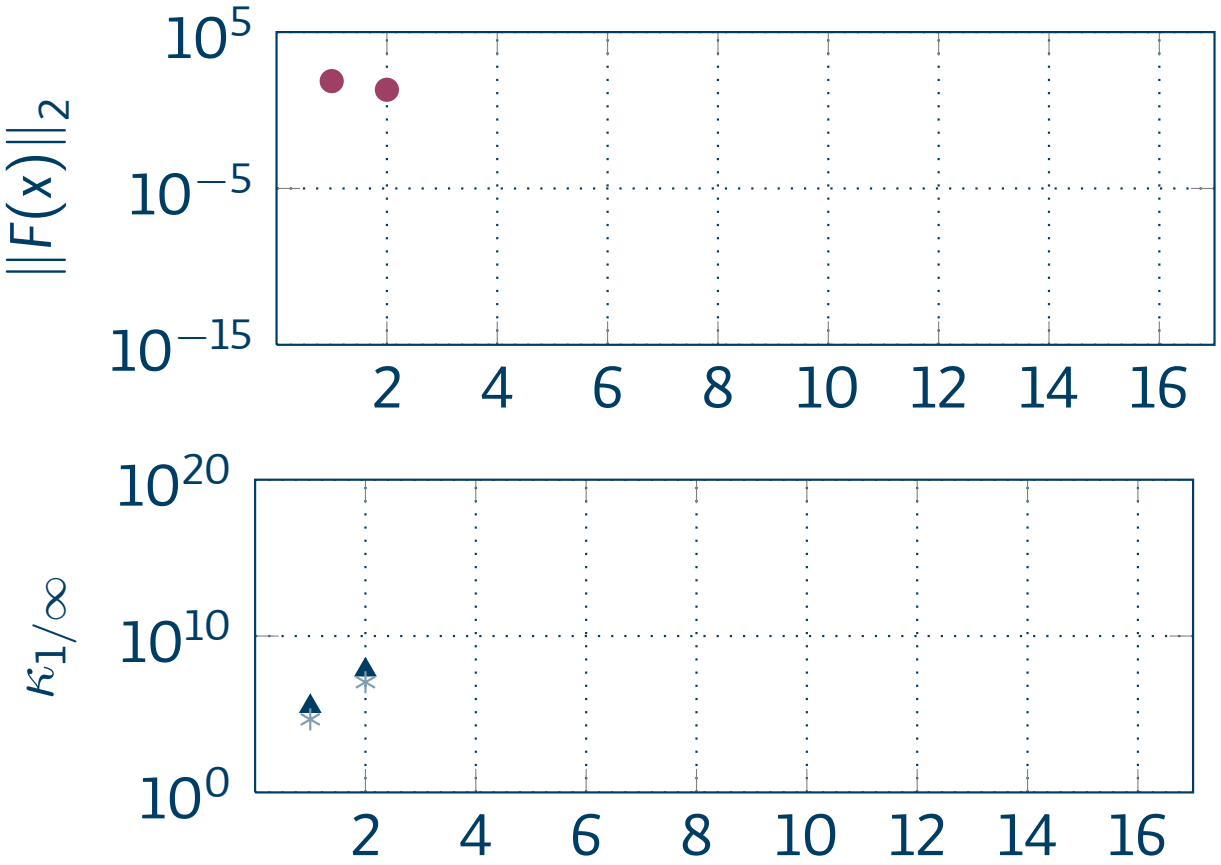


Figure: Newton iteration history, with bordering (here: with *LU* solves for the linear equation system).

Newton with bordered Jacobian



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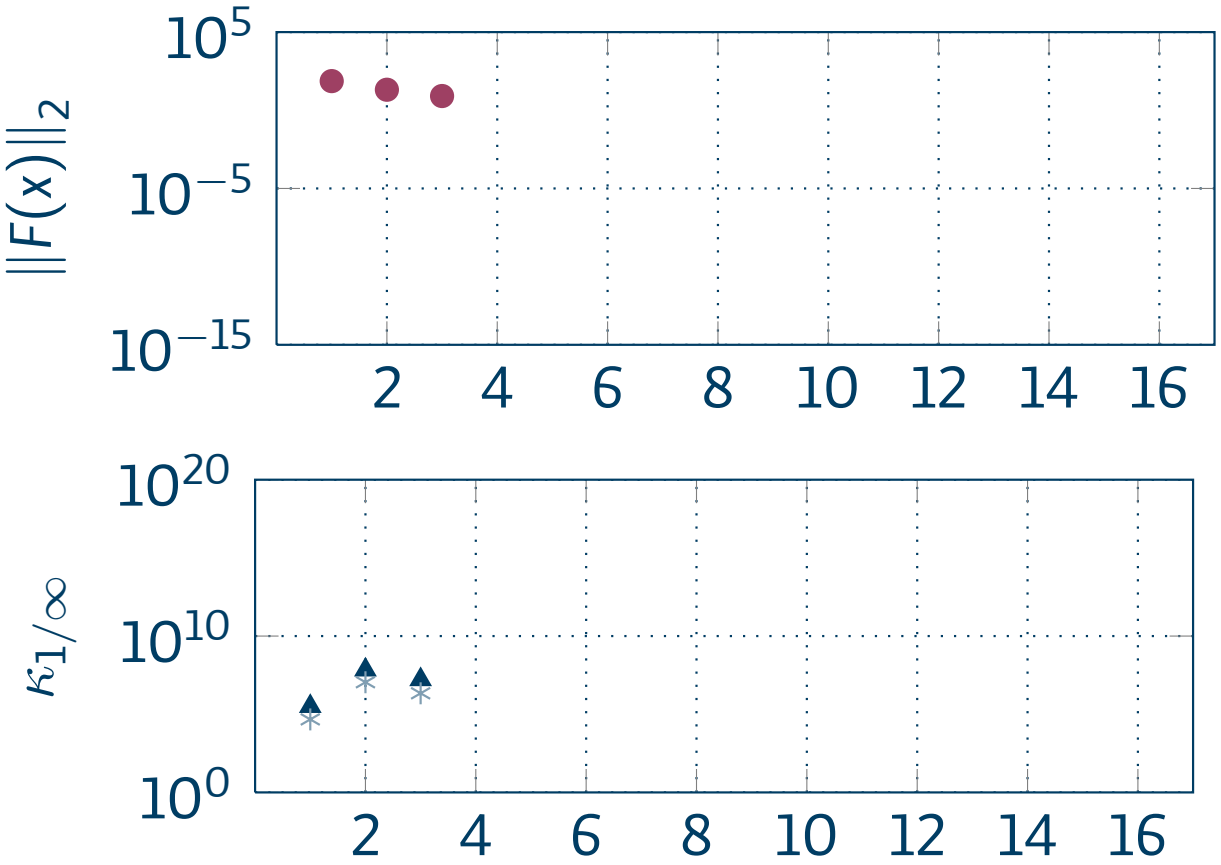

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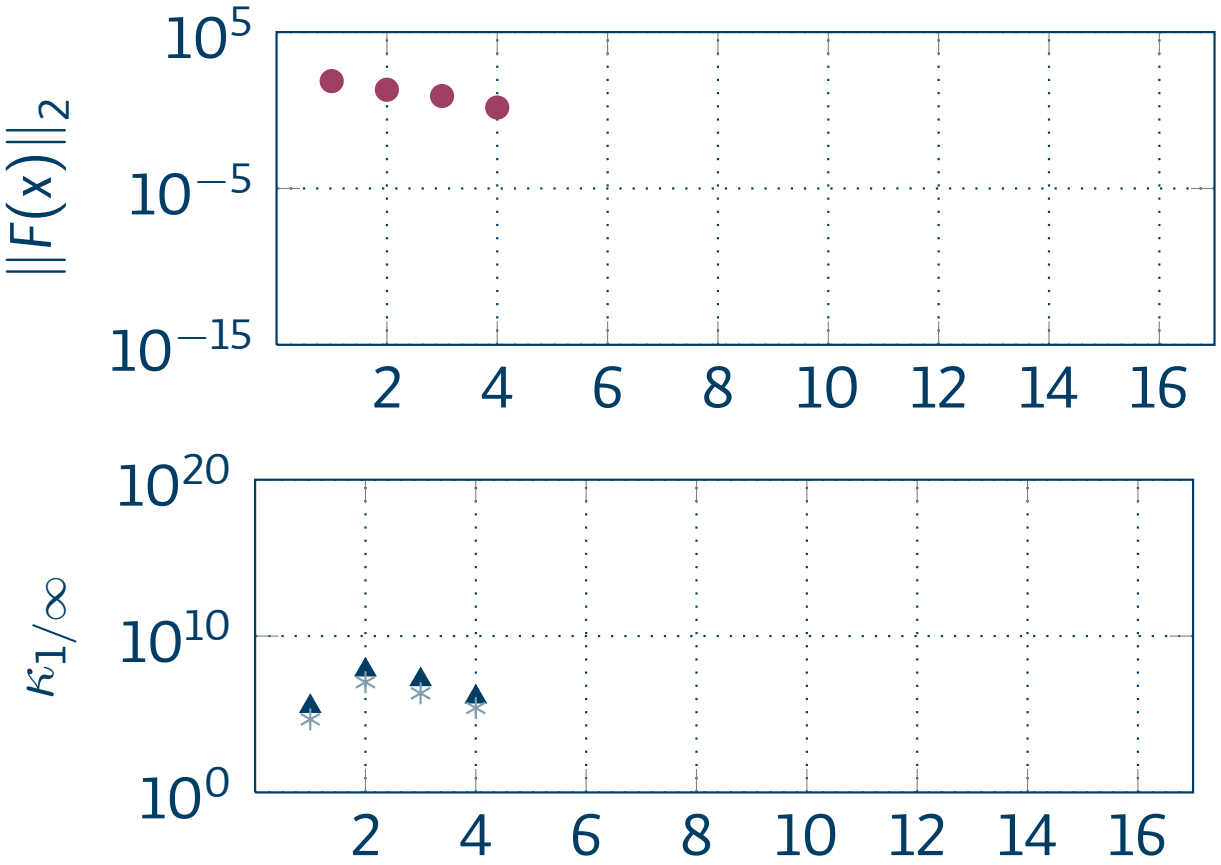
Newton with bordered Jacobian



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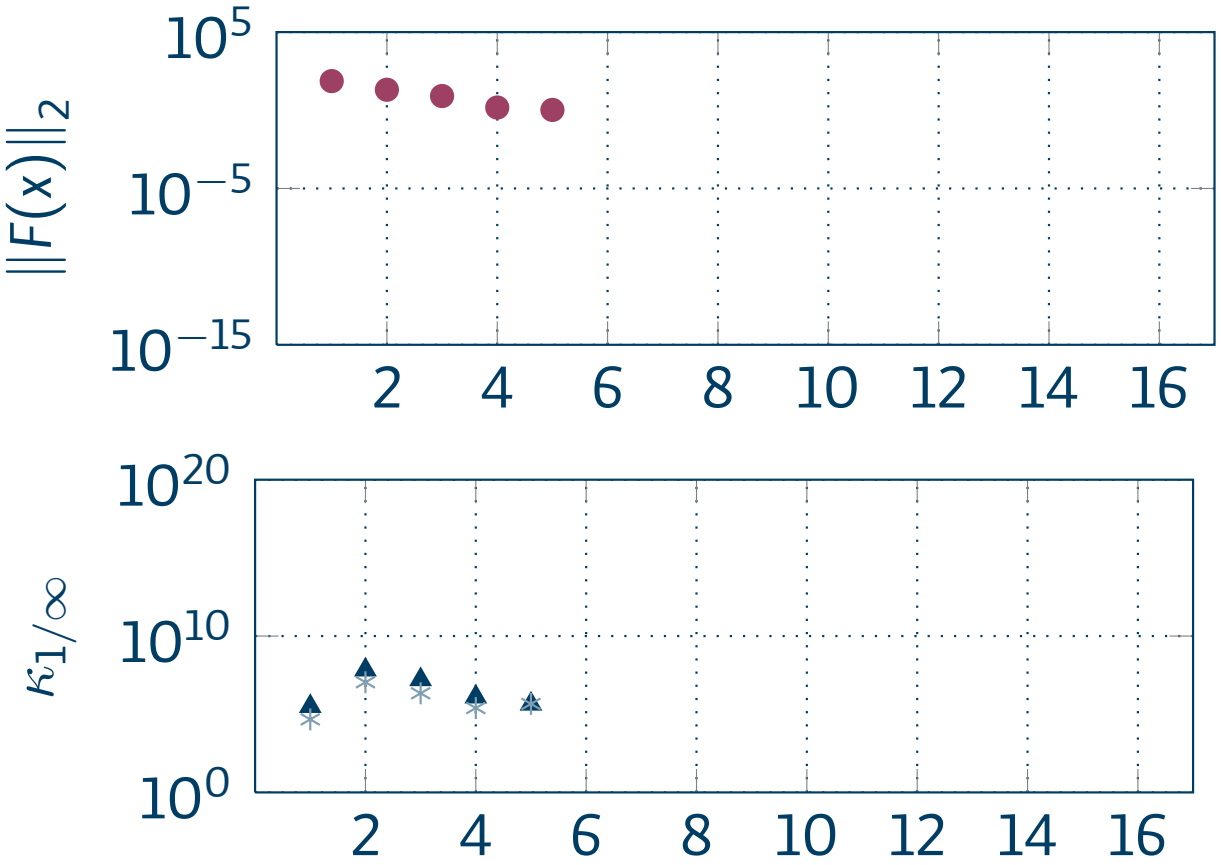

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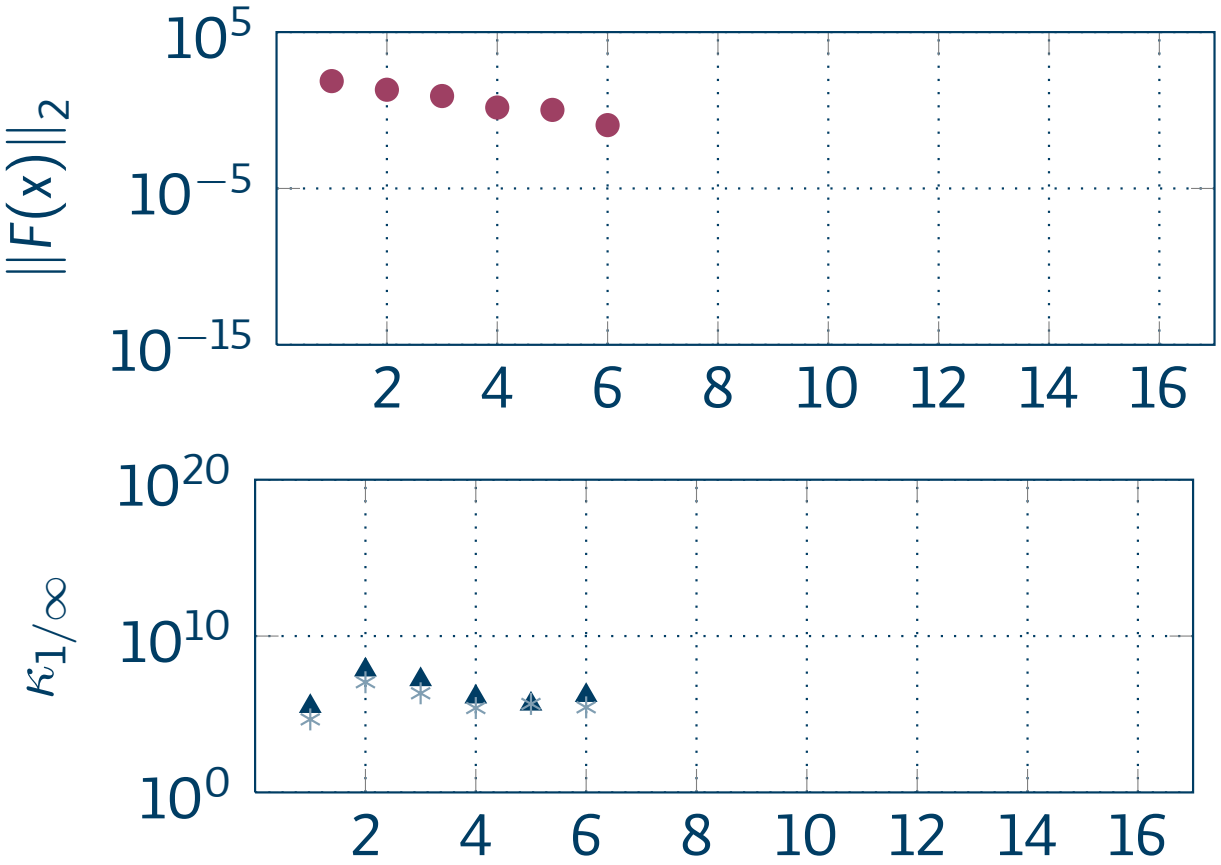
Newton with bordered Jacobian



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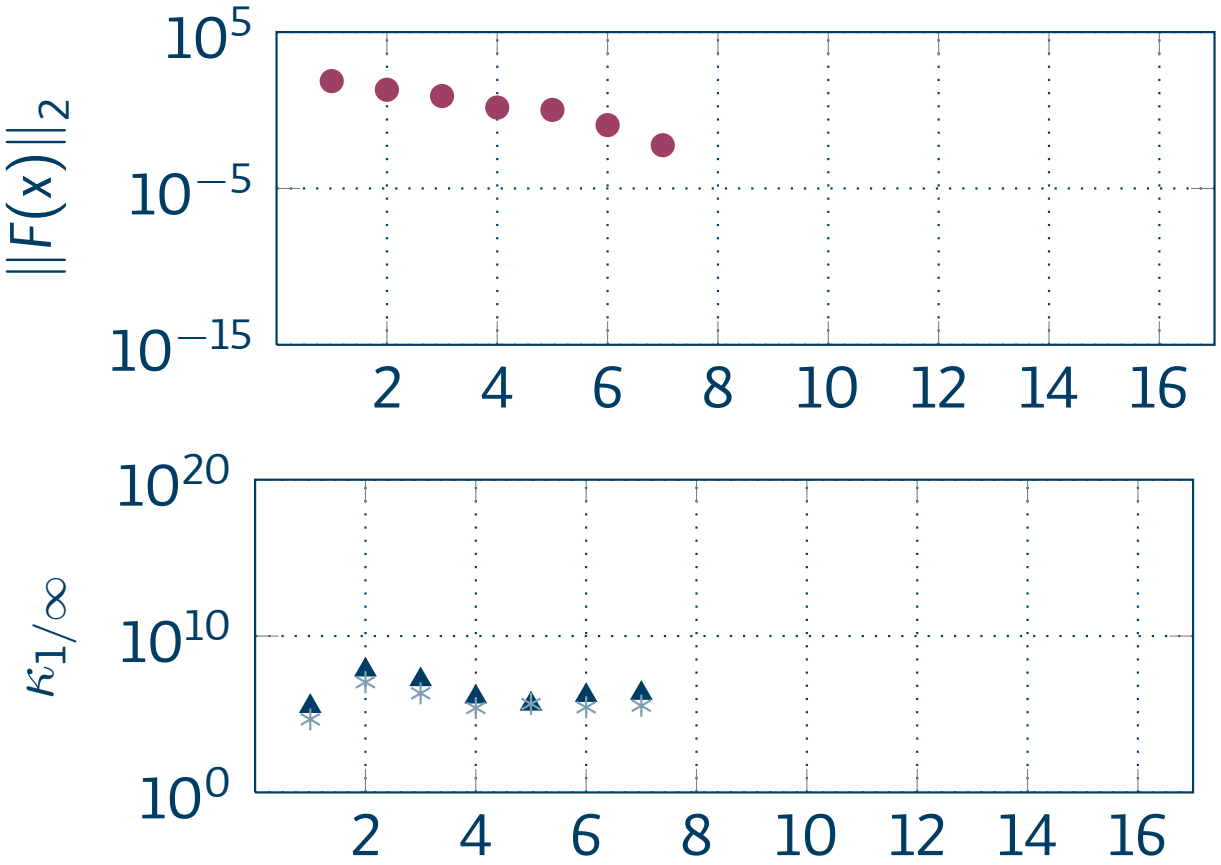
Newton with bordered Jacobian



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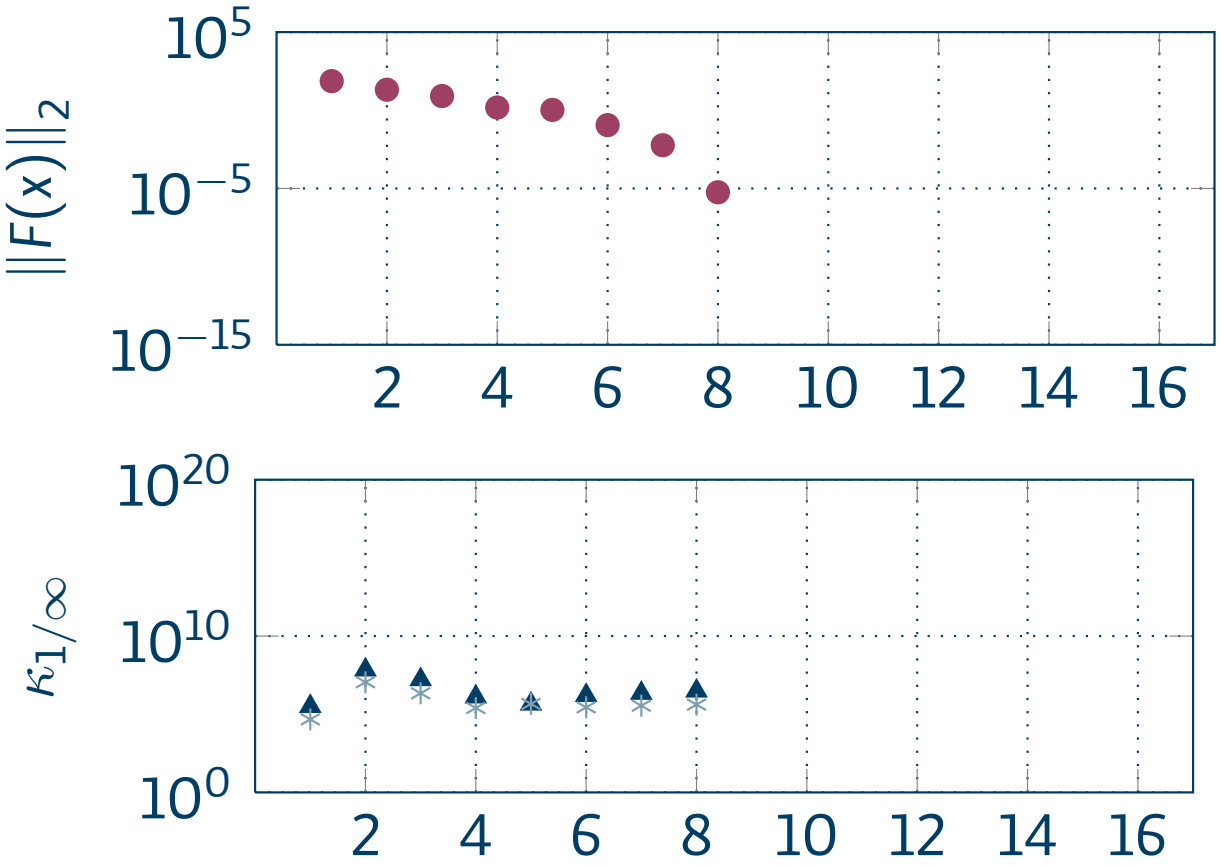
Newton with bordered Jacobian



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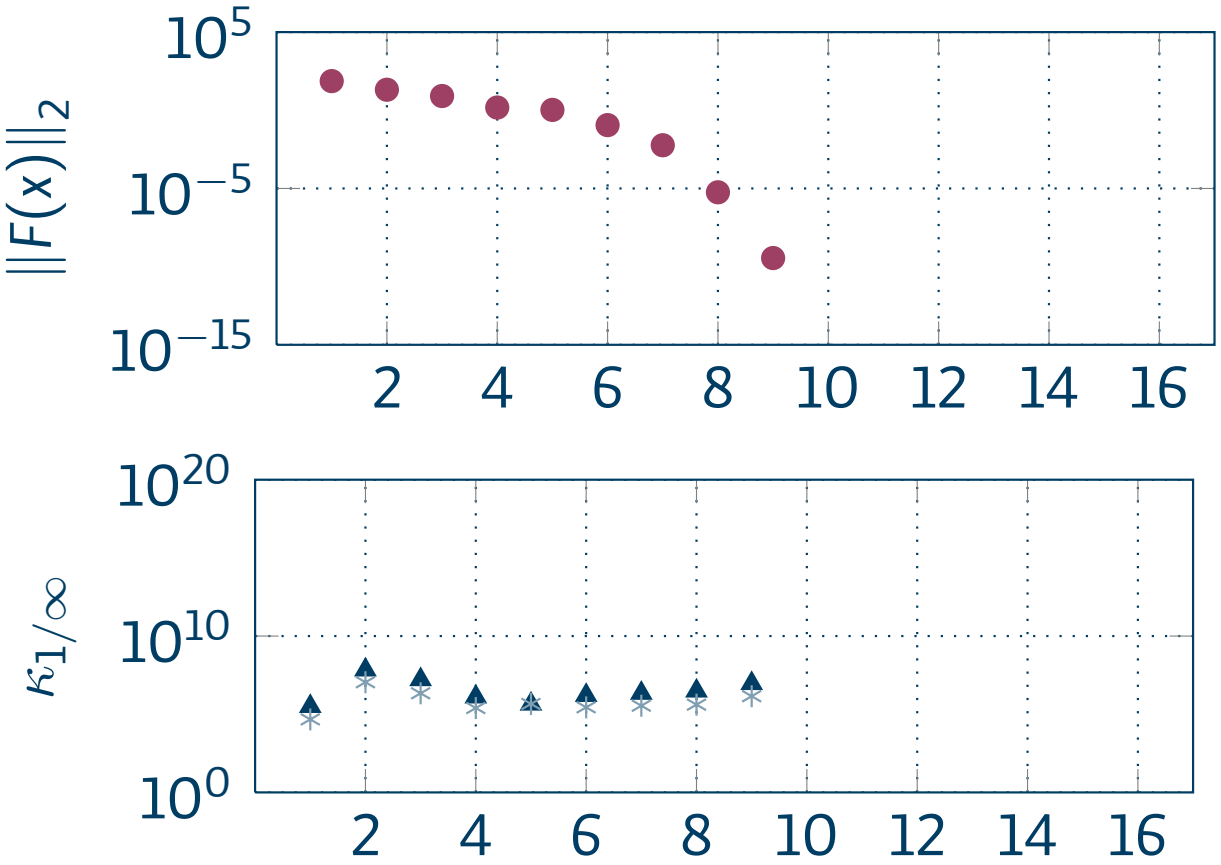
Newton with bordered Jacobian



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Newton with bordered Jacobian

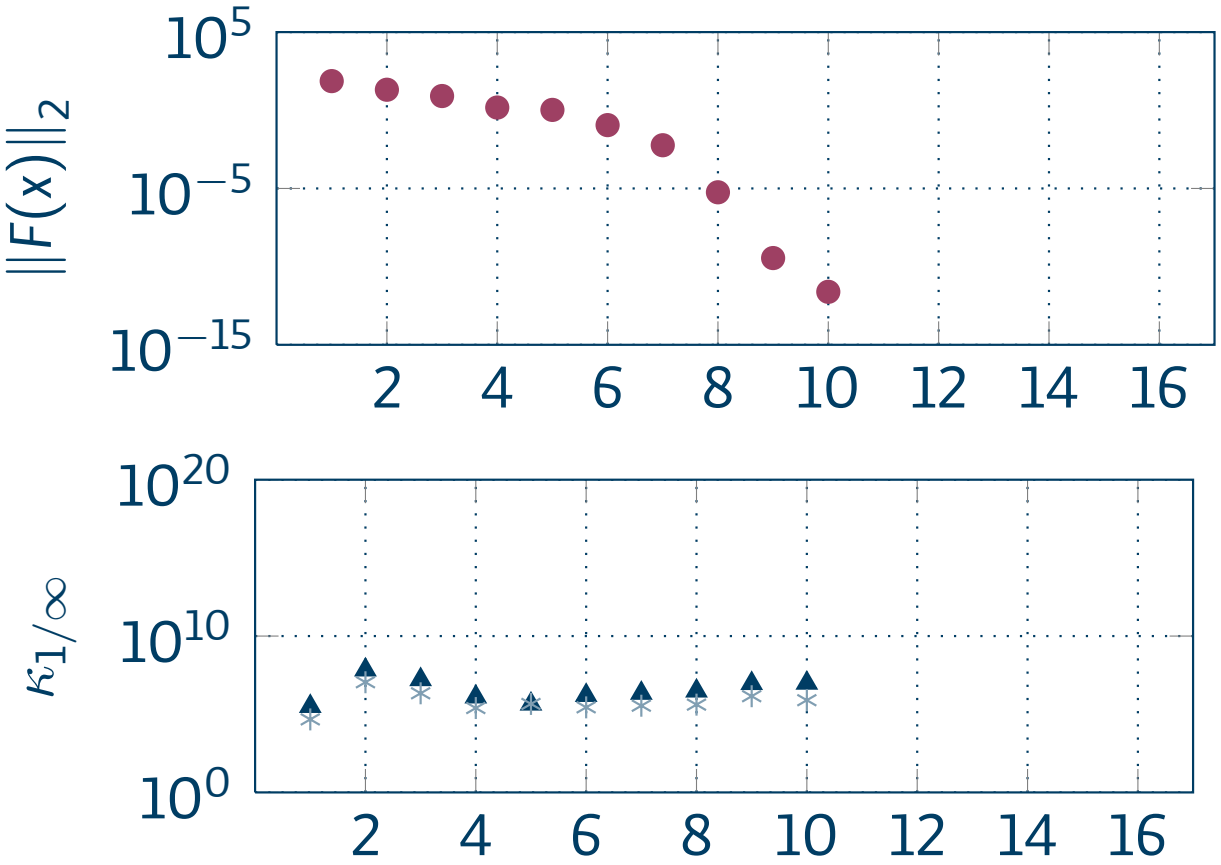


Figure: Newton iteration history, with bordering (here: with *LU* solves for the linear equation system).

How to solve bordered systems?

$$\begin{bmatrix} J & A \\ B^T & C \end{bmatrix} \begin{bmatrix} X \\ Y \end{bmatrix} = \begin{bmatrix} F \\ G \end{bmatrix}$$

- Rearrange:

$$\begin{bmatrix} C & B^T \\ A & J \end{bmatrix} \begin{bmatrix} Y \\ X \end{bmatrix} = \begin{bmatrix} G \\ F \end{bmatrix}.$$

- QR of the first block row $[C, B^T] = [R^T, 0]Q^T$ yields

$$\begin{bmatrix} R^T & 0 \\ [A & J]Q \end{bmatrix} \begin{bmatrix} Z_Y \\ Z_X \end{bmatrix} = \begin{bmatrix} G \\ F \end{bmatrix}.$$

How to solve bordered systems? (cont.)

- $$\begin{bmatrix} R^T & 0 \\ [A & J]Q \end{bmatrix} \begin{bmatrix} Z_Y \\ Z_X \end{bmatrix} = \begin{bmatrix} G \\ F \end{bmatrix}.$$

- $$Z_Y = R^{-T}G,$$
$$[A \;\; J]Q \begin{bmatrix} 0 \\ Z_X \end{bmatrix} = F - [A \;\; J]Q \begin{bmatrix} Z_Y \\ 0 \end{bmatrix} \quad \Leftrightarrow \quad PZ_X = \widetilde{F}$$

  where
$$P = J + UV^T.$$

Newton's method

$x \leftarrow x0$
$res \leftarrow f(x)$
while $\|r\| > \tau$ **do**
  solve system $J_x x_{\text{update}} = -res$
  $x \leftarrow x + x_{\text{update}}$
  $res \leftarrow f(x)$
end

Algorithm 1: Newton's method

The Jacobian

$$J_\psi \varphi = \Big(\underbrace{(-\mathrm{i}\nabla - \mathbf{A})^2}_{K} \underbrace{-1 + 2|\psi|^2}_{D_1} \Big) \varphi + \underbrace{\psi^2}_{D_2} \overline{\varphi}.$$

Properties of the Jacobian operator

The Jacobian

$$J_\psi \varphi = (K + D_1)\,\varphi + D_2 \overline{\varphi}.$$

- J_ψ is **linear** over $H^2(\Omega)$ as $\mathbb{R}$-vector space;
- J_ψ is **self-adjoint** ("symmetric") w.r.t.

$$\langle [\cdot], [\cdot] \rangle = \Re \langle \cdot, \cdot \rangle_{H^2(\Omega)} ;$$

- J_ψ is **not generally definite**.

Iterative solvers for J_ψ

J_ψ self-adjoint? CG/MINRES!

$r_0 \leftarrow b - Ax_0, p_0 \leftarrow r_0, k \leftarrow 0$
while $\|r_k\| > \tau$ **do**
  $\alpha_k \leftarrow \|r_k\|^2 / \langle p_k, Ap_k \rangle$
  $x_{k+1} \leftarrow x_k + \alpha_k p_k$
  $r_{k+1} \leftarrow r_k - \alpha_k A p_k$
  $\beta_k \leftarrow \|r_{k+1}\|^2 / \|r_k\|^2$
  $p_{k+1} \leftarrow r_{k+1} + \beta_k p_k$
end

Algorithm 2: Conjugate gradients.

Iterative solvers for J_ψ

J_ψ self-adjoint? CG/MINRES!

$r_0 \leftarrow b - Ax_0, p_0 \leftarrow r_0, k \leftarrow 0$
while $\|r_k\| > \tau$ **do**
  $\alpha_k \leftarrow \|r_k\|^2 / \Re\langle p_k, Ap_k\rangle$
  $x_{k+1} \leftarrow x_k + \alpha_k p_k$
  $r_{k+1} \leftarrow r_k - \alpha_k A p_k$
  $\beta_k \leftarrow \|r_{k+1}\|^2 / \|r_k\|^2$
  $p_{k+1} \leftarrow r_{k+1} + \beta_k p_k$
end

Algorithm 3: Conjugate gradients.

Iterative solvers for J_ψ (cont.)

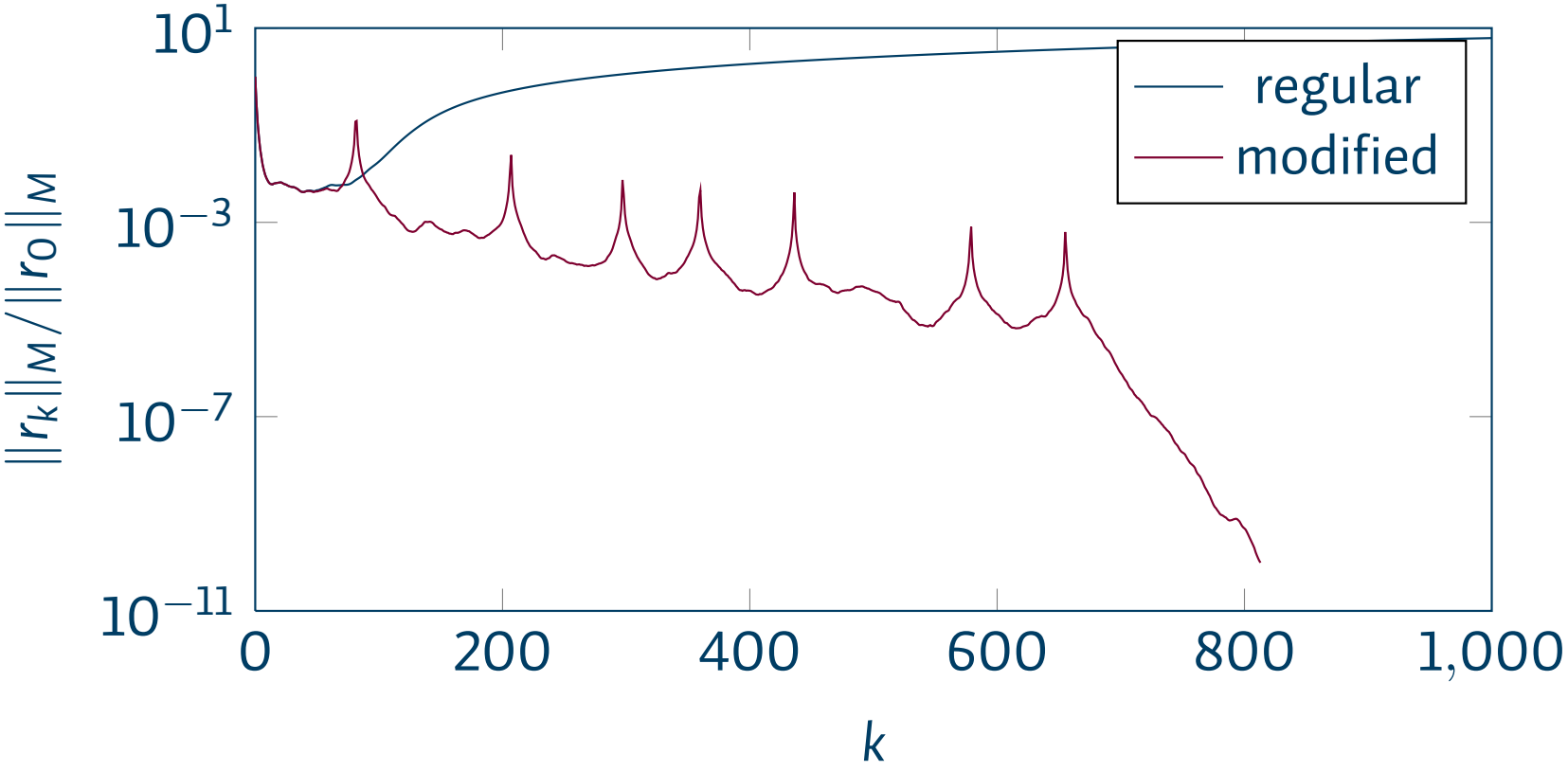


Figure: CG convergence for J.

Preconditioning the Jacobian

The GL Jacobian

$$J_\psi^{(h)}\varphi = \big(K + D_1\big)\varphi + D_2\overline{\varphi}.$$

Possible ideas for preconditioning:

- diagonal

$$P_{\mathrm{d}}\varphi = \big(\,\mathrm{diag}(K) + D_1\big)\varphi + D_2\overline{\varphi}.$$

$$\alpha\varphi_k + \beta\overline{\varphi}_k = \gamma \quad \Rightarrow \quad \varphi_k = (\overline{\alpha}\gamma - \beta\overline{\gamma})/(|\alpha|^2 - |\beta|^2)$$

- kinetic energy operator $K = (-\mathrm{i}\nabla - \mathbf{A})^2$

$$P_{\mathrm{K}}\varphi = K\varphi.$$

Preconditioners compared

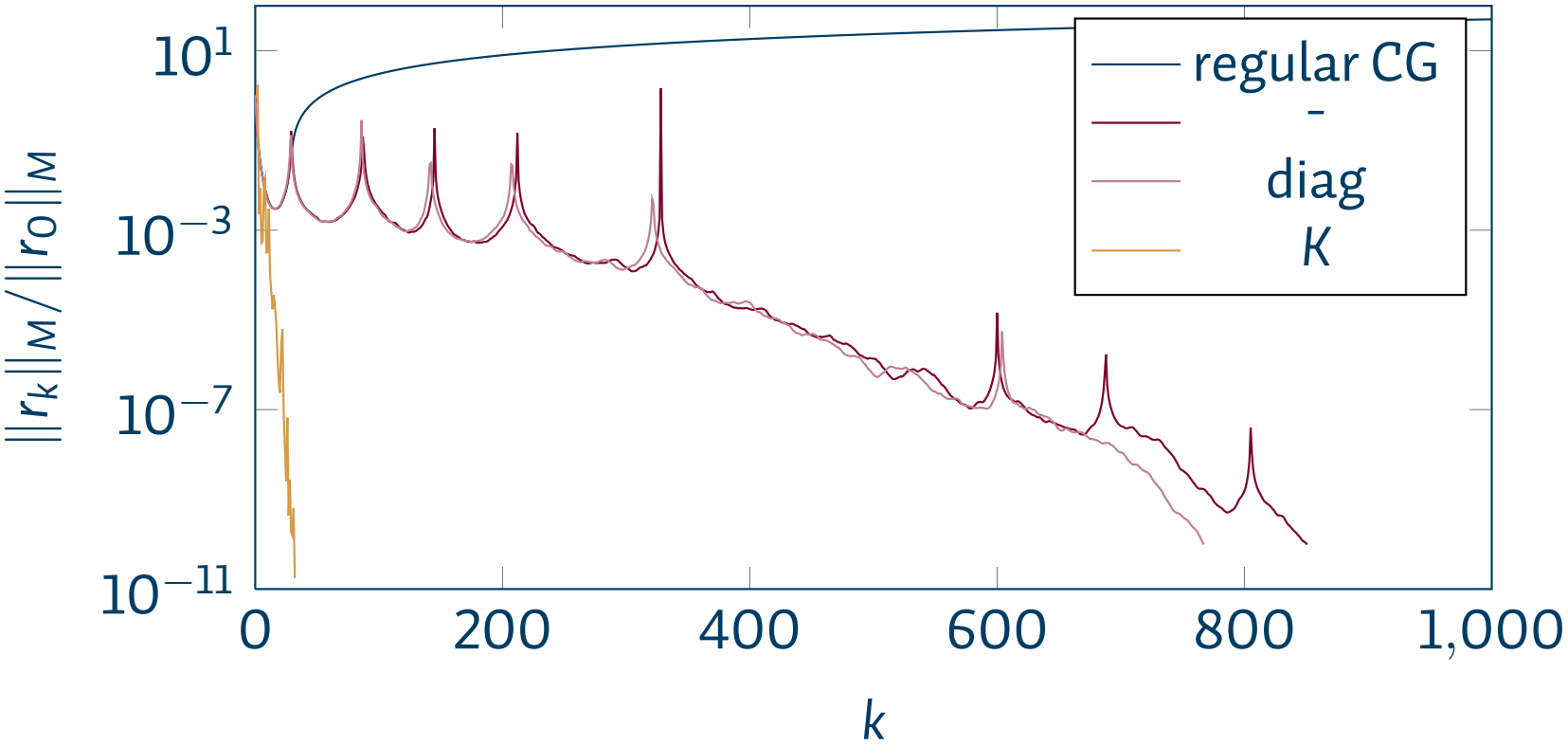


Figure: Convergence of CG. RHS $= 0$, initial guess random, ψ random, $\mu = 0.01$.

K^{-1} generally good?

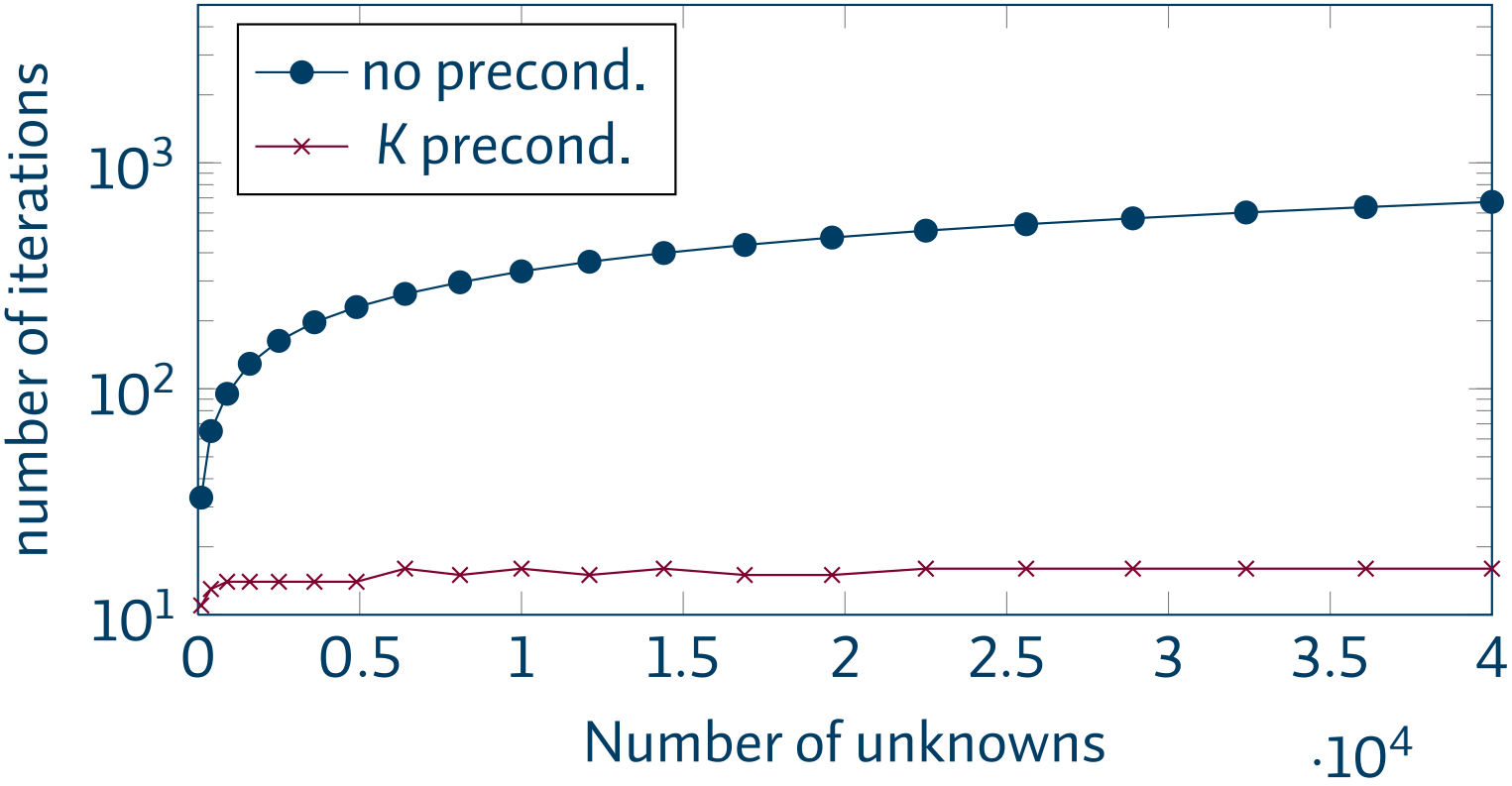
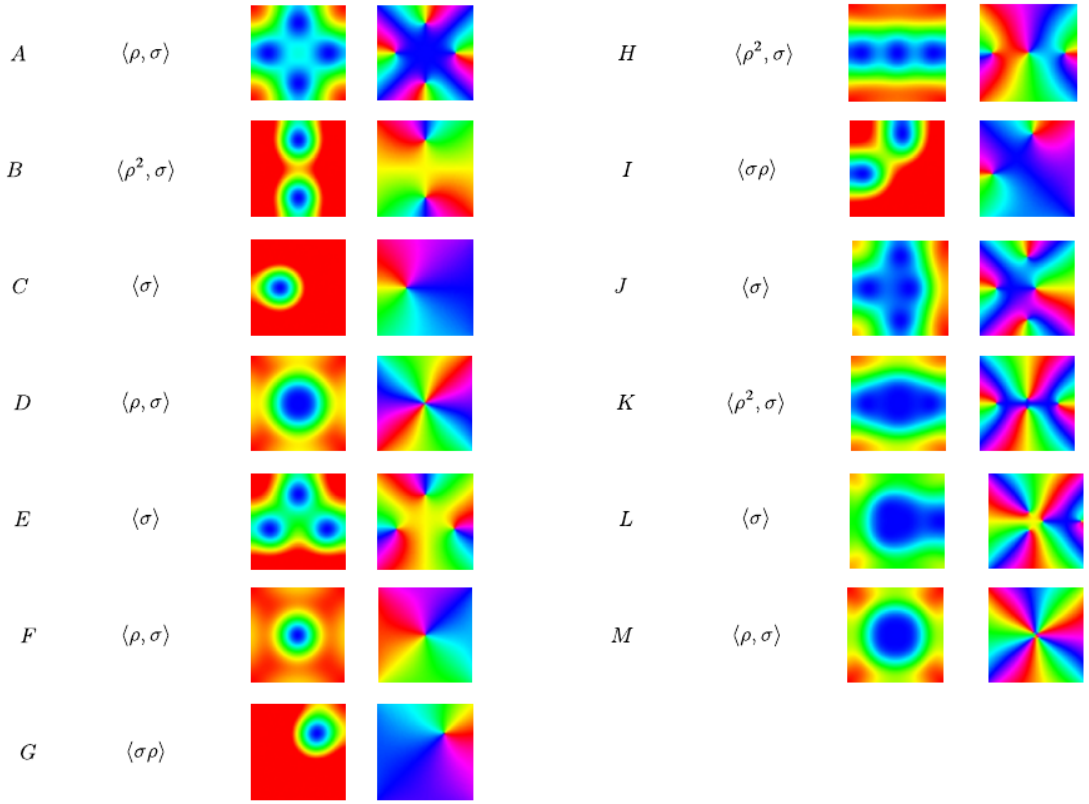


Figure: Performance of the K^{-1}-preconditioner for different **number of unknowns**.

K^{-1} generally good? (cont.)

J_ψ depends on ψ, K does **not**. Problem?



K^{-1} generally good? (cont.)

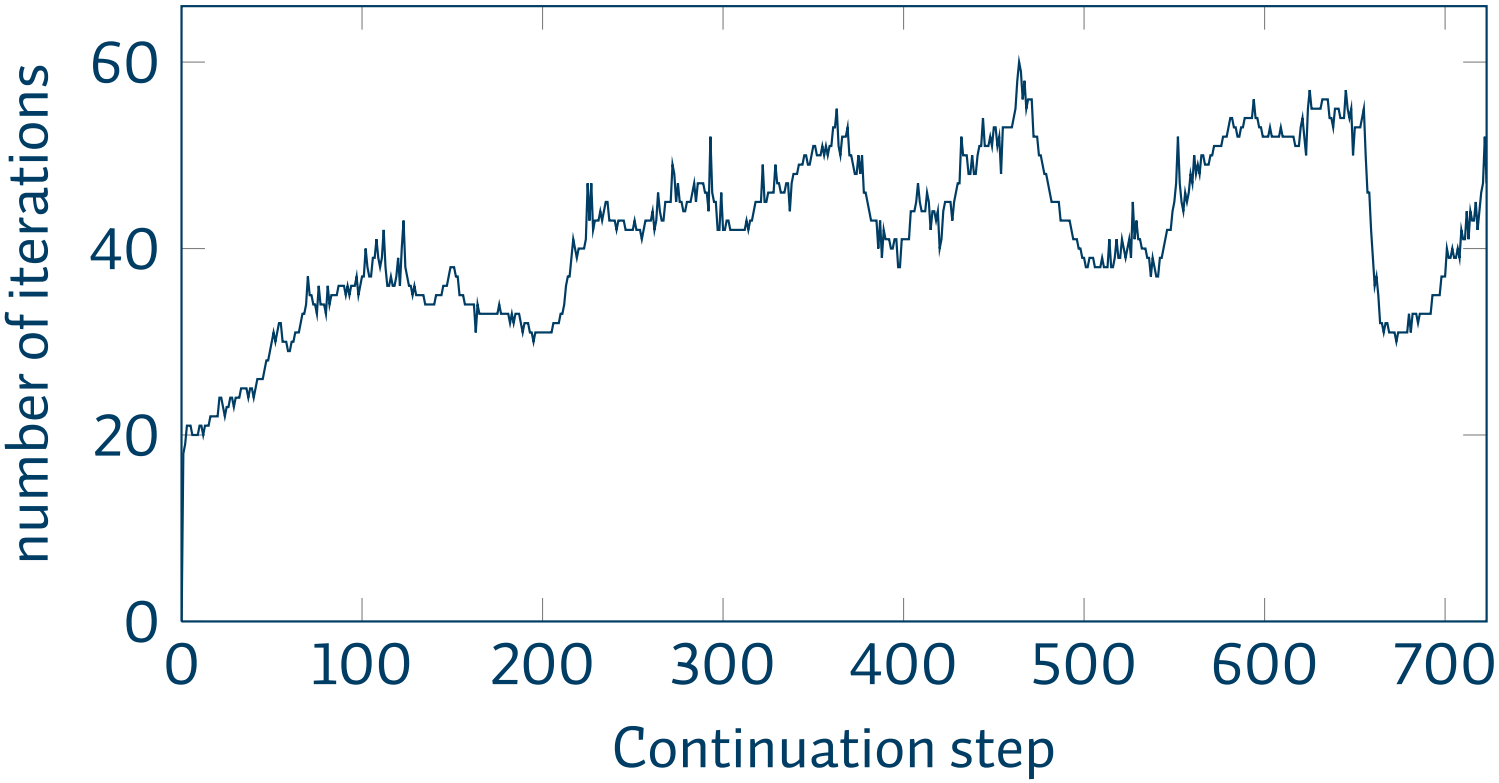


Figure: Number of K^{-1}-preconditioned CG iterations throughout a numerical continuation run in μ (**different states** ψ).

Moving over to solving K

Message

Moved the problem of solving a system with

$$J_\psi \varphi = \left((-\mathrm{i}\nabla - \mathbf{A})^2 - 1 + 2|\psi|^2\right)\varphi + \psi^2\overline{\varphi}$$

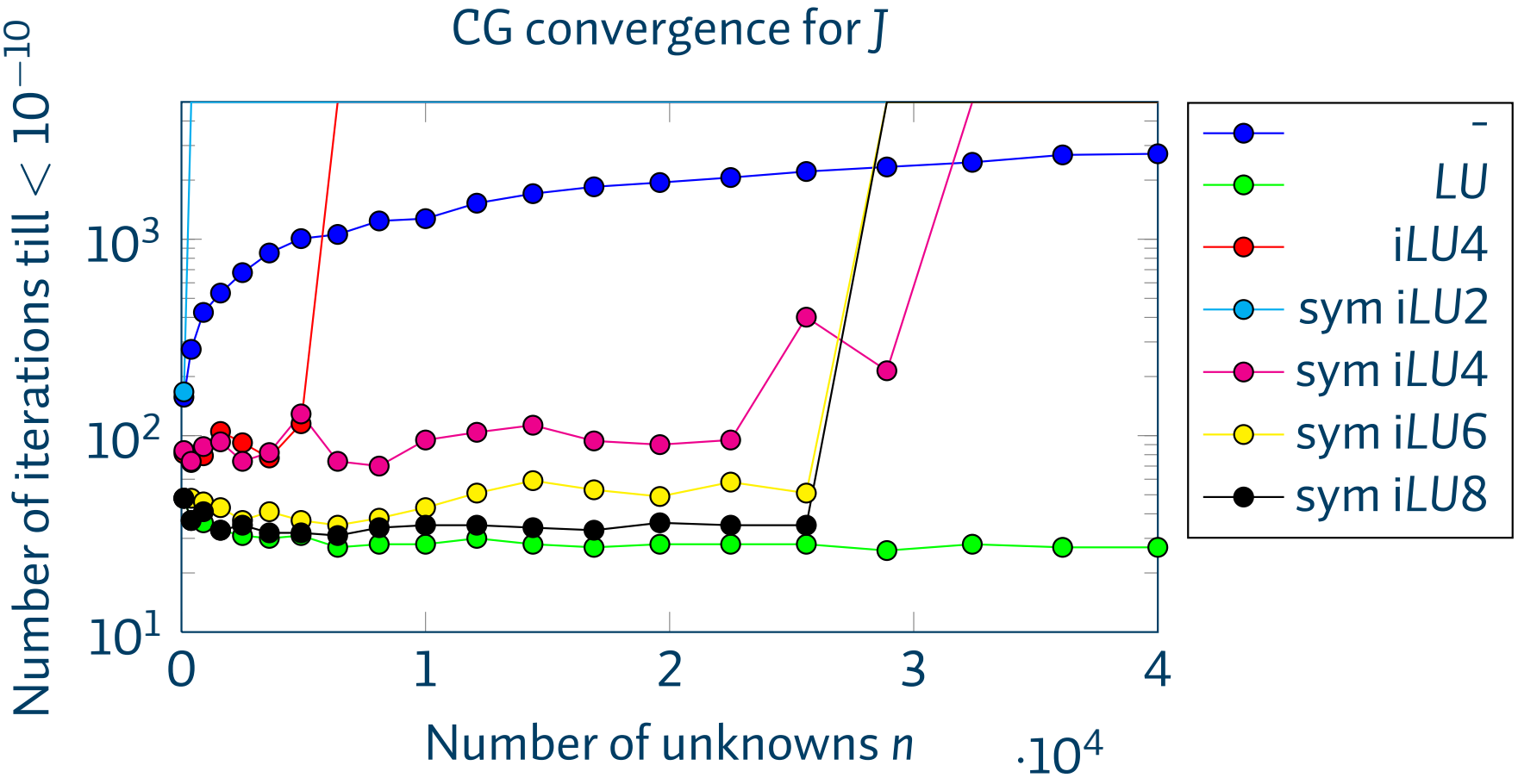
to solving a system with

$$K\varphi = (-\mathrm{i}\nabla - \mathbf{A})^2\varphi.$$

Much nicer, because K is

- structurally similar to ∇^2,
- representable by a matrix,
- self-adjoint,
- **positive (semi-)definite**

How to solve K^{-1}?



The kinetic energy operator

Kinetic energy operator

$$K\varphi = (-\mathrm{i}\nabla - \mathbf{A})^2\varphi.$$

- complex-valued,
- **self-adjoint** (Hermitian),
- **positive semi-definite**,
- has eigenvalue 0 iff $\mathbf{A} = 0$,
- simple structure (FVM discretization):

$$K\varphi = \sum_{\text{“neighbors” } k} -\mathrm{i}|P|\frac{\widetilde{U}_h\varphi_k - \varphi}{\|\mathbf{x}_k - \mathbf{x}\|}, \quad \widetilde{U}_h = \exp\left\{-\mathrm{i}\int_{\text{edge } \mathbf{e}} \mathbf{A}\cdot\mathbf{e}\right\}$$

Multigrid

...for

$$K\varphi = (-\mathbb{i}\boldsymbol{\nabla} - \mathbf{A})^2\varphi.$$

Scott P. MacLachlan, Cornelis W. Oosterlee.
Algebraic multigrid solvers for complex-valued matrices.
SIAM Journal on Scientific Computing, 30:1548–1571, 2008.

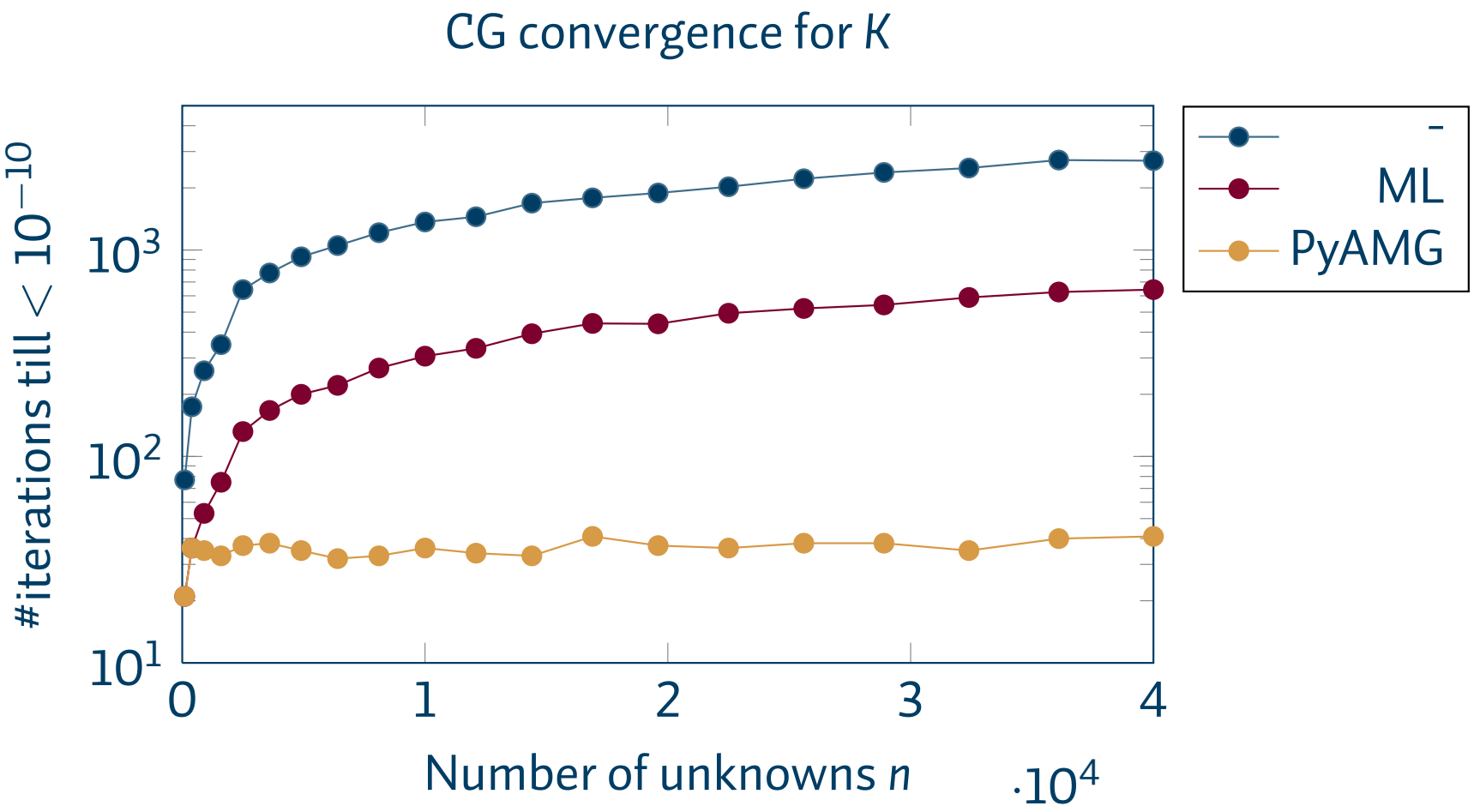
PyAMG (sequential)

Smoothed aggregation, Block-Gauß-Seidel smoother, Hermitian symmetry, standard aggregation

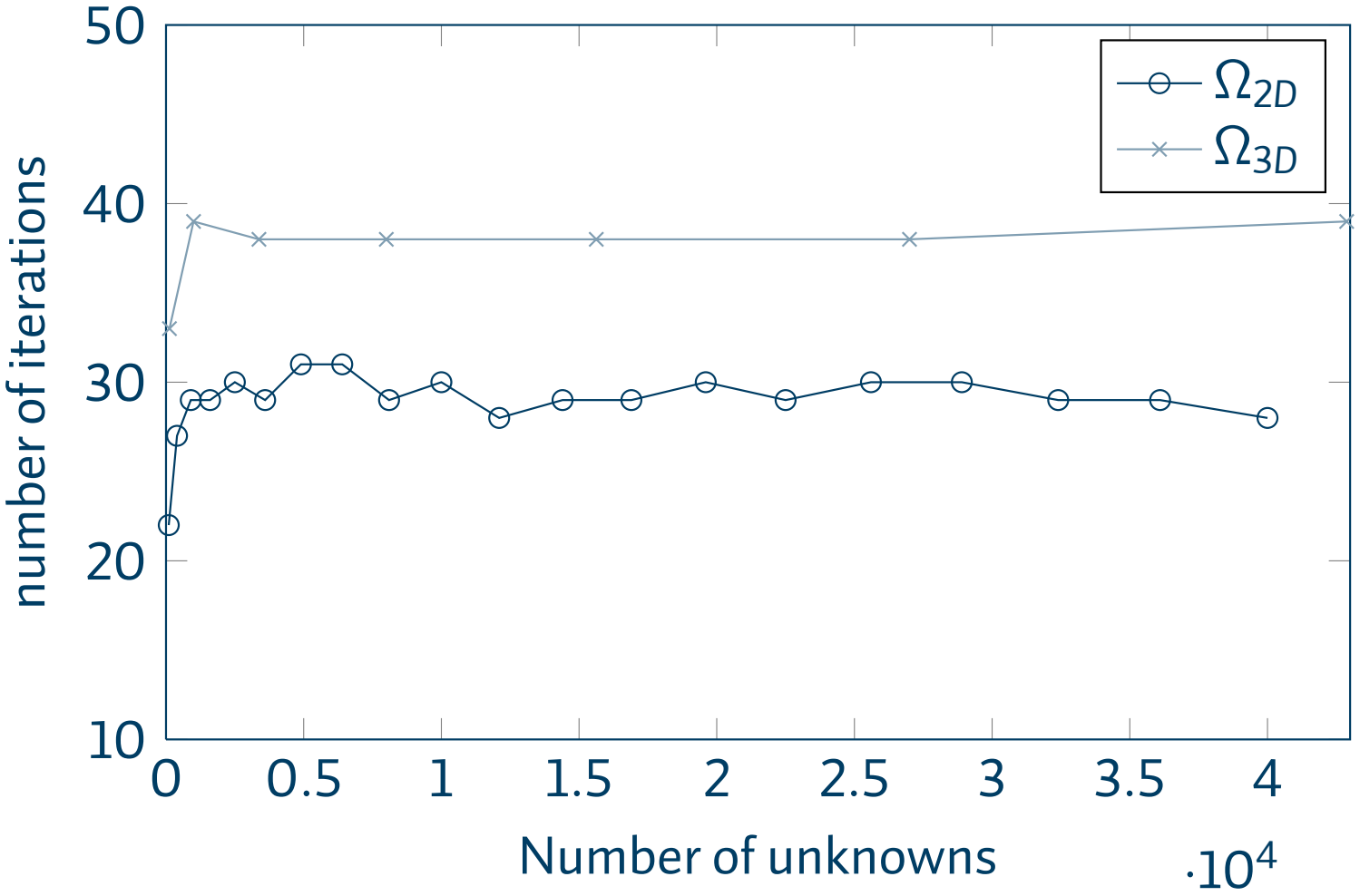
ML/Trilinos (parallel)

Smoothed aggregation, Chebyshev smoother, uncoupled aggregation

Multigrid


CG convergence for K
#iterations till $< 10^{-10}$
10^3
10^2
10^1
0
1
2
3
4
Number of unknowns n
$\cdot 10^4$
-
ML
PyAMG

K^{-1} multigrid for production problems



More involved test cases

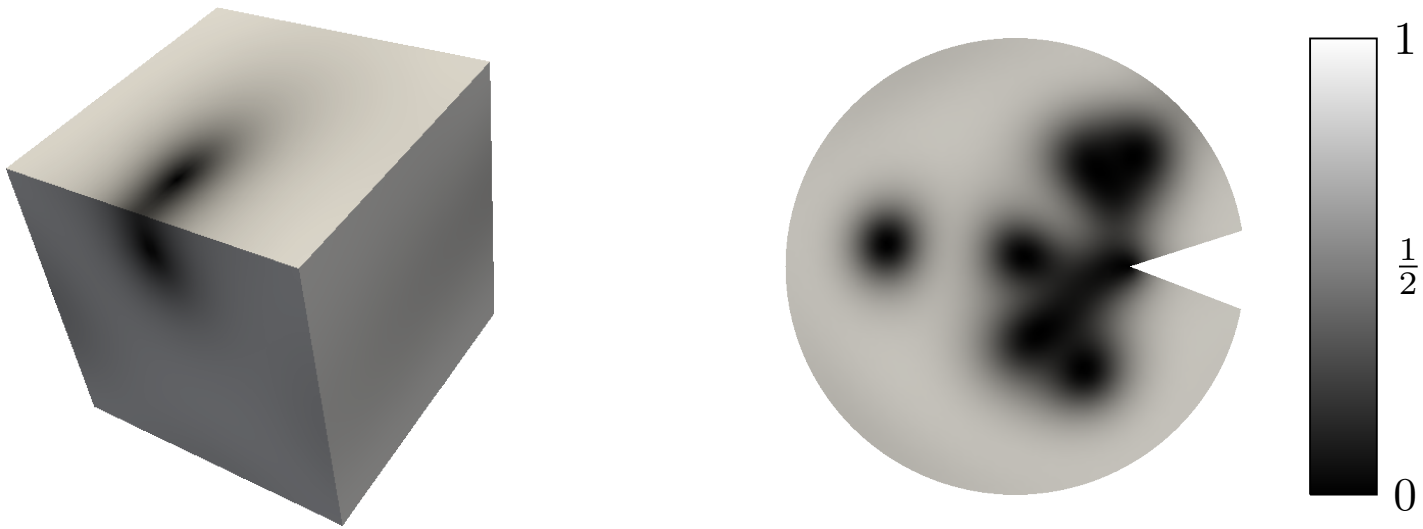


Figure: Typical solutions $|\psi|^2$ of the Ginzburg–Landau equations (2M, 200K DOF).

Preconditioning: conclusions

Solve $\mathcal{GL}(\psi)$ with **Newton**

Solve J_ψ with **MINRES**

Precondition with **kinetic energy operator** K^{-1}, solved by

MG-preconditioned CG

Message

Preconditioning J_ψ for all $\mathbf{A} \neq 0$ delivers an algorithm which is

- independent of the size equation system
- computationally scalable (comfirmed on 4000+ cores)

This makes

- 2D calculations feasible (e.g., numerical continuation)
- 3D calculations **possible**.

Technicalities

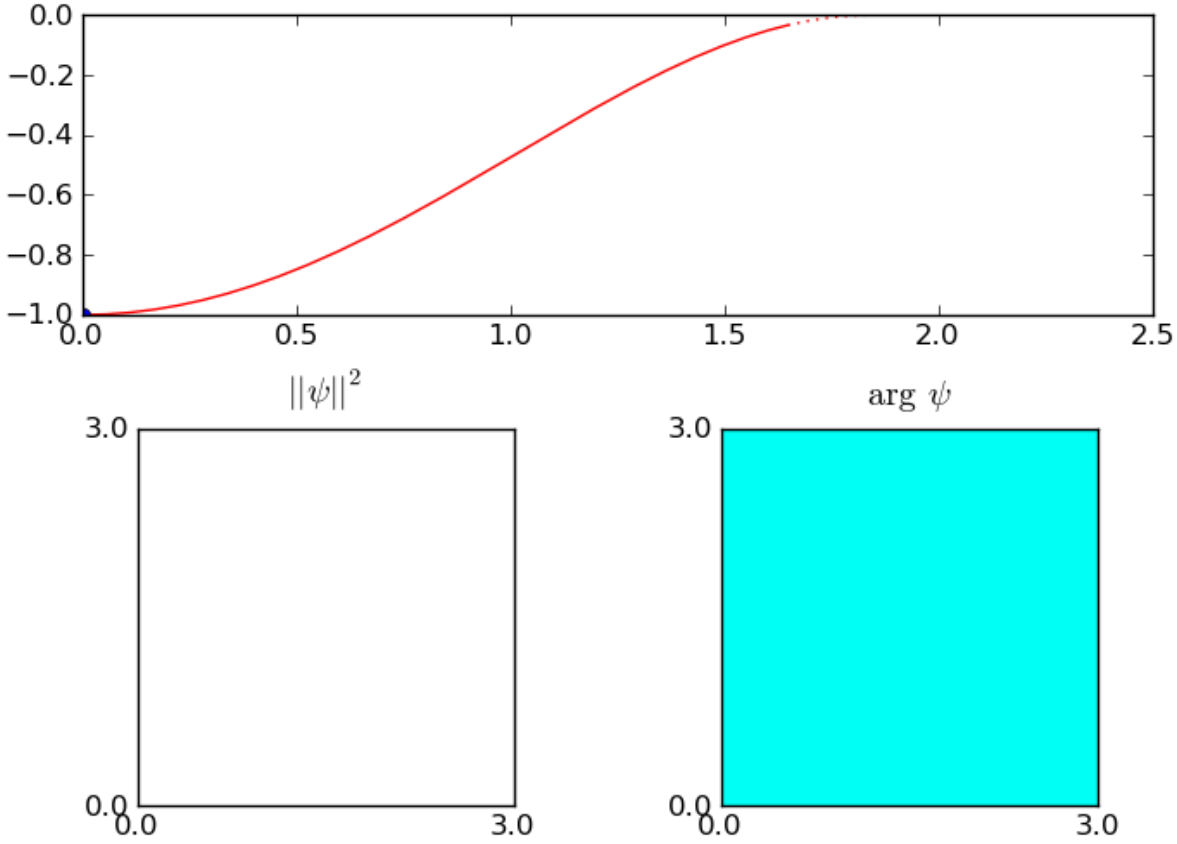
- Continuation: Arc-length, adaptive step sizes
- Nonlinear solves: Newton
- Linear solves: MINRES + K^{-1} + AMG

Software in use:

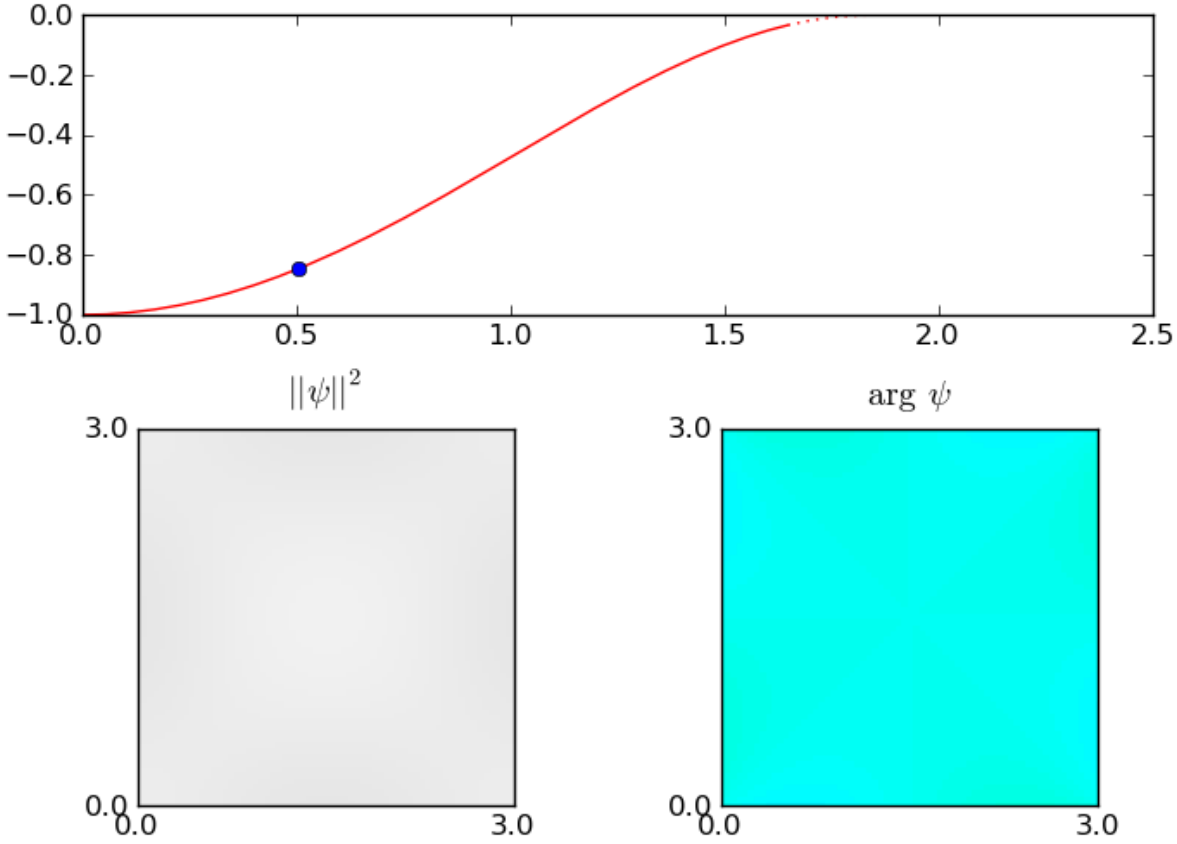
- Trilinos: **LOCA**, NOX

Andy Salinger, Eric Phipps (Sandia National Labs)

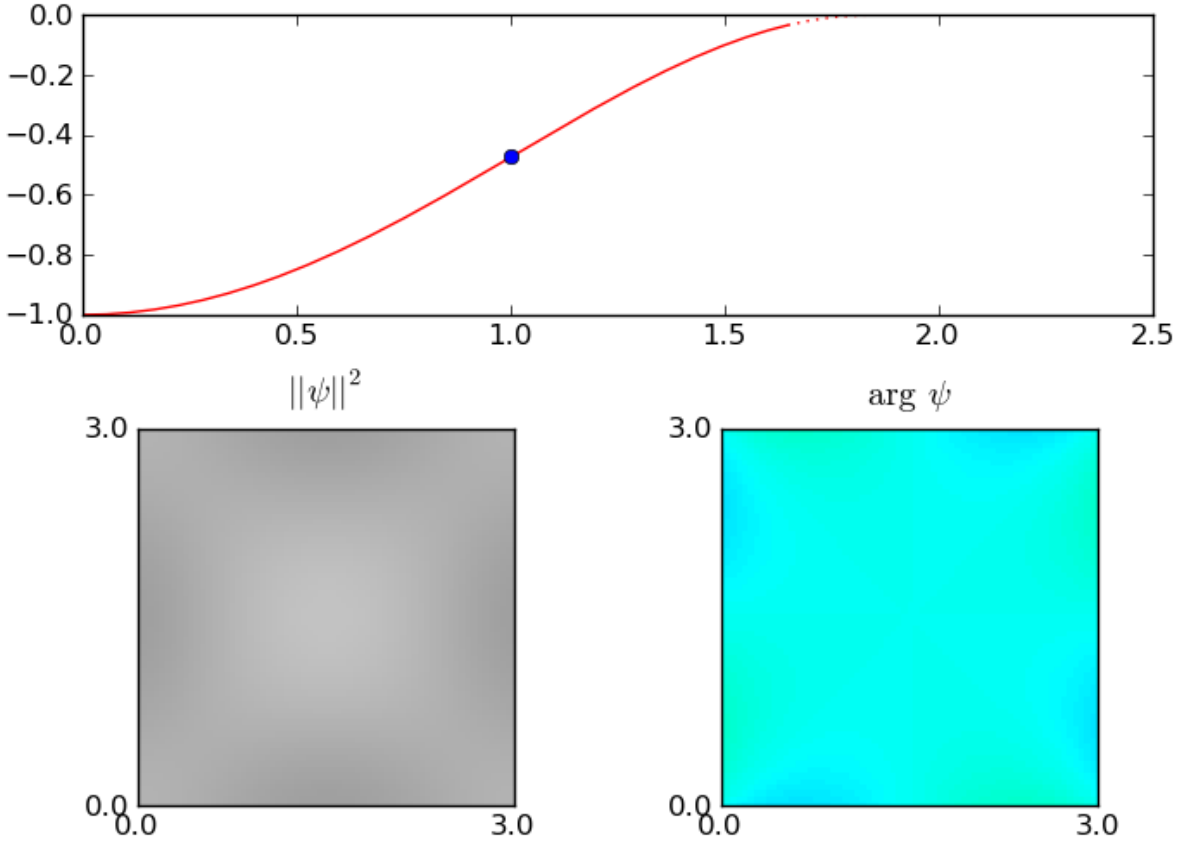
Calculation



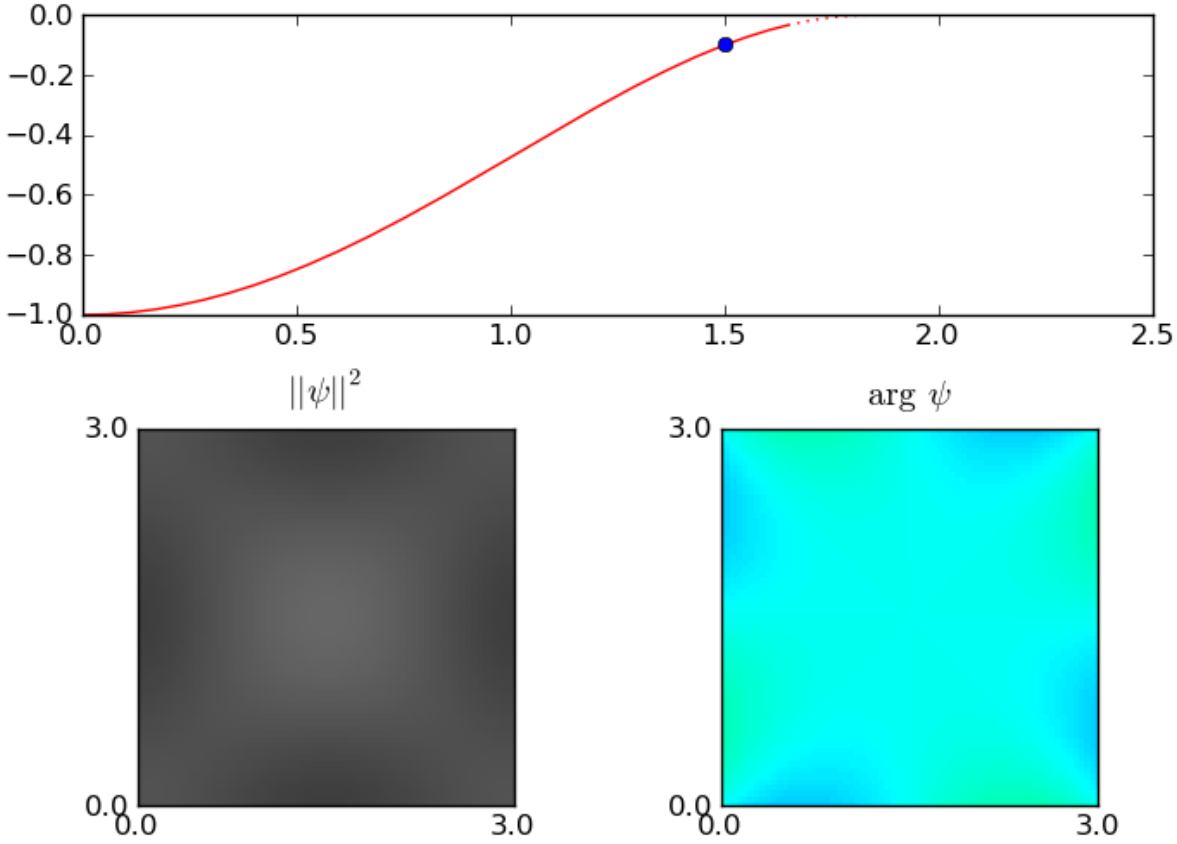
Calculation



Calculation



Calculation



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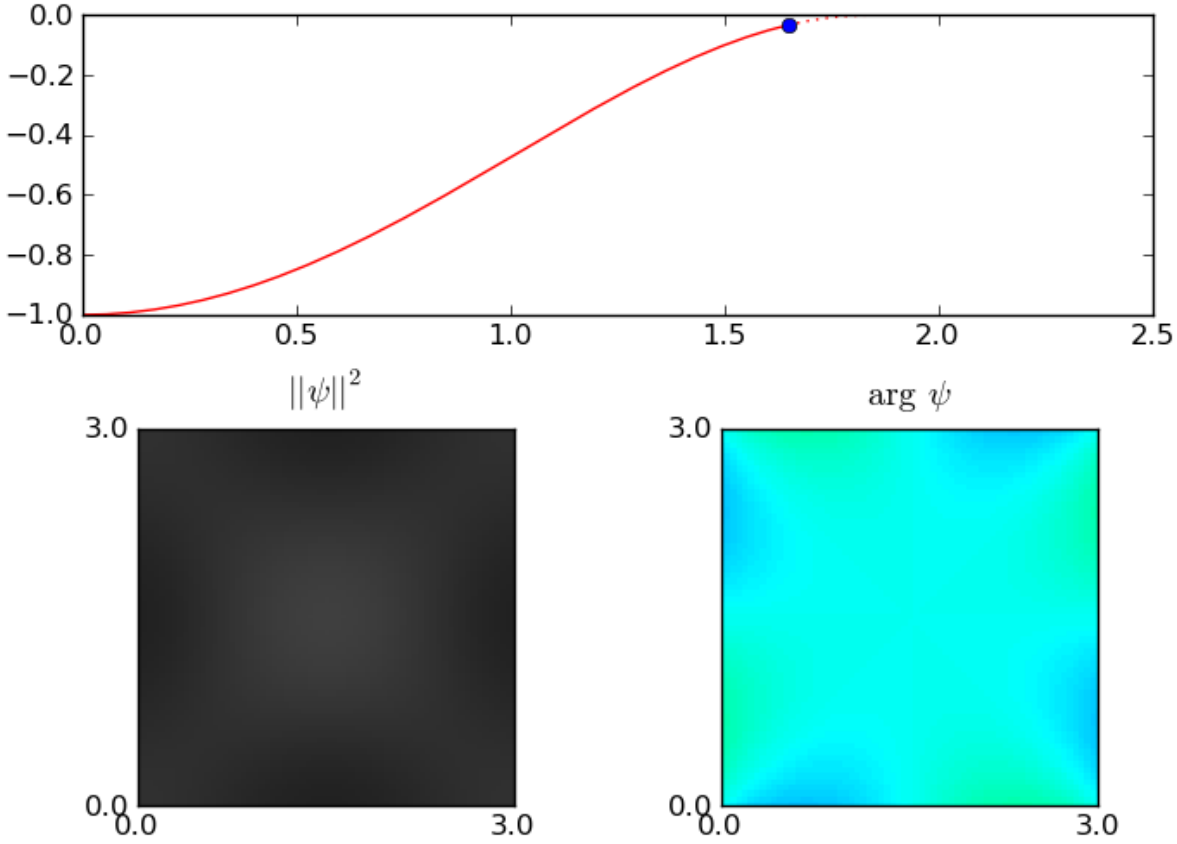
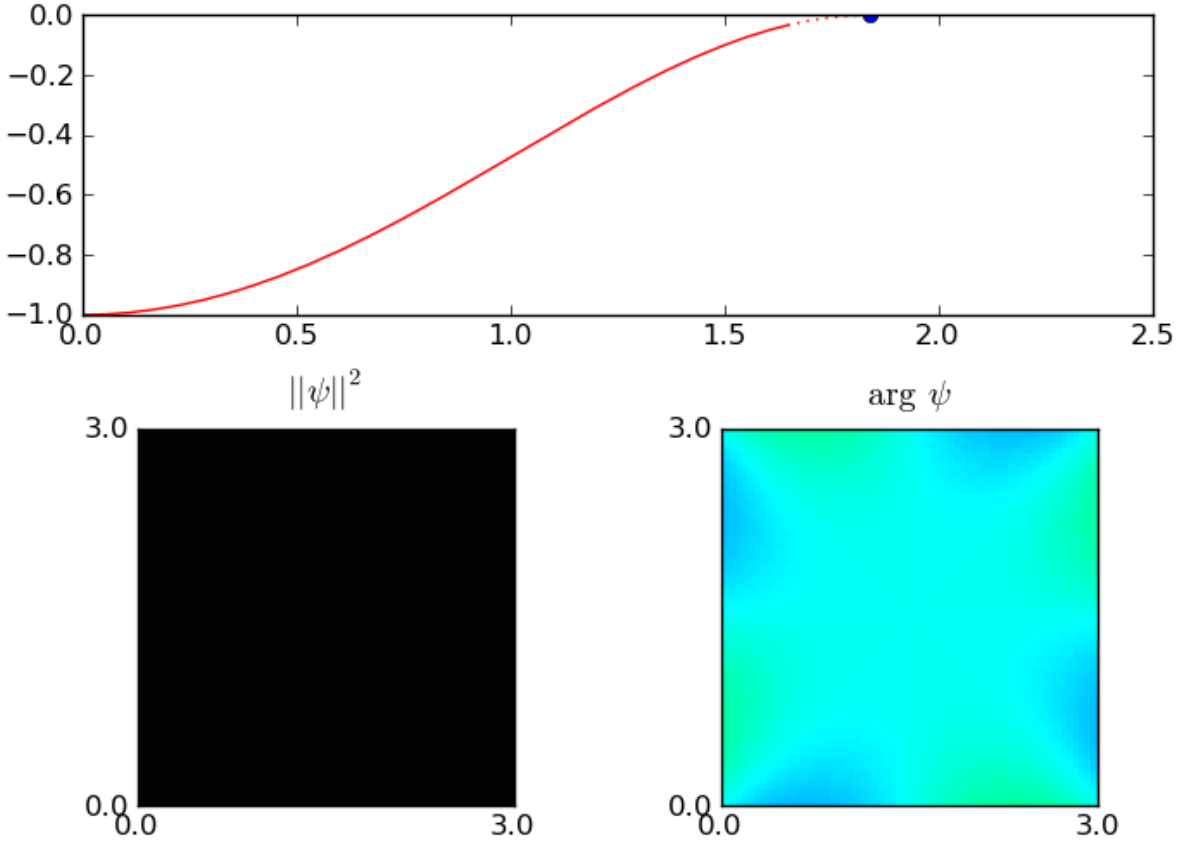
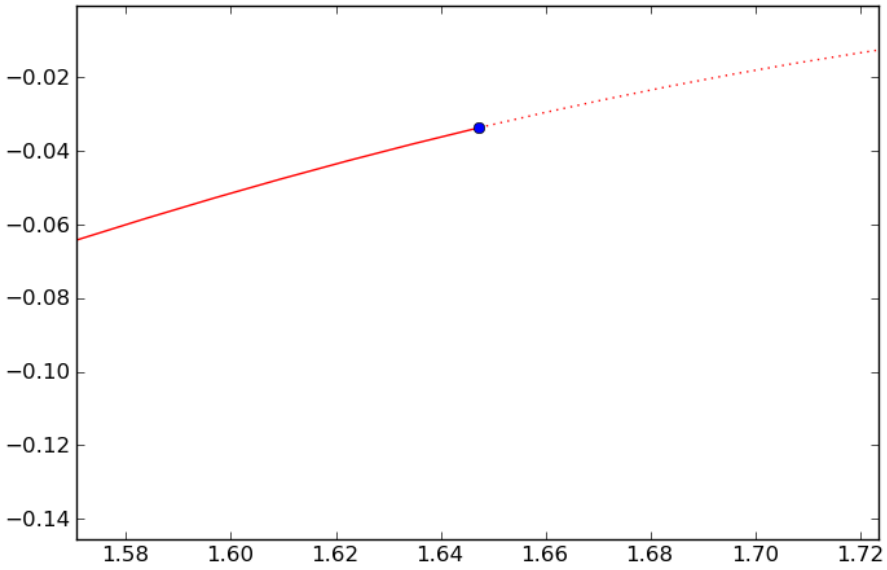


Calculation



Branch point at $H_0 \approx 1.64$



Two eigenvalues going unstable.

$\Longrightarrow$ Branching!

Branch point at $H_0 \approx 1.64$ (cont.)

Application of the **equivariant branching lemma**.

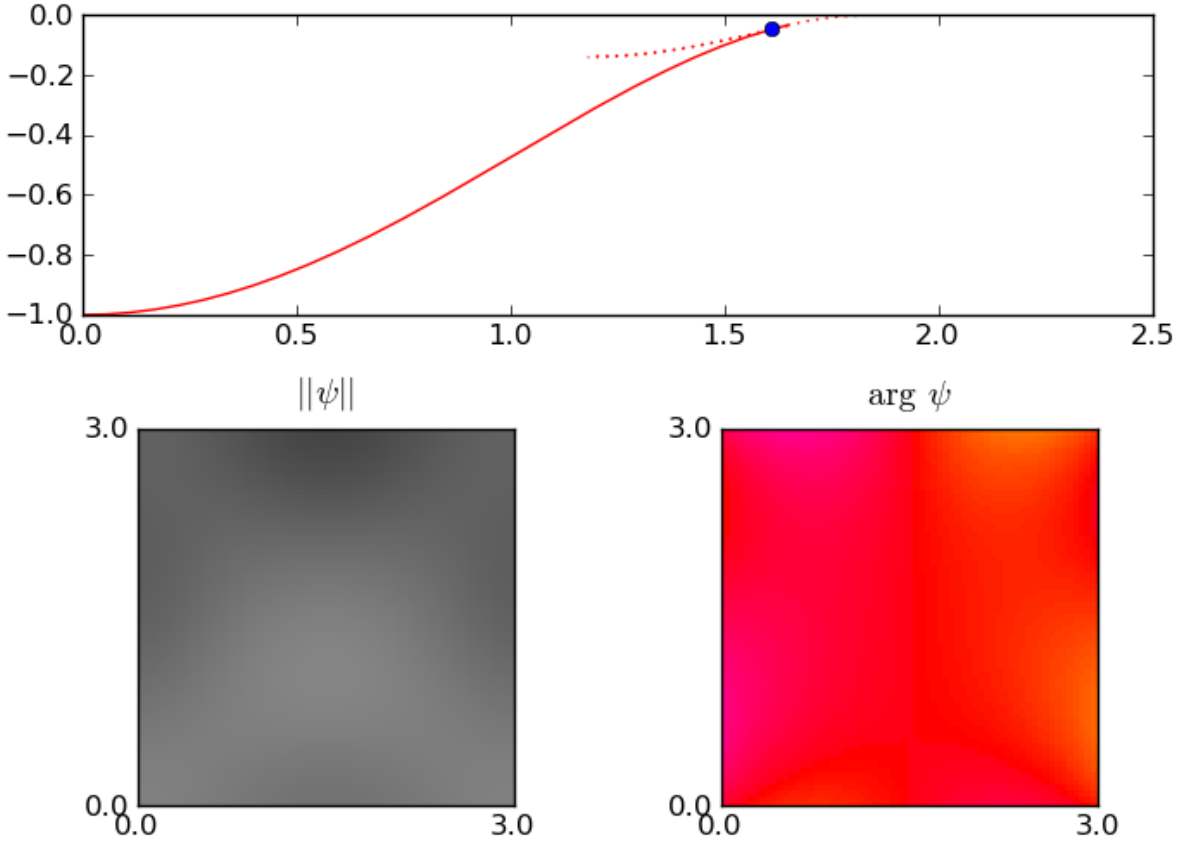
Main questions:

- Which representation has the model "chosen"?
- What are the axial subgroups in this representation?
  - $\langle \sigma \rangle$ (conjugated flip)
  - $\langle \rho\sigma \rangle$ (conjugated flip along diagonal)

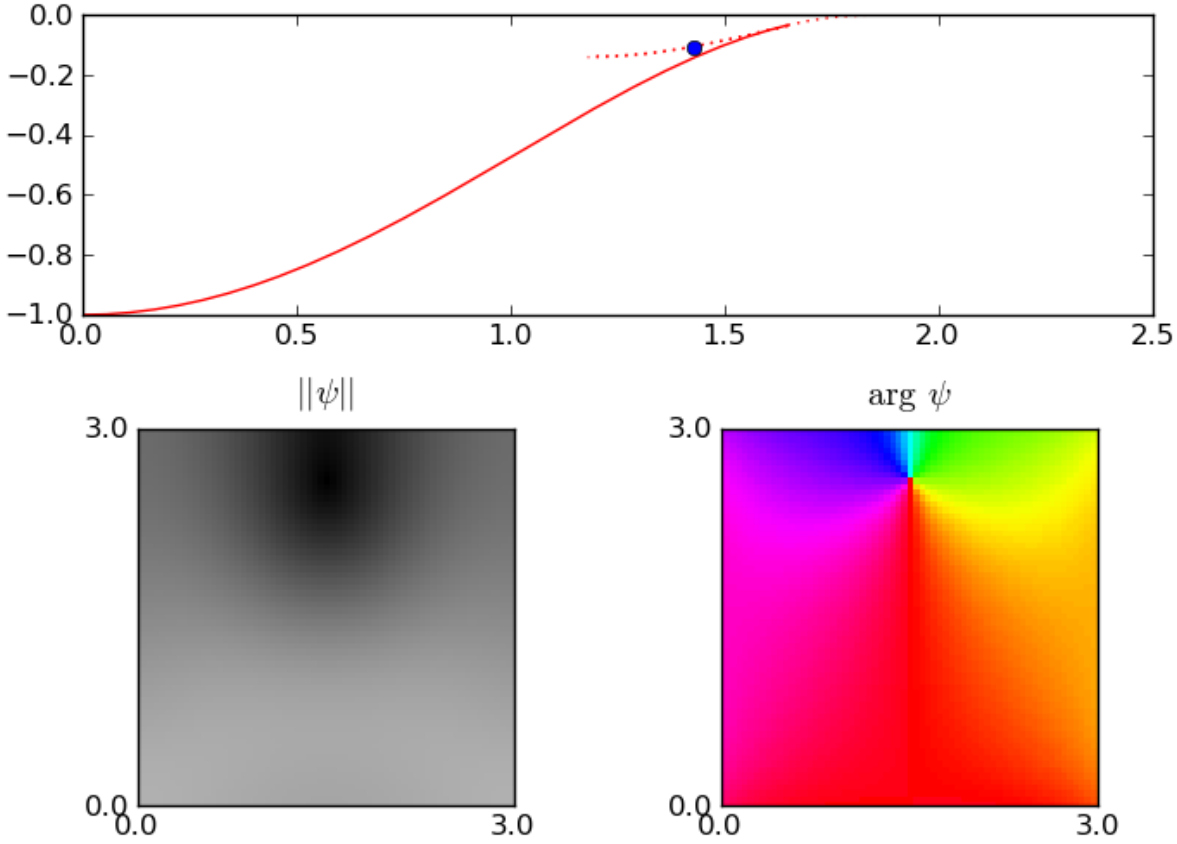
Then guaranteed:

There are unique solution branches with symmetry $\langle \sigma \rangle$, $\langle \rho\sigma \rangle$.

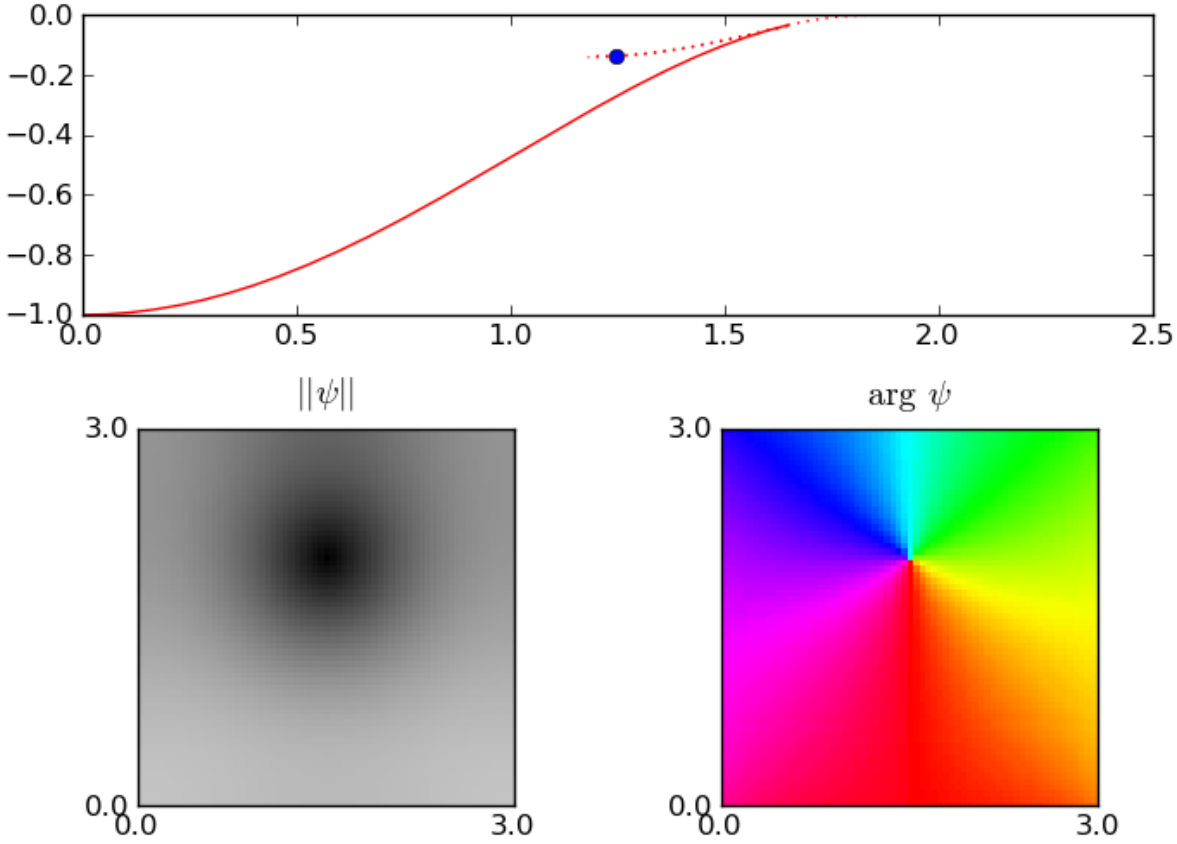
Branch 1



Branch 1



Branch 1



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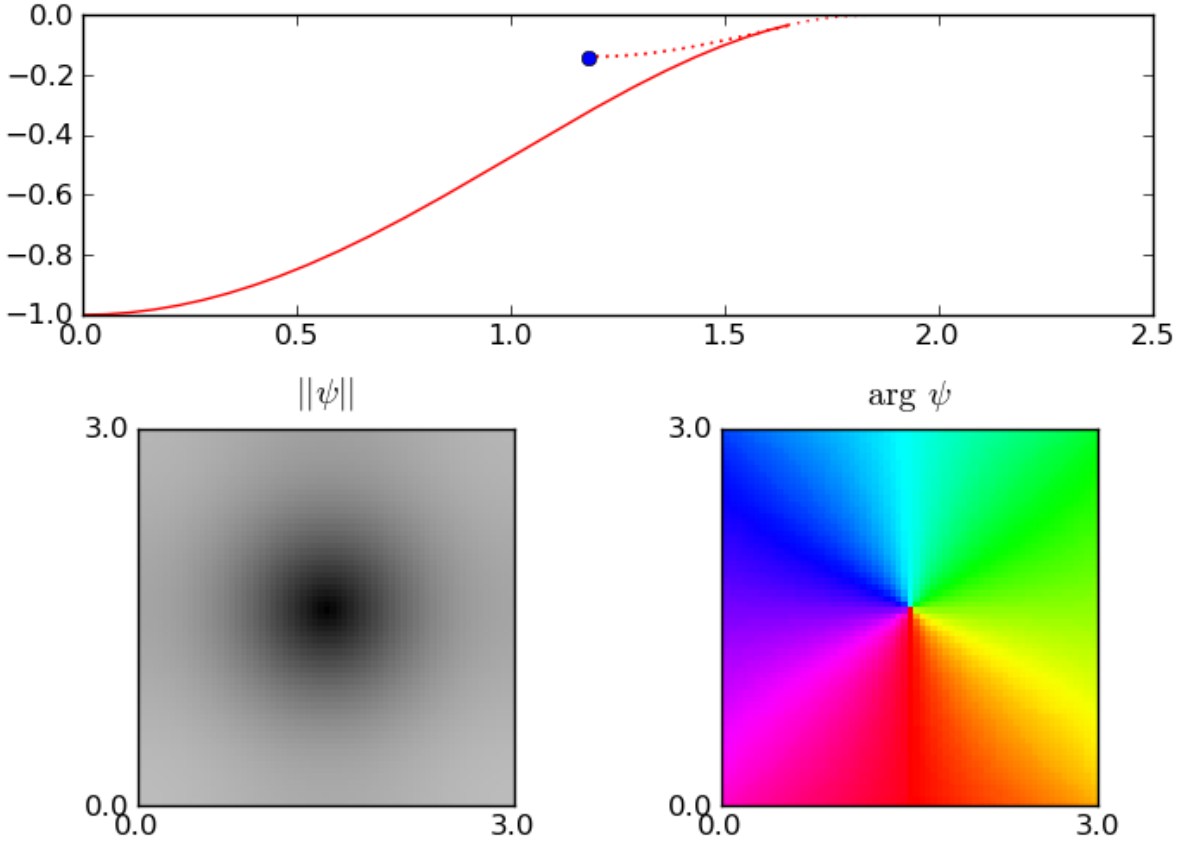
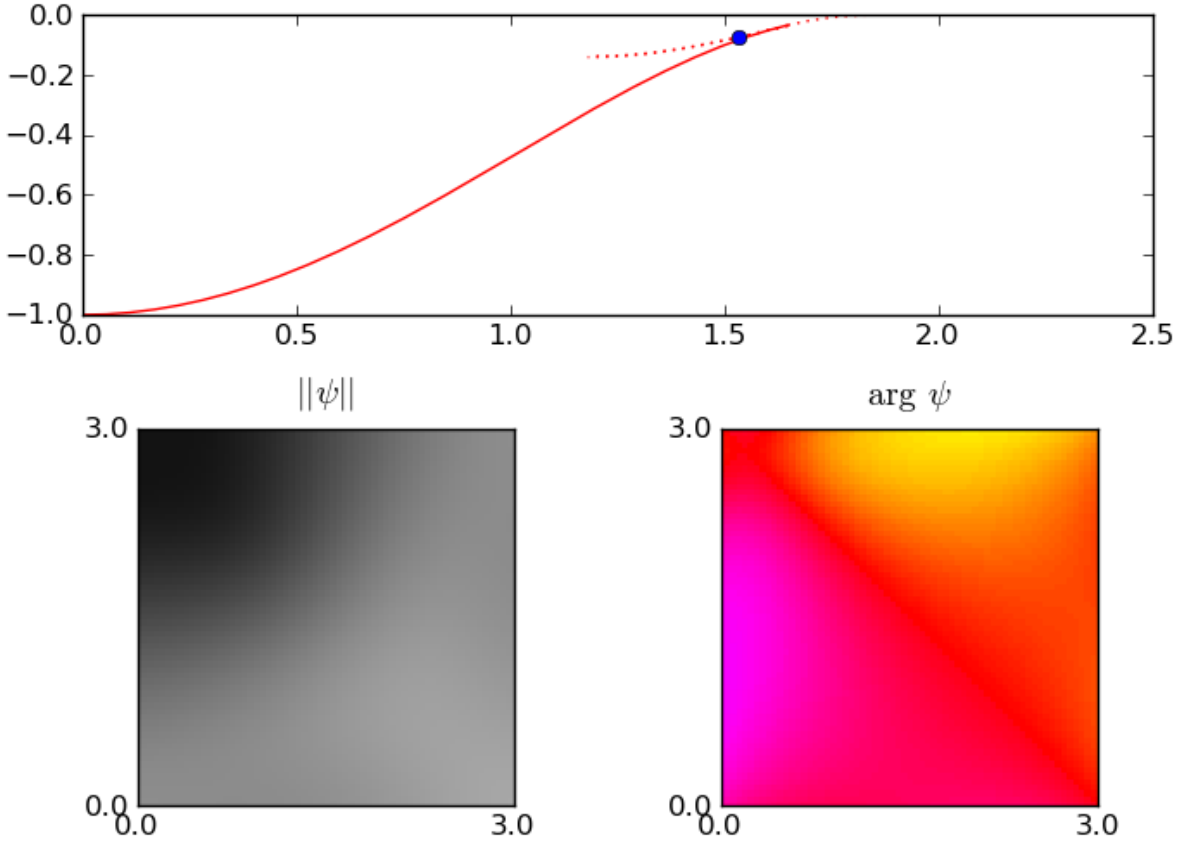
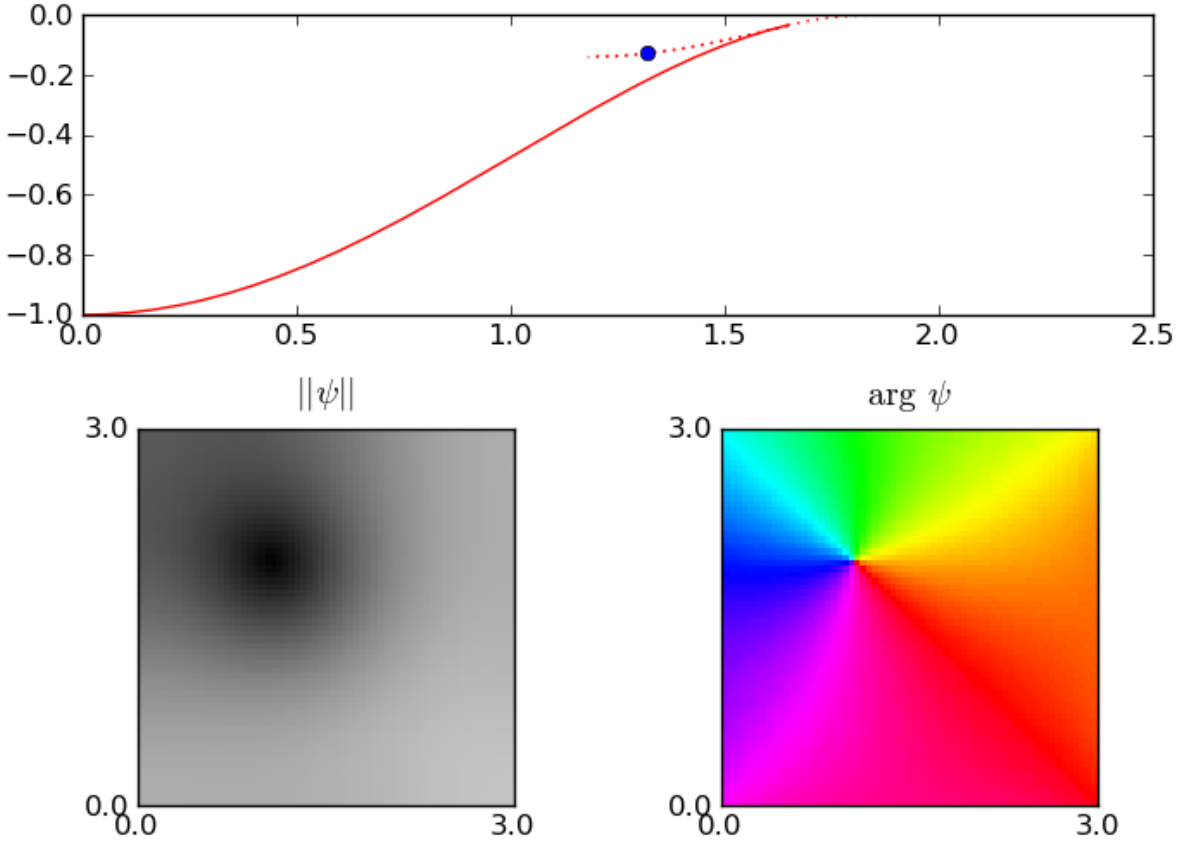


Branch 2



Branch 2



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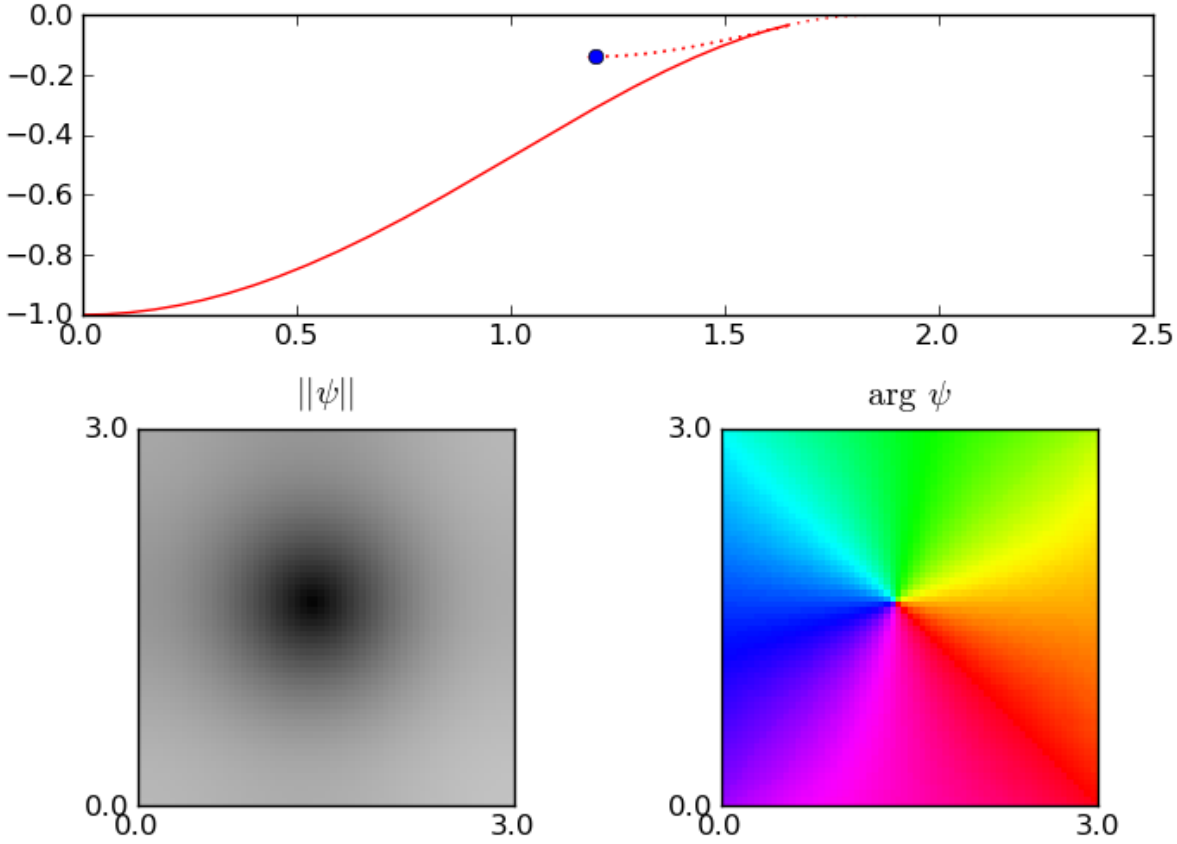
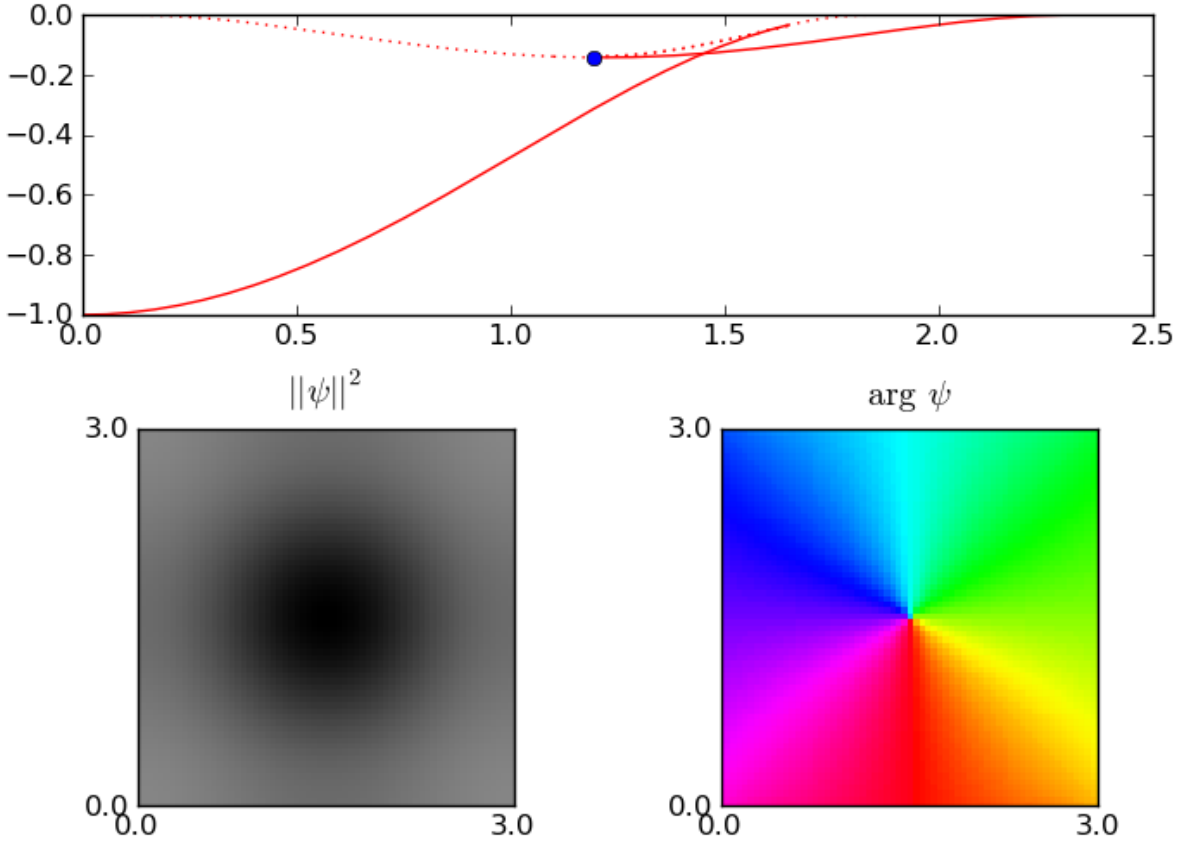


One-vortex solution



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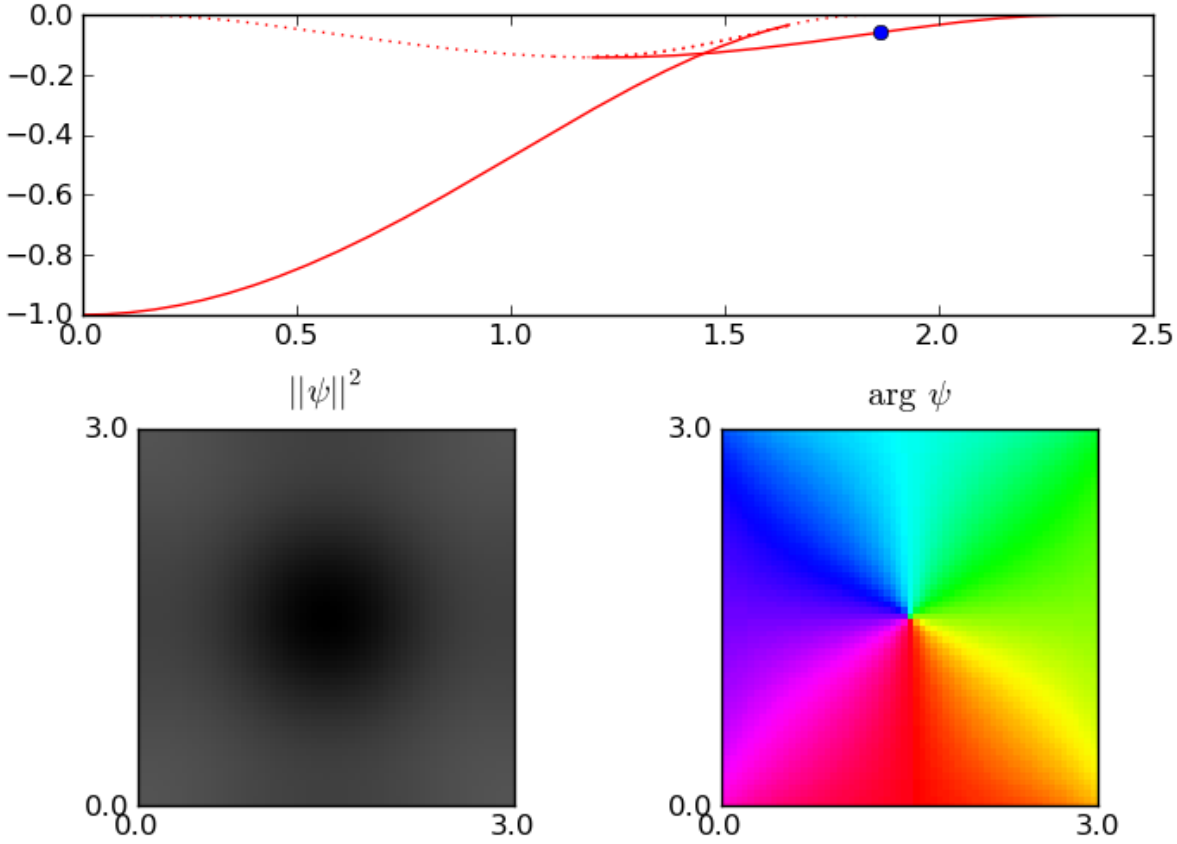
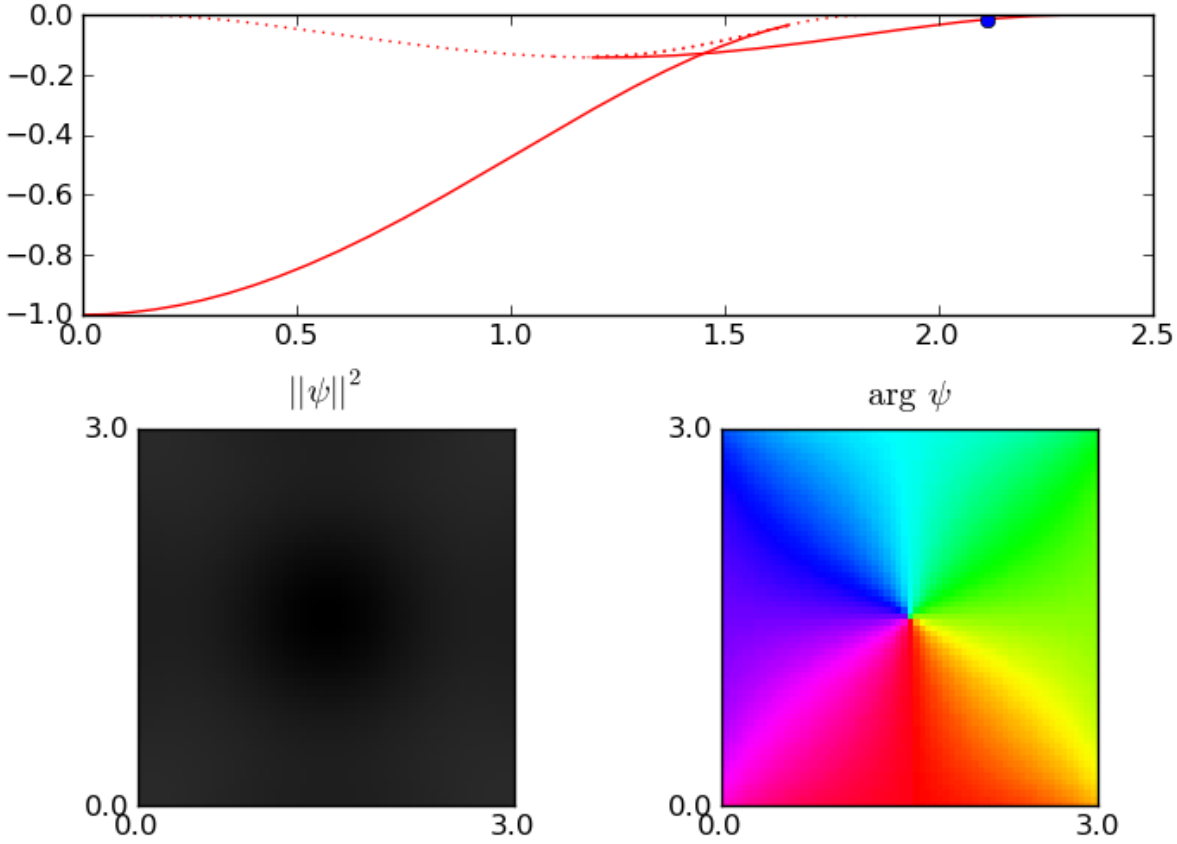
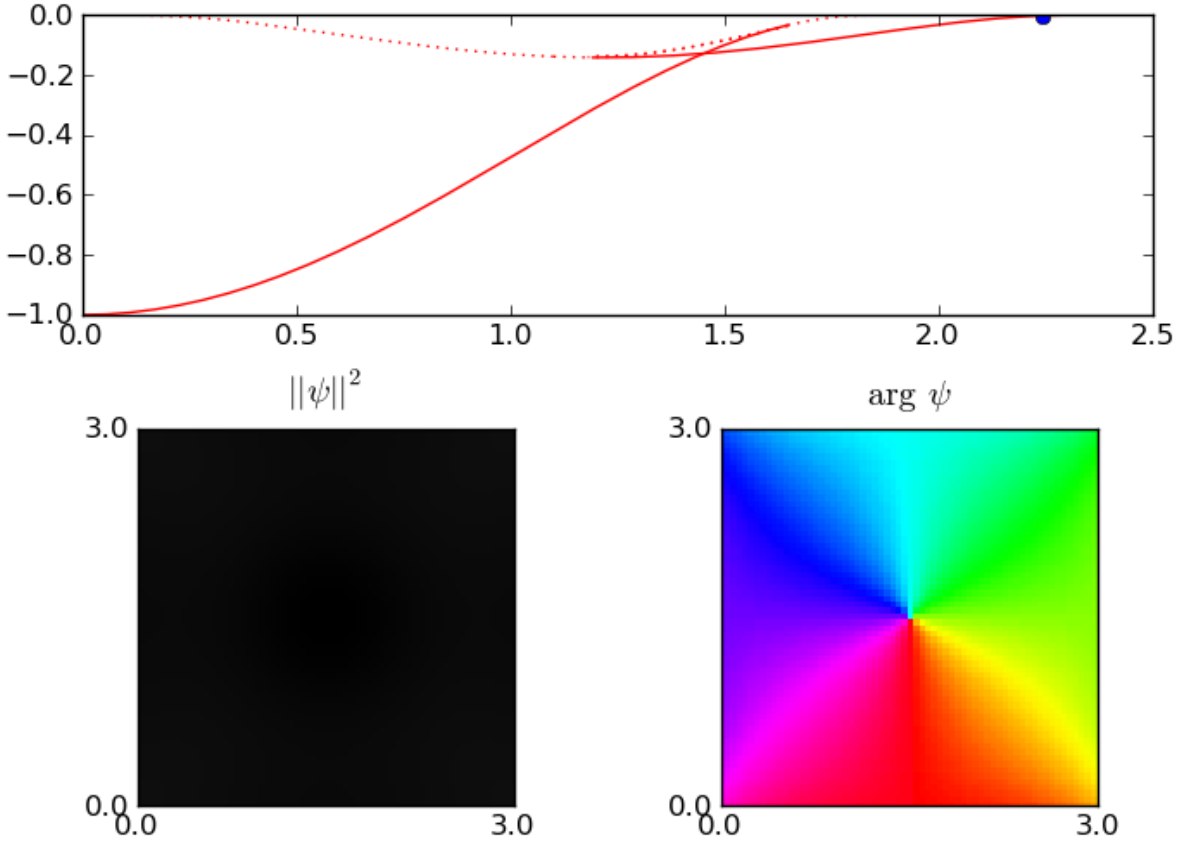


One-vortex solution



One-vortex solution



Outlook

The full GL problem:

$$\begin{cases} (-\mathrm{i}\nabla - \mathbf{A})^2 \psi = \psi \left(1 - |\psi|^2\right) & \text{on } \Omega_1 \\ -\nabla \times (\nabla \times \mathbf{A}) = \dfrac{1}{\kappa^2} \left(\dfrac{1}{2\mathrm{i}} \left(\overline{\psi} \nabla \psi - \psi \nabla \overline{\psi}\right) - |\psi|^2 \mathbf{A} \right) & \text{on } \mathbb{R}^n \\ \mathbf{n} \left(-\mathrm{i}\nabla - \mathbf{A}\right) \psi|_\Gamma = 0, & \text{on } \Gamma \\ \lim\limits_{\mathbf{x} \to \infty} \nabla \times \mathbf{A} = \mathbf{H}_0. \end{cases}$$

- Preconditioning the full equations?