Solving sign problems with physics-informed kernels

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IsoQuant SFB1225

STRUCTURES CLUSTER OF EXCELLENCE

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Central task in computations of lattice field theories

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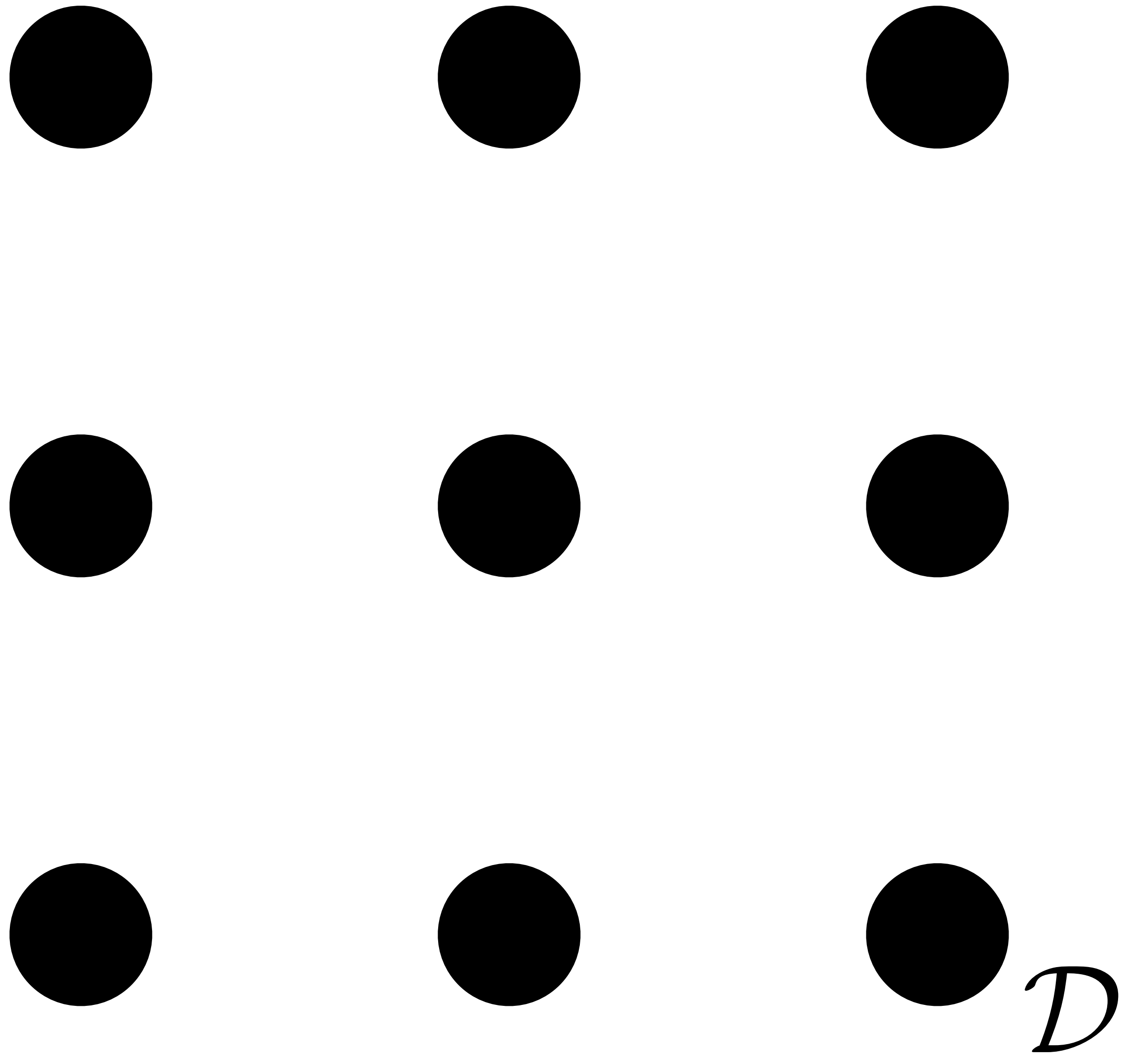

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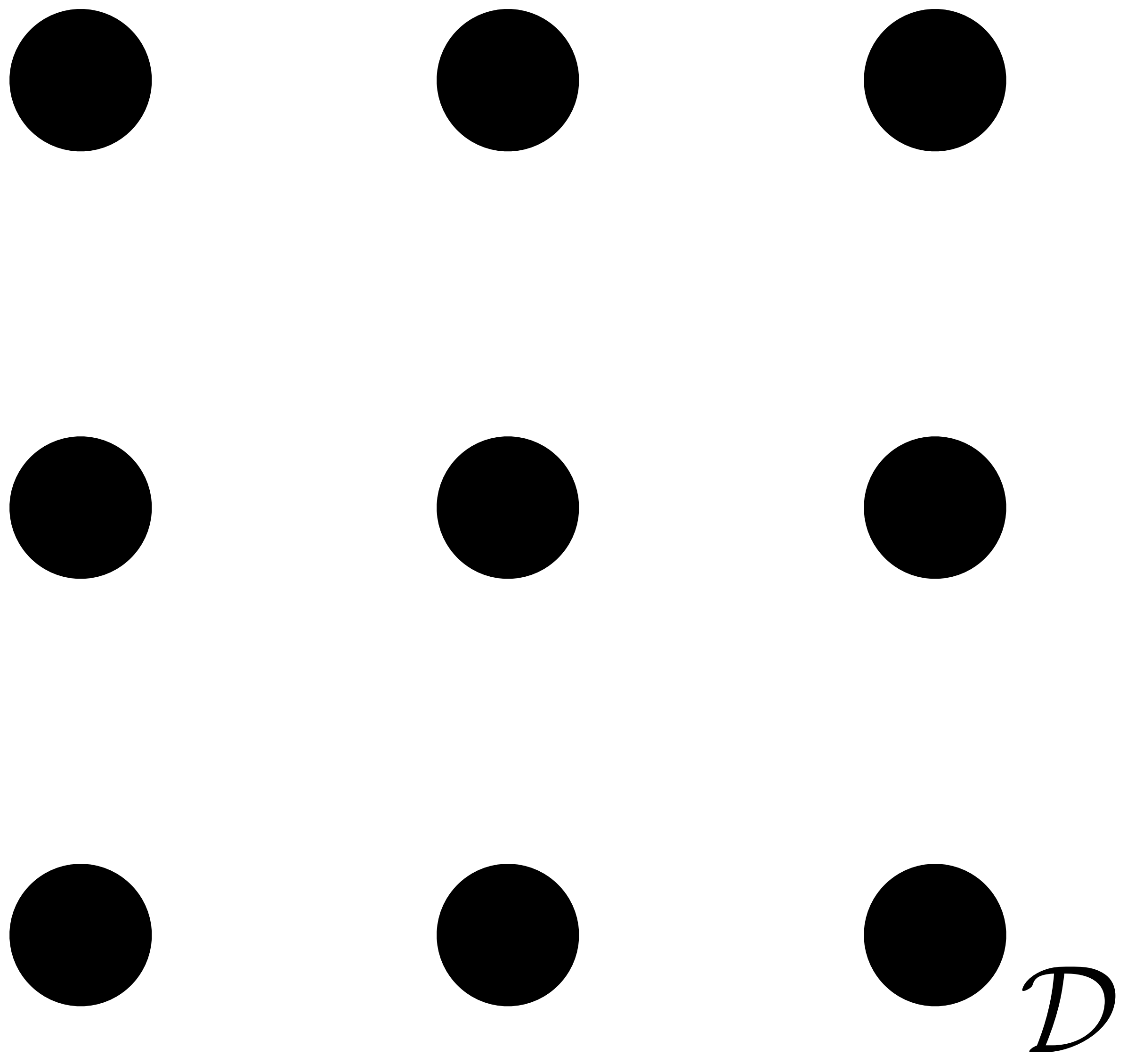

Central Step

$$\langle \mathcal{O} \rangle = \int D\phi \, p(\phi) \, \mathcal{O}(\phi) = \mathop{\mathbb{E}}_{\phi \sim p} \left[\mathcal{O}(\phi) \right]$$

When p is a probability distribution

But generally $p(\phi) \in \mathbb{C}$ and not $p(\phi) \in [0, 1]$

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$$\langle \mathcal{O} \rangle = \int D\phi \, p(\phi) \, \mathcal{O}(\phi) \qquad \phi \in \mathbb{R}^{\mathcal{D}}$$

Euclidean $p(\phi) = \frac{1}{\mathcal{N}} e^{-\hat{S}(\phi)} = e^{-S(\phi)}$

Real-time $p(\phi) = \frac{1}{\mathcal{N}} e^{i\hat{S}(\phi)} = e^{iS(\phi)}$

using Markov chain Monte Carlo

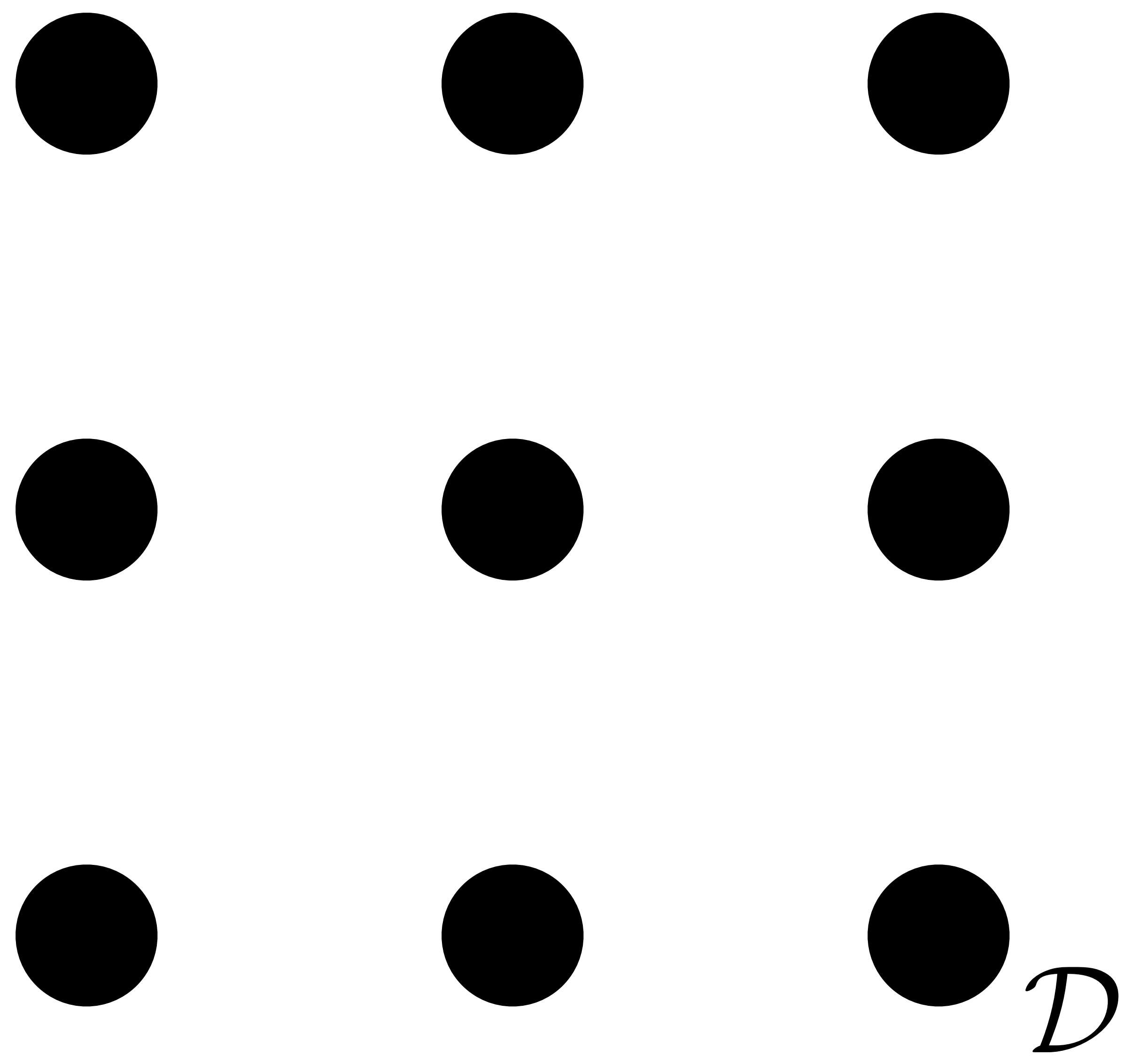

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Illustration at the example of naïve reweighting

$$\langle \mathcal{O} \rangle = \frac{\int D\phi \left[\mathcal{O}(\phi) e^{-i\hat{S}_I(\phi)} \right] e^{-\hat{S}_R(\phi)}}{\int D\phi \left[e^{-i\hat{S}_I(\phi)} \, e^{-\hat{S}_R(\phi)} \right]} = \frac{\underset{\phi \sim |p|}{\mathbb{E}} \left[\mathcal{O} e^{-i\hat{S}_I(\phi)} \right]}{\underset{\phi \sim |p|}{\mathbb{E}} \left[e^{-i\hat{S}_I(\phi)} \right]}$$

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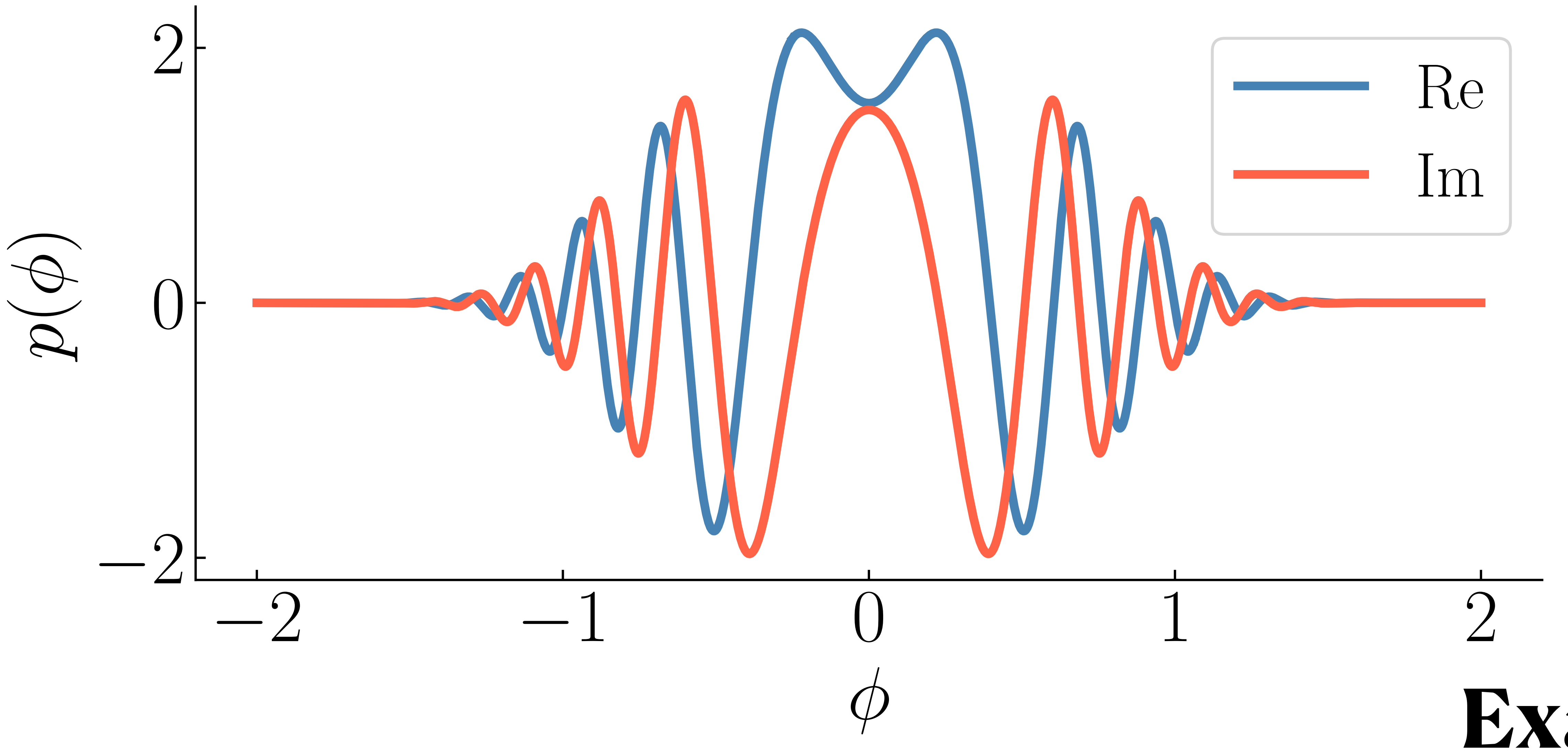

Example action

$$S(\phi) = \sum_{x\in\mathcal{D}} \left[\frac{1}{2}(m^2 + i\gamma)\phi_x^2 + \frac{1}{4}\lambda\phi_x^4 \right]$$

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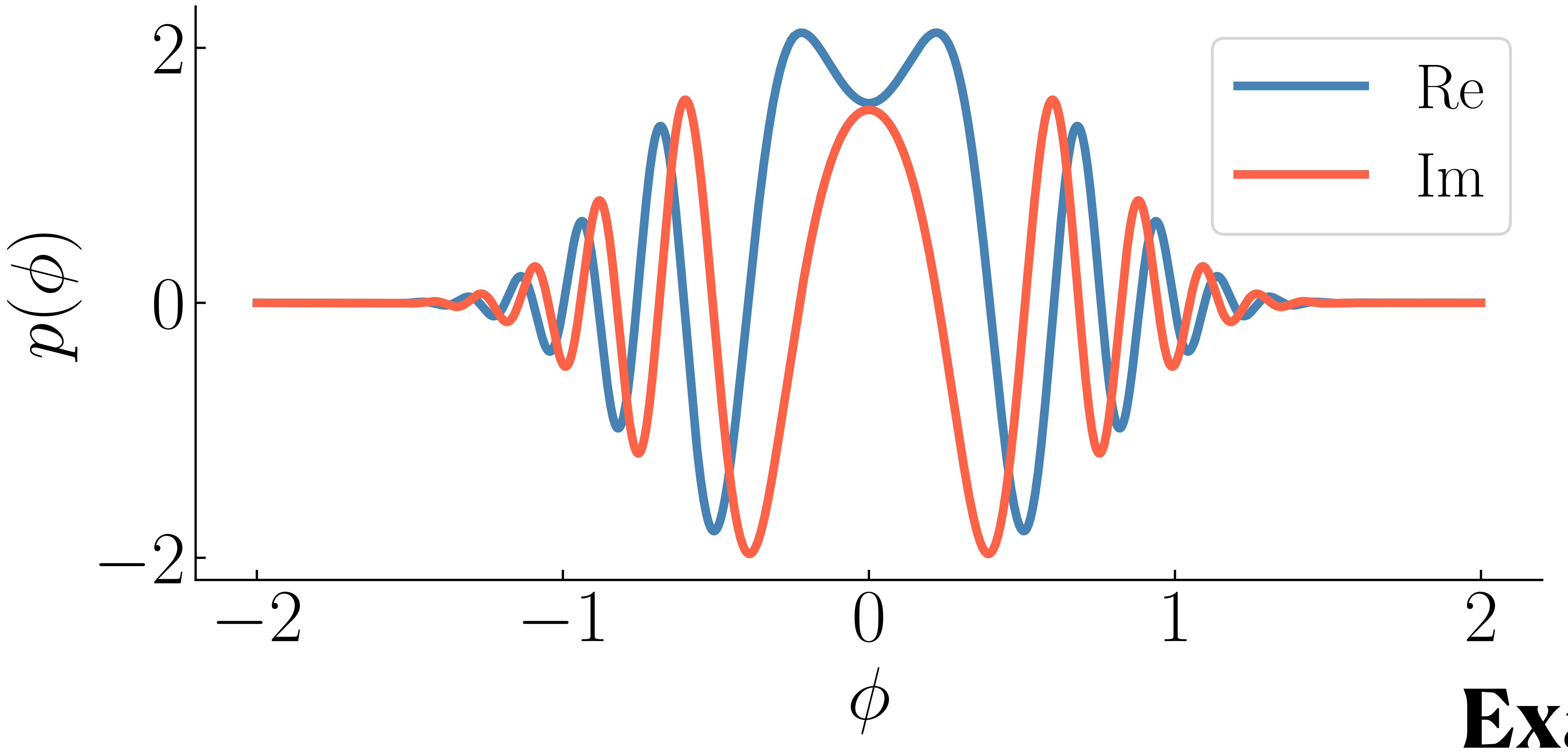

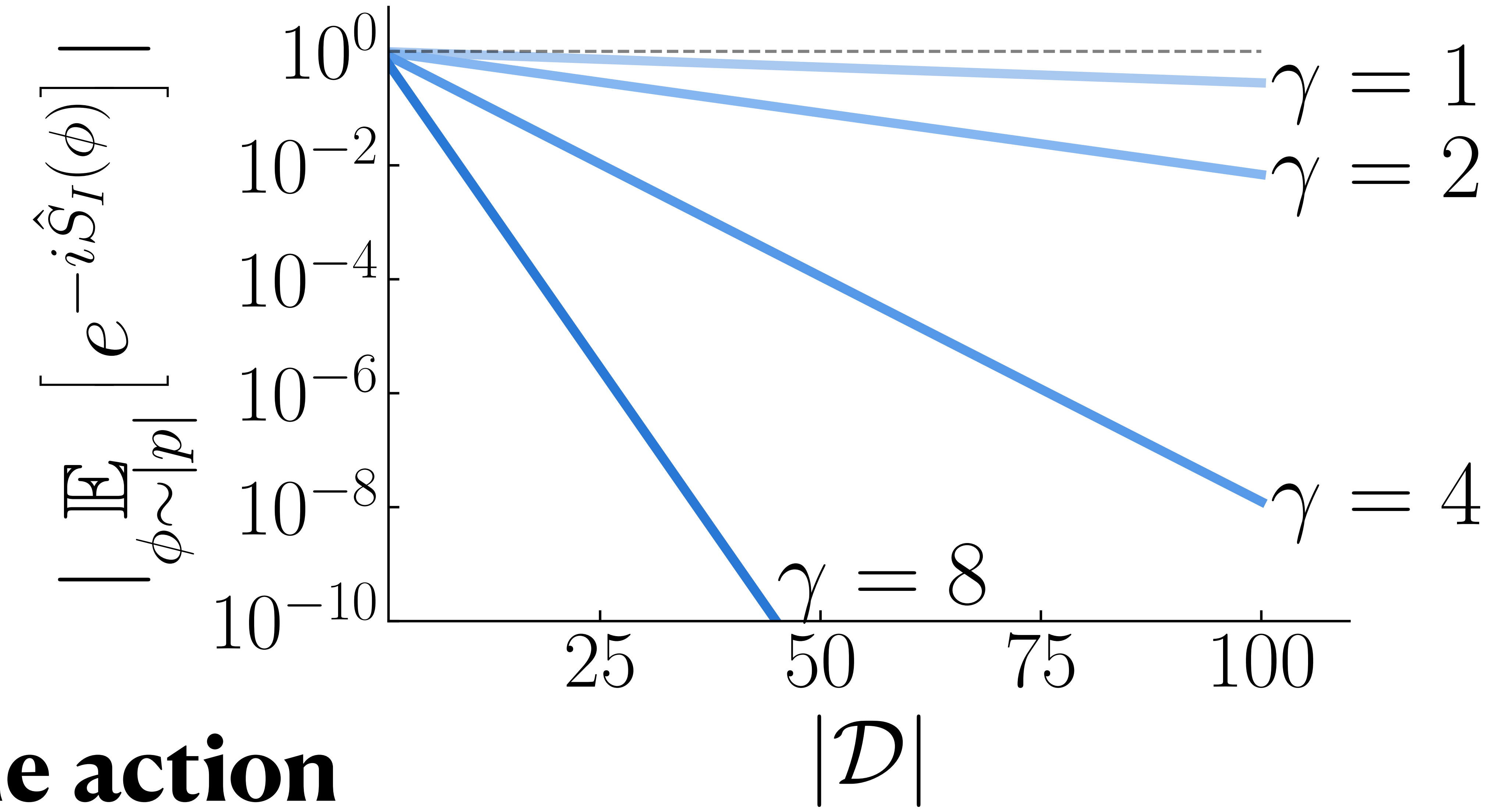

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Complex Langevin

e.g.

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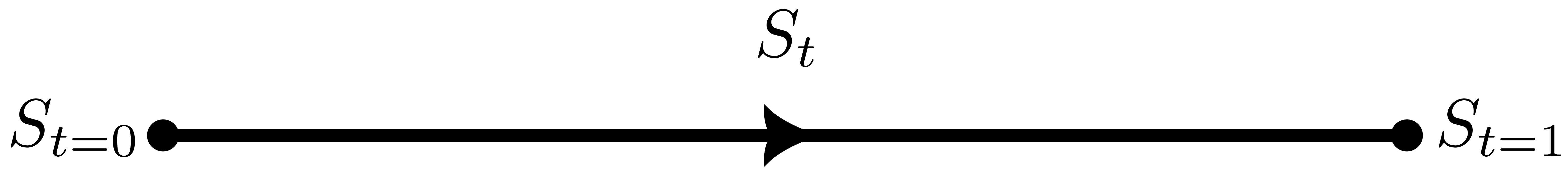
$S_1 = S$

Physics-Informed Kernels



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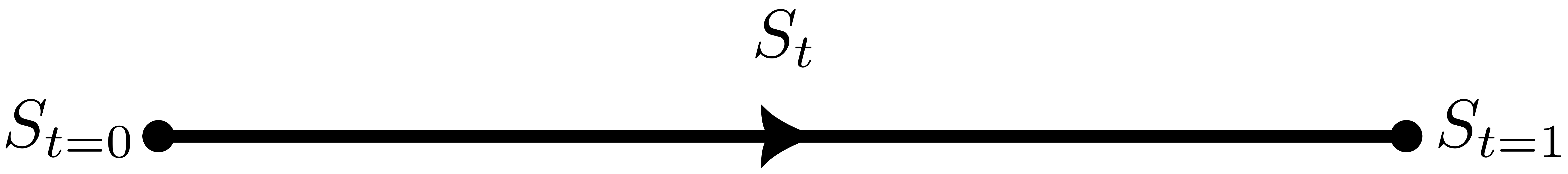

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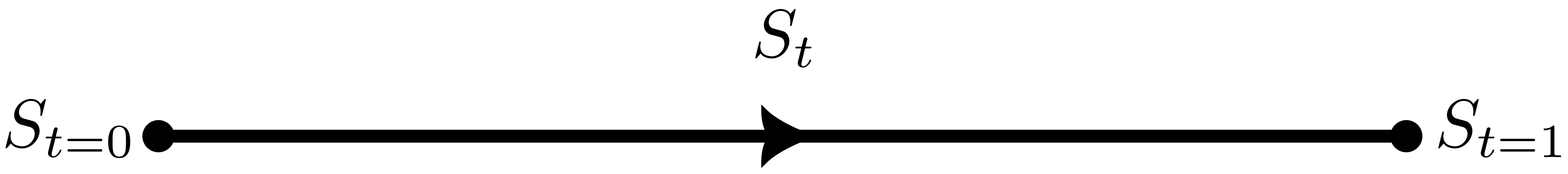

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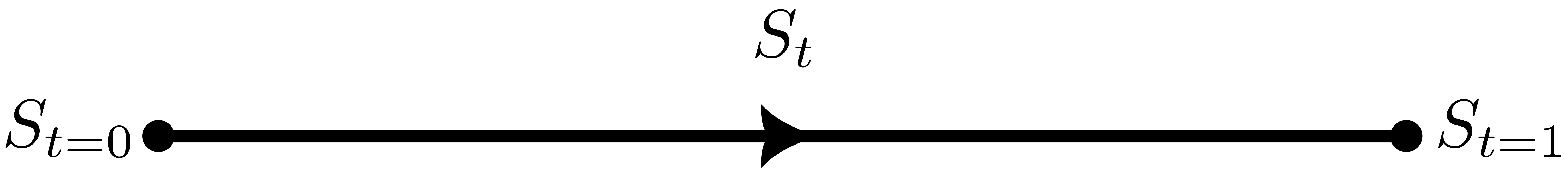

Analytically set (unnormalised) action path

e.g. $\hat{S}_t(\phi) = \frac{1}{2}\phi^T \Sigma^{-1} \phi + t\frac{\lambda}{4}\sum_{i\in\mathcal{D}} \phi_i^4$

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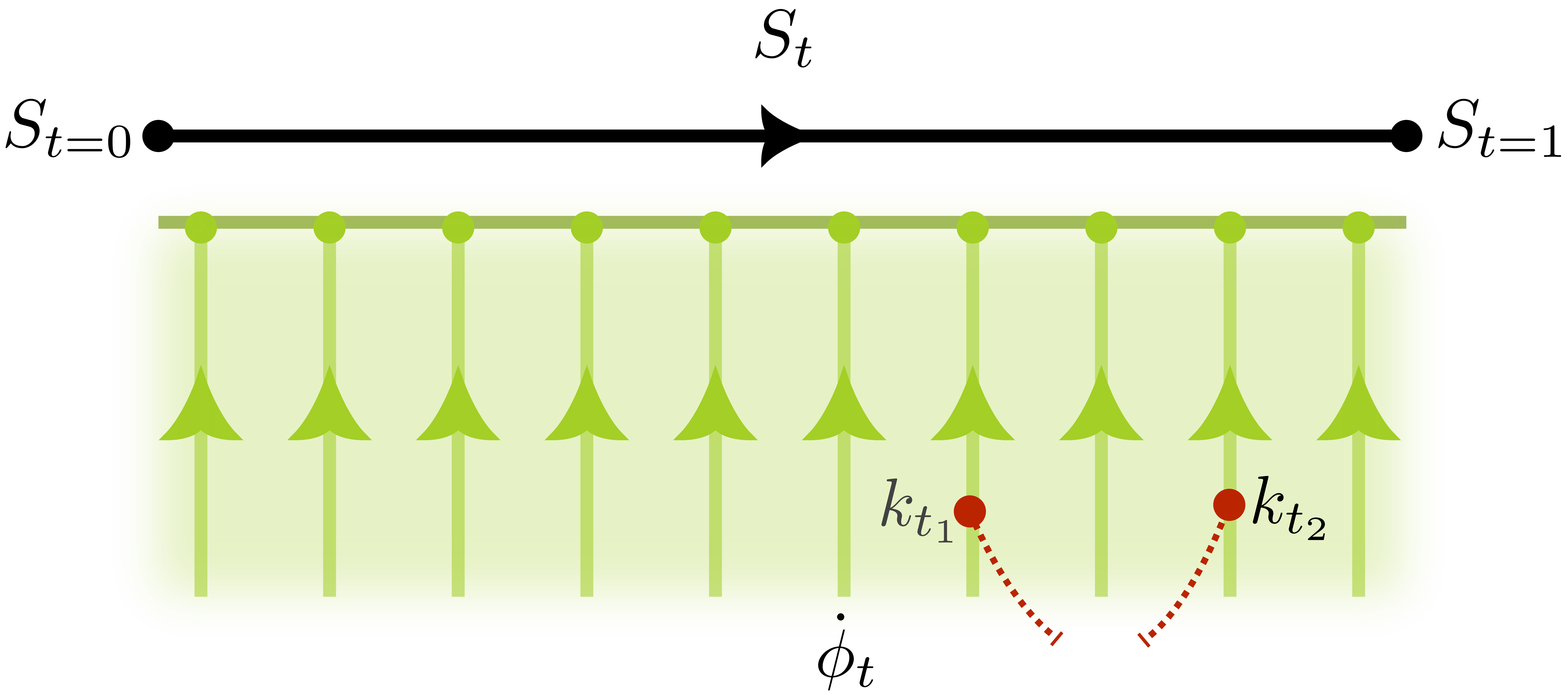

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see also

Liu, Wang, arXiv: 1608.04471
Lawrence, Yamauchi, PRD 103(114509), 2021.
Bonanno, Bulgarelli, Cellini et al., arXiv:2601.20708
Albergo, Boffi, Vanden-Eijnden, arXiv:2303.08797
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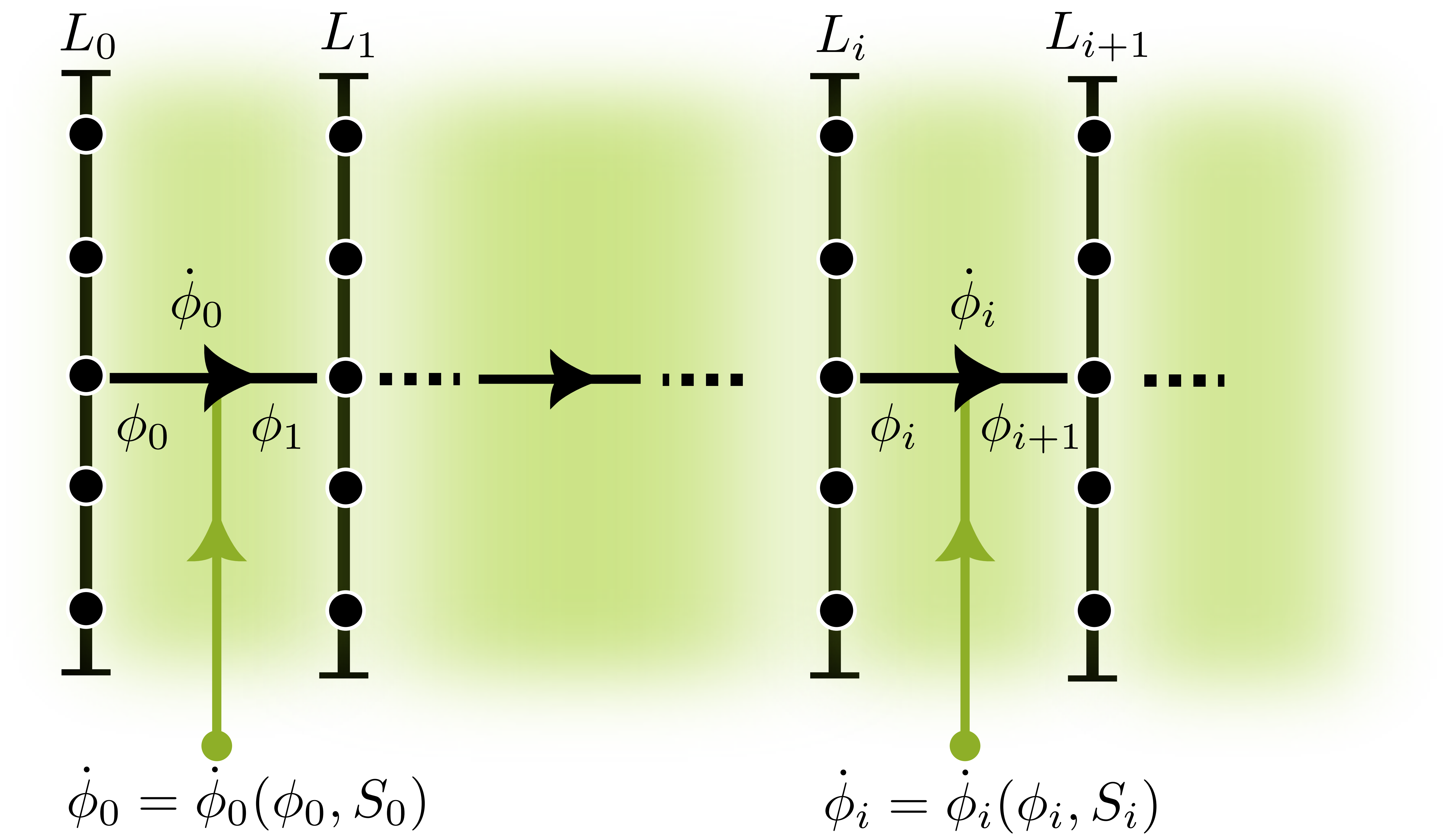

Dissecting: Measure transport now translated into independent sub-problems.

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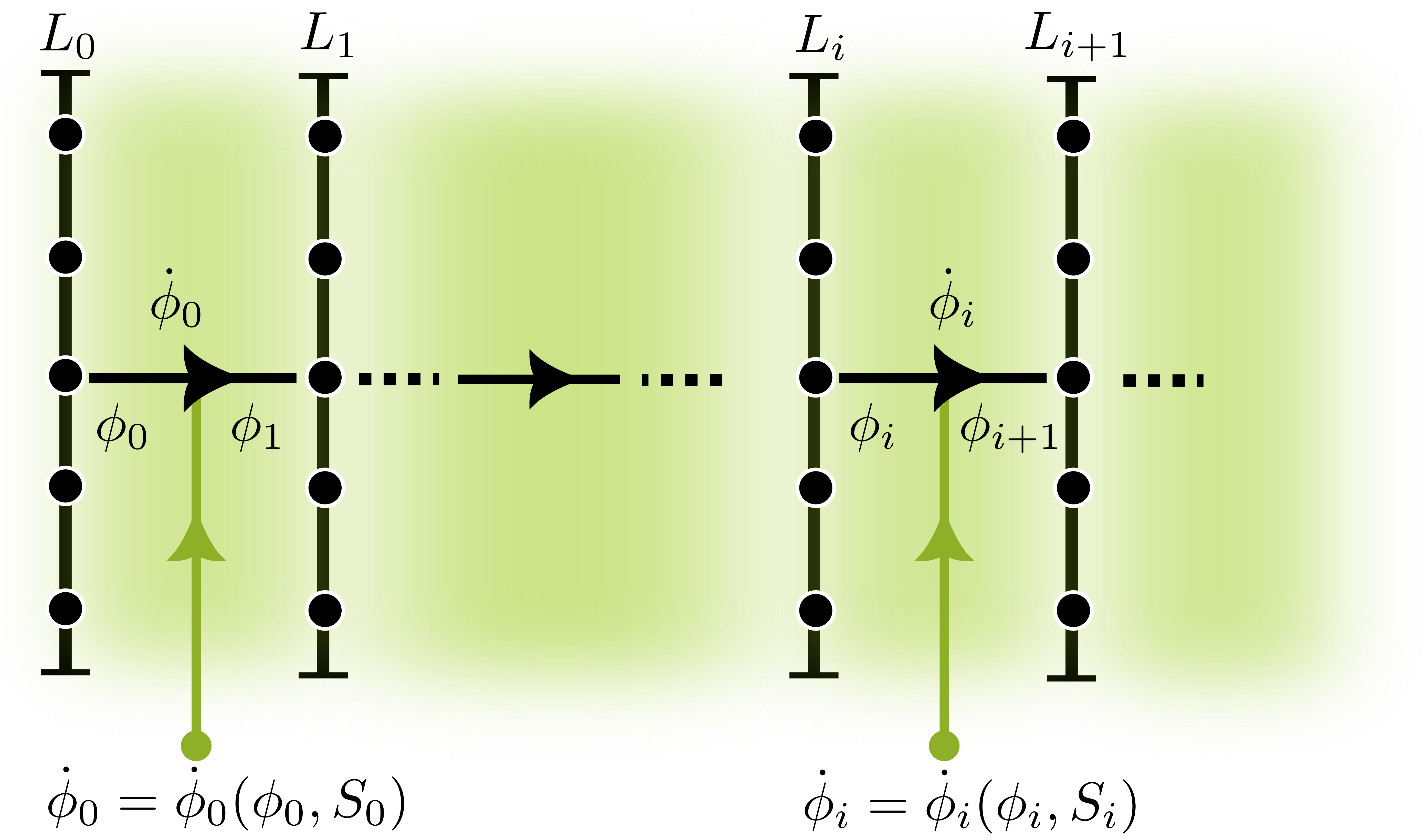

Dissecting: Measure transport now translated into independent sub-problems.

Kind of problem: Each sub-problem does not require the notion of a *statistical divergence* but boils down to a *linear high-dimensional PDE.*

PIKfolds: An instructive example

$$\hat{S}_t(\phi) = \frac{1}{2}m_t^2\phi^2 + \frac{1}{4}\lambda_t\phi^4$$

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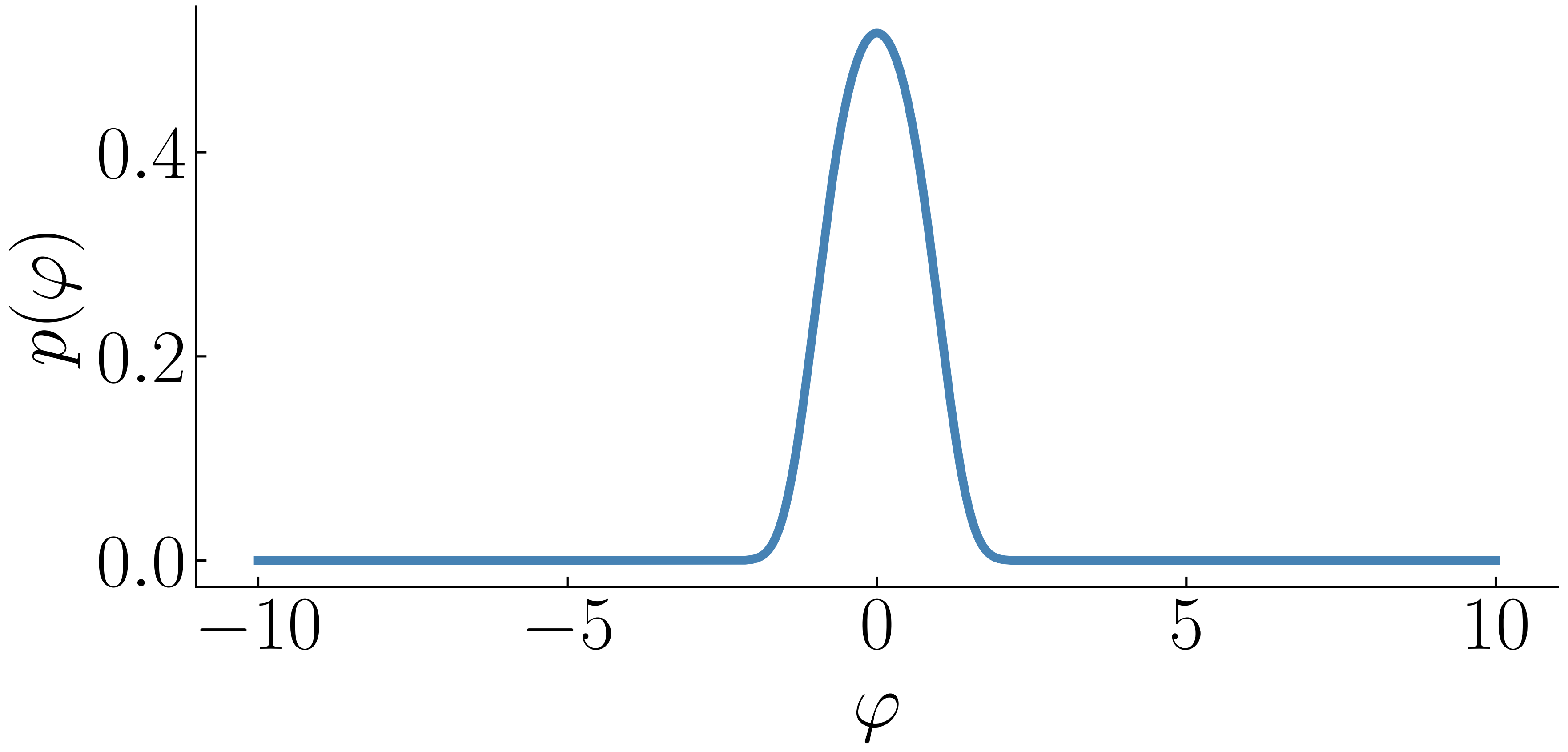

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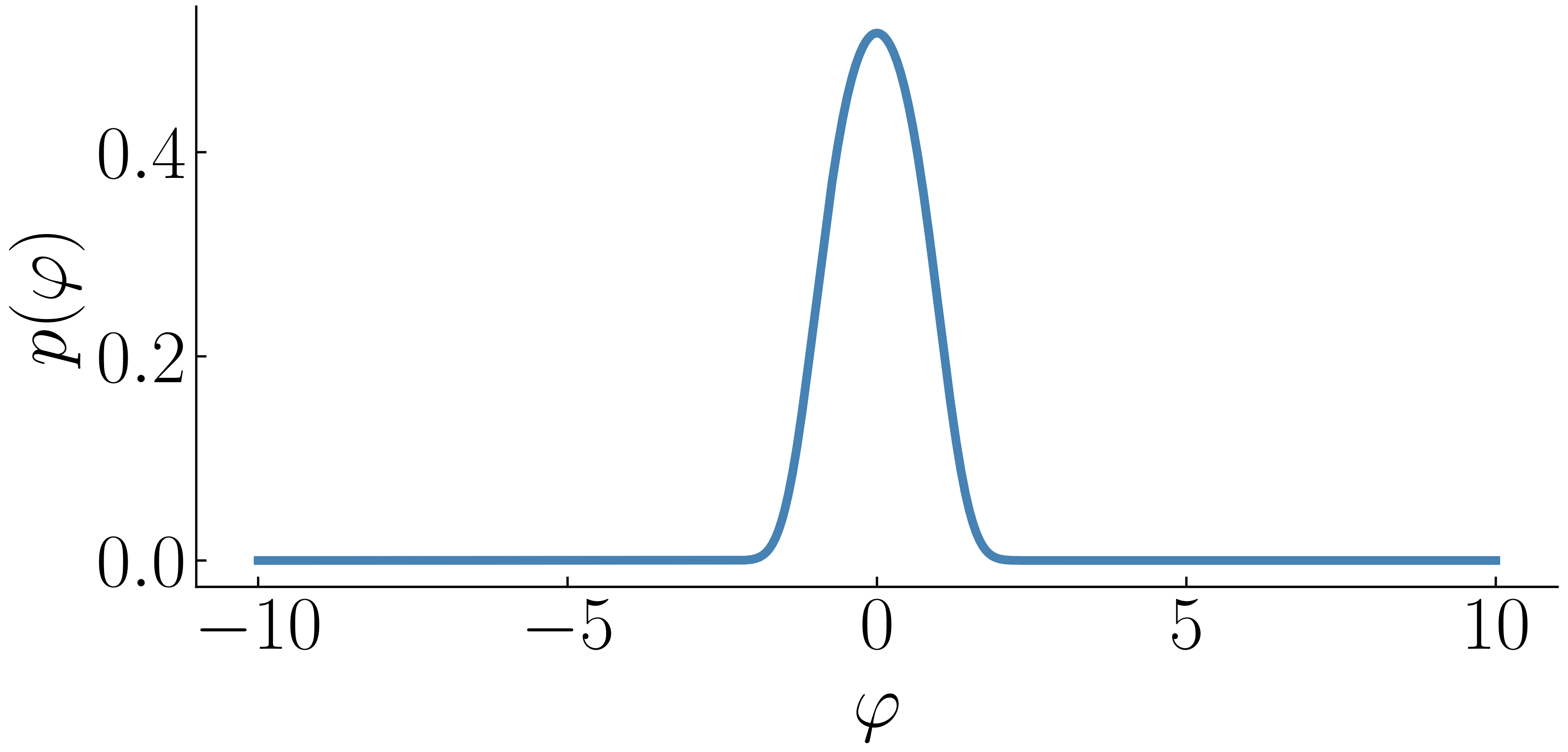
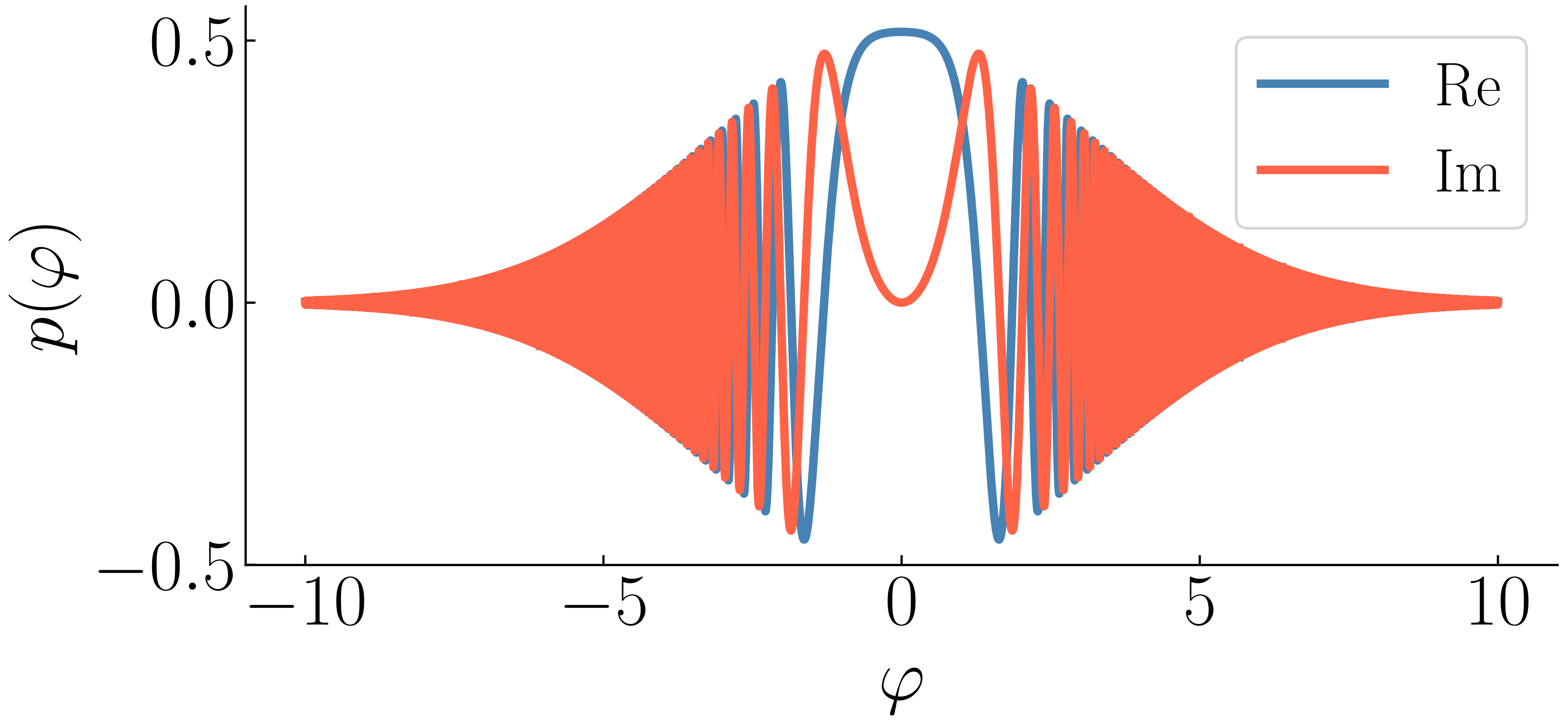
e^{-S} $S_0(\phi_0)$

$S_1(\phi_1)$ e^{iS}





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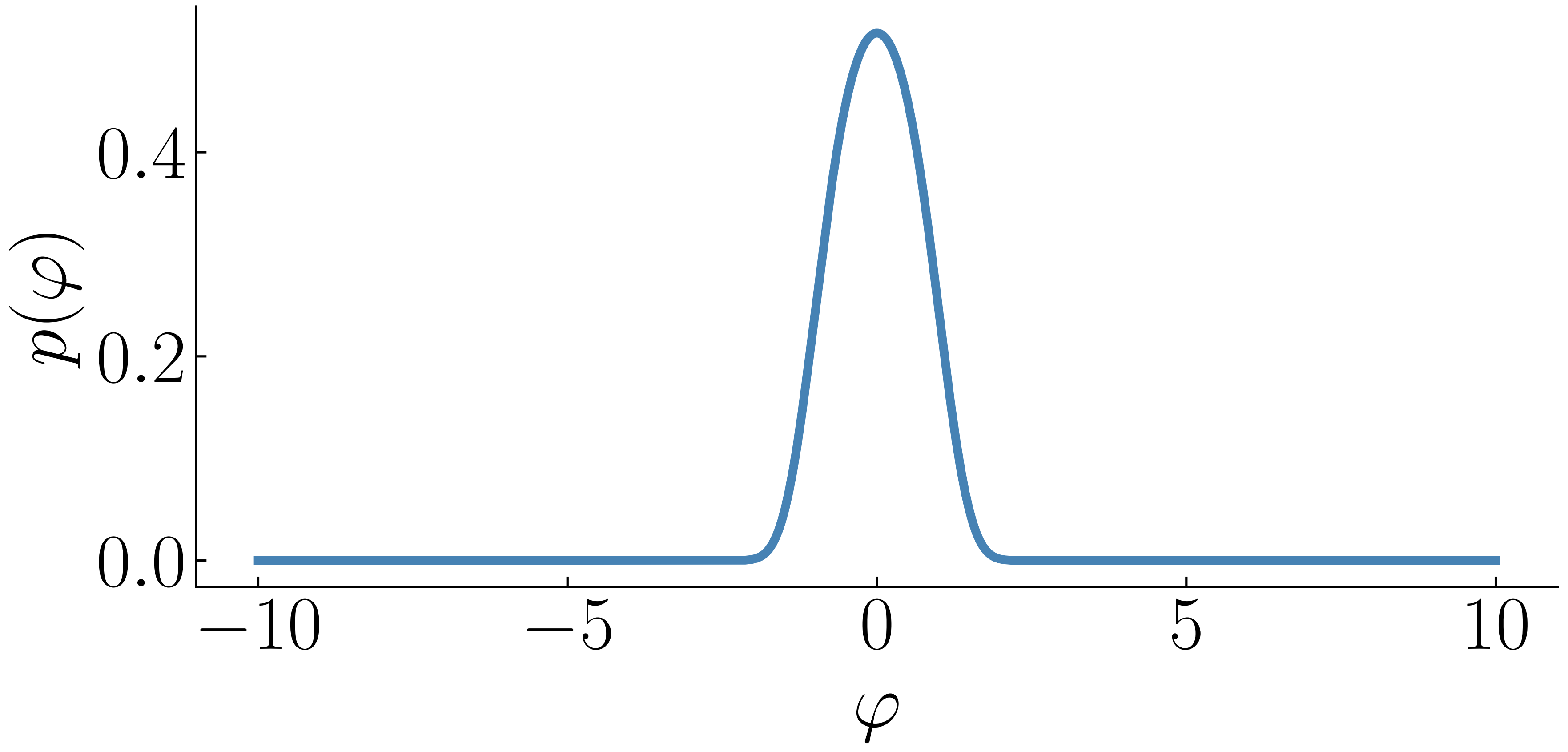

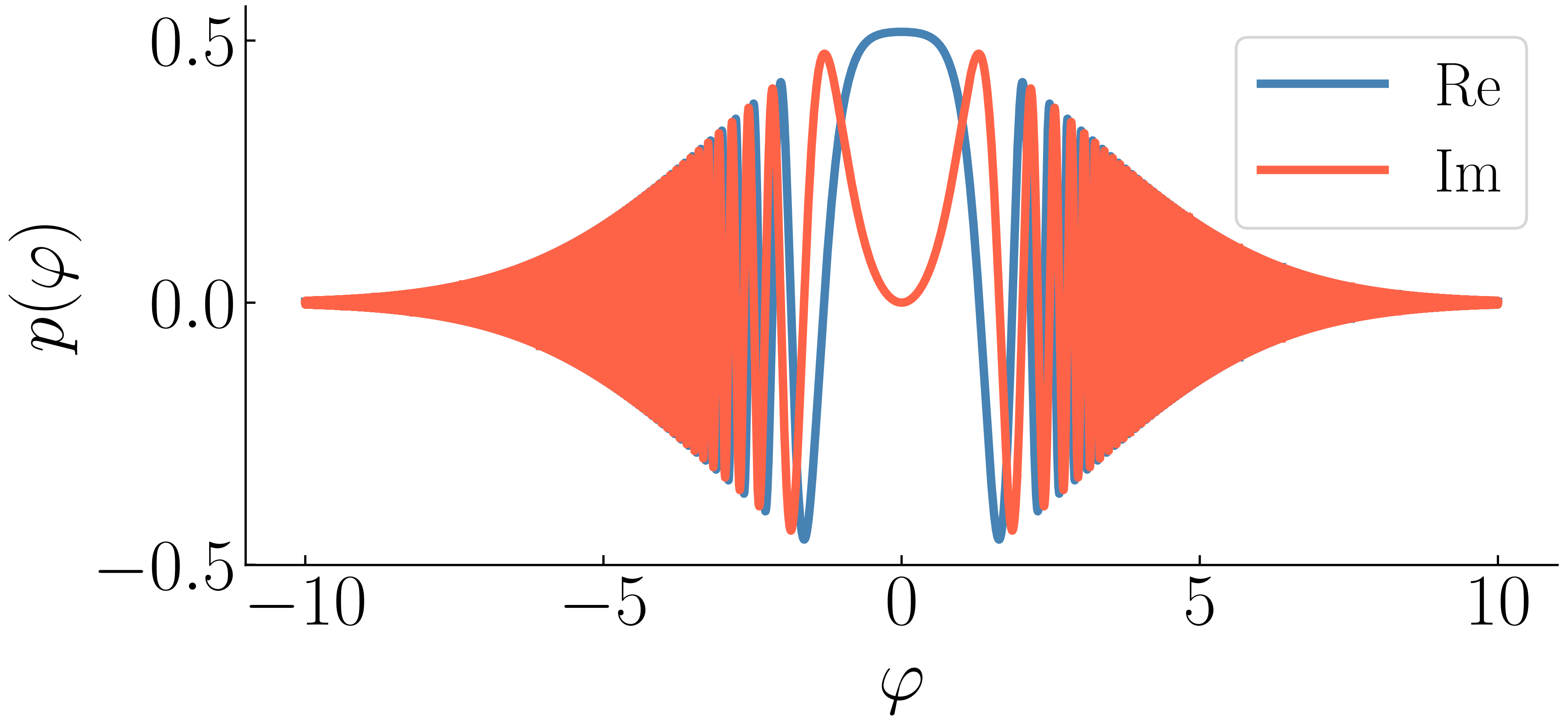

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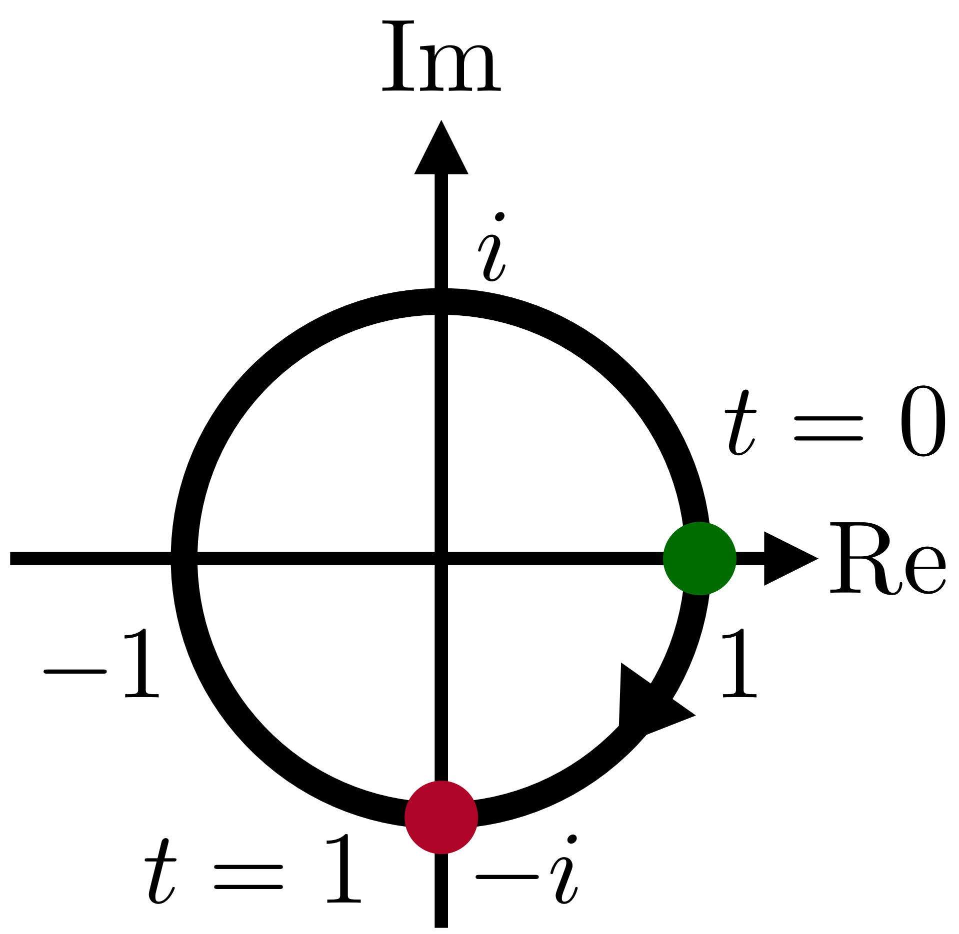

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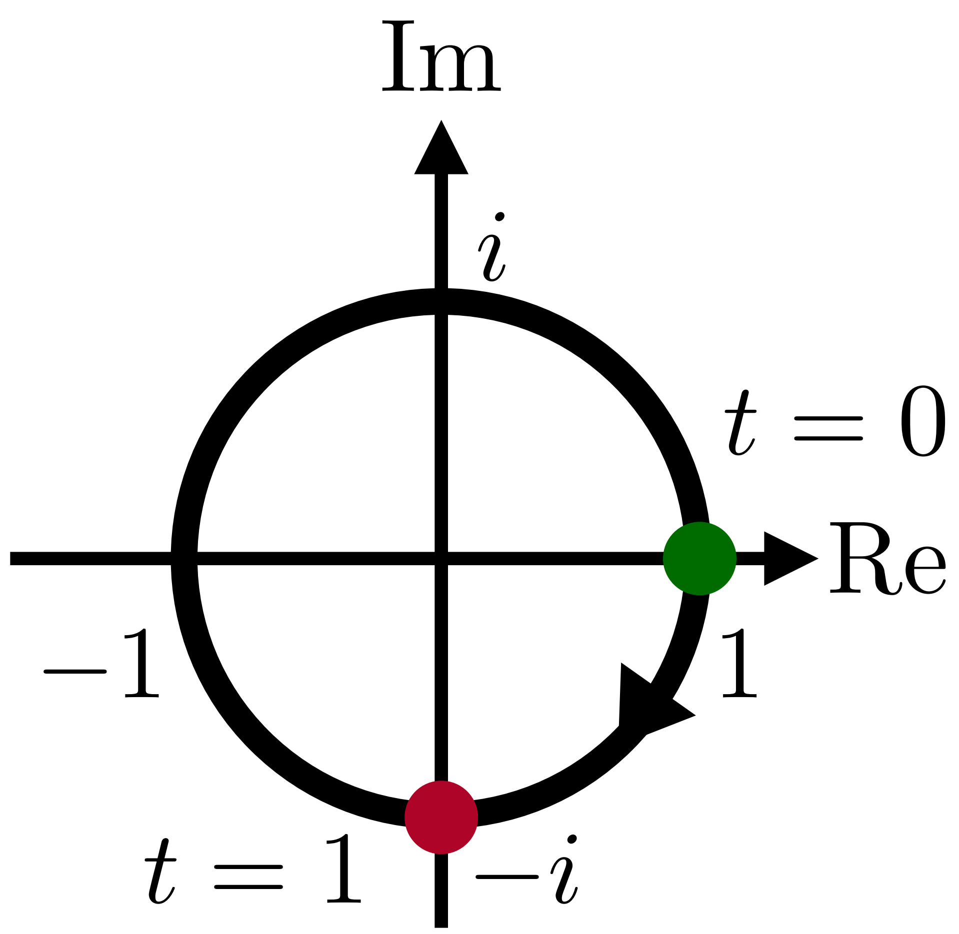

Change in the couplings

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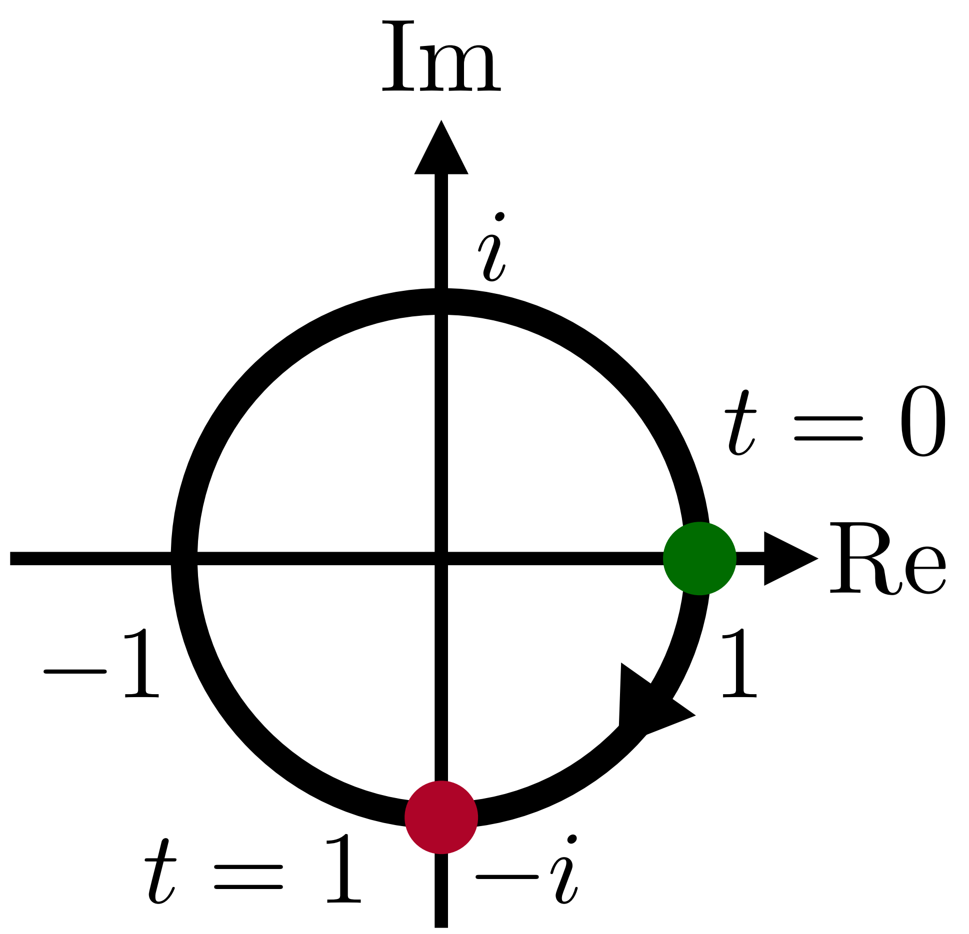

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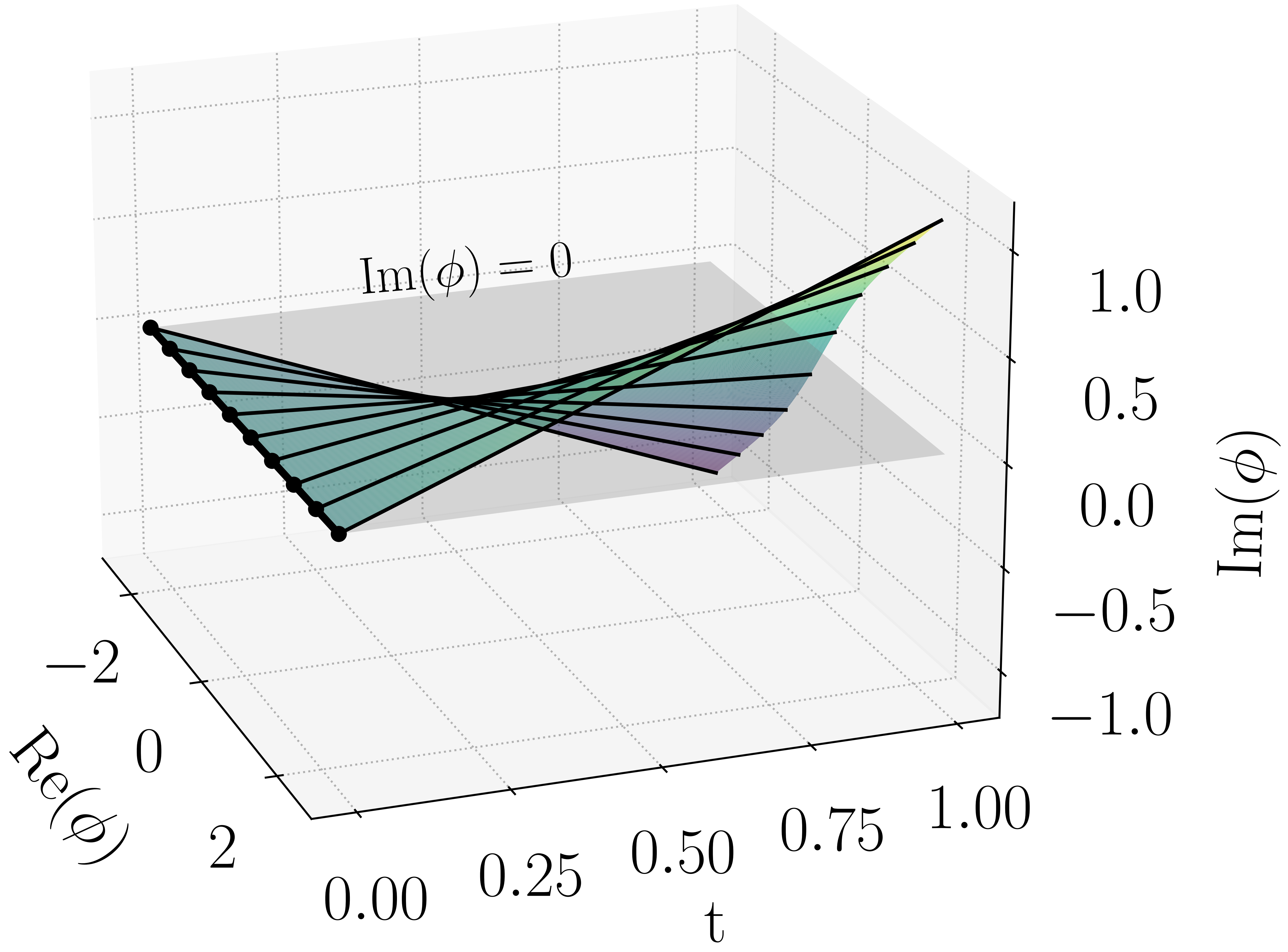

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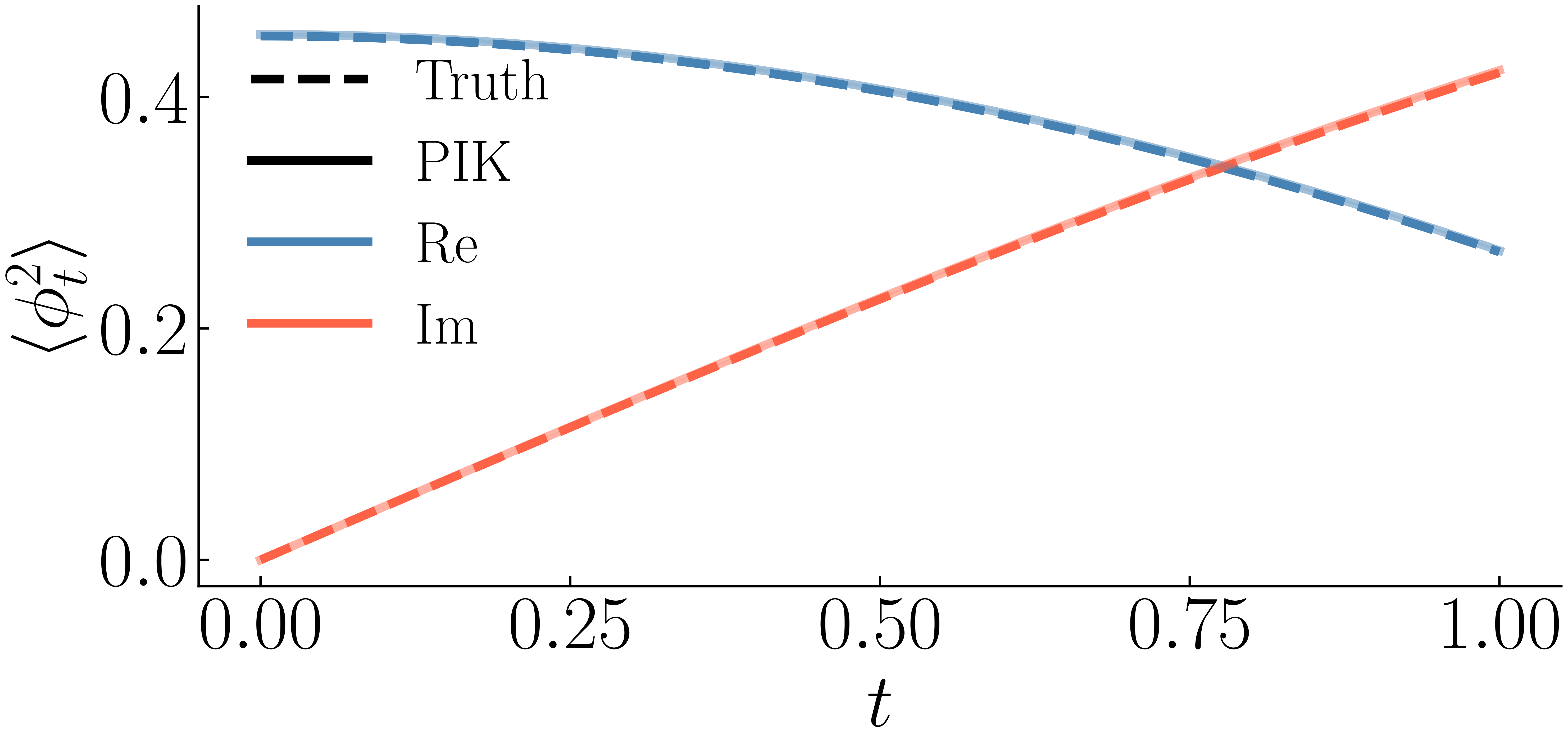

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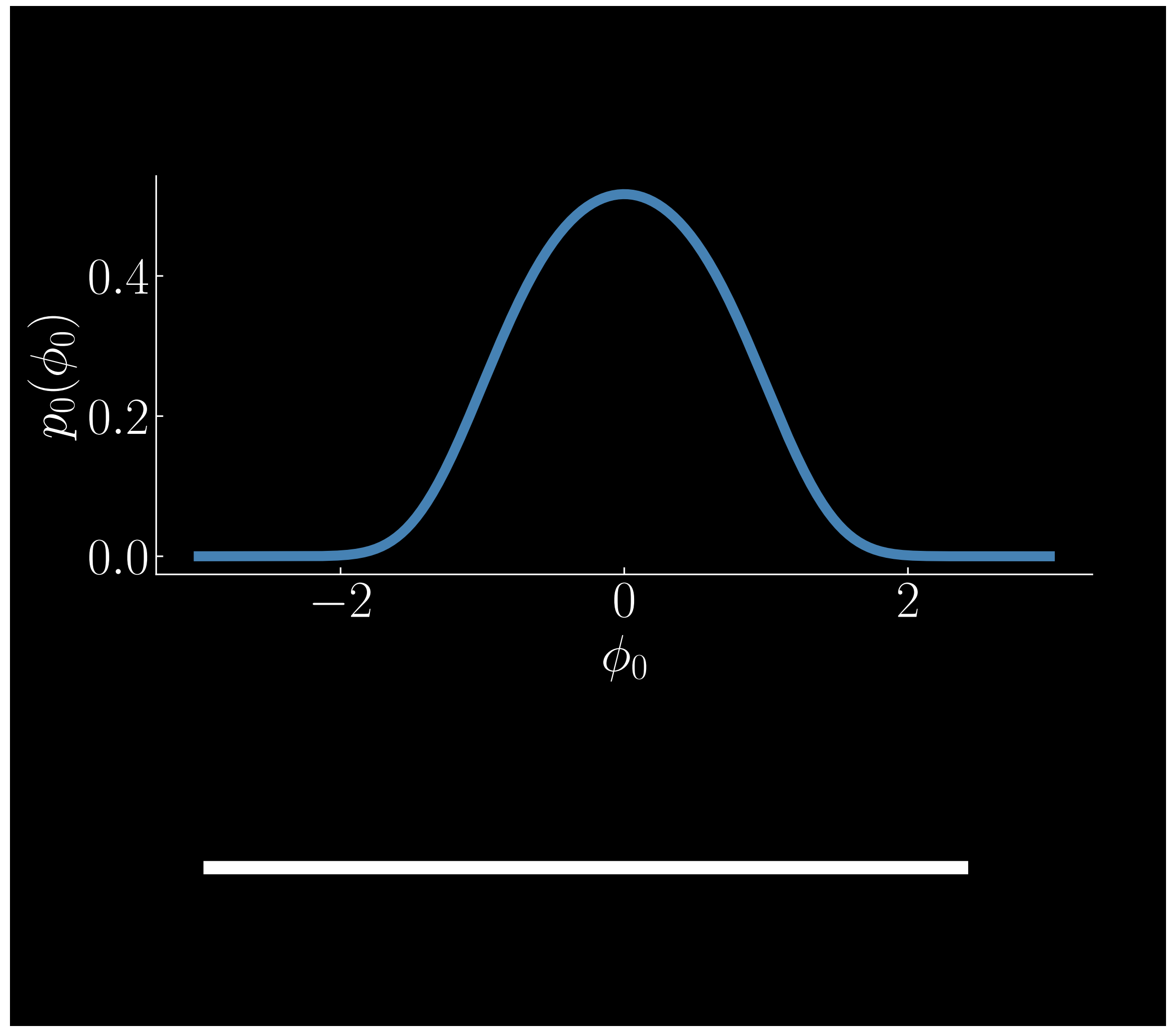

$$(p_0, \mathcal{M}_0)$$

Typically

$$p_0(\phi_0) \in \mathbb{R}$$
$$\mathcal{M}_0 = \mathbb{R}^{\mathcal{D}}$$

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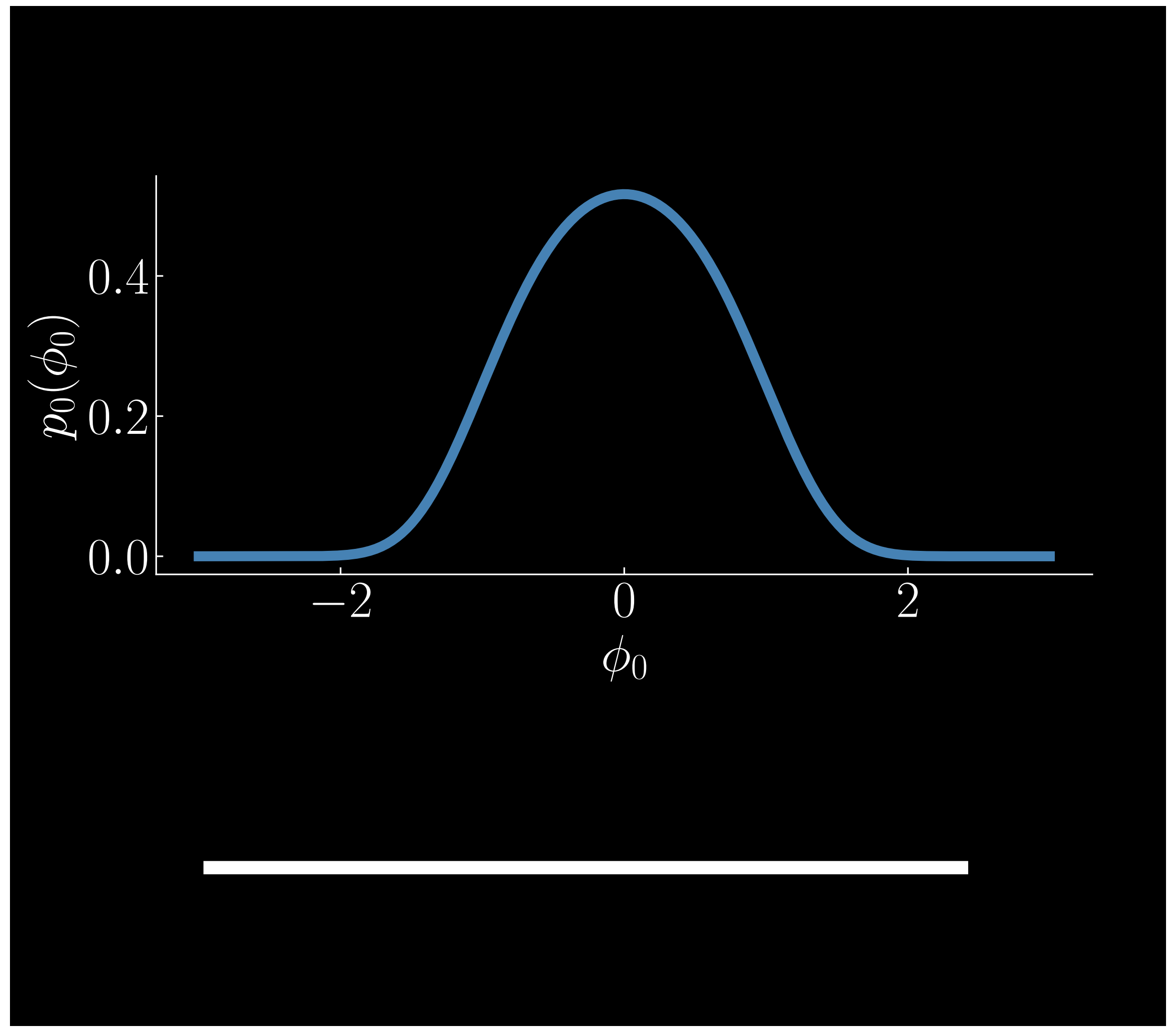

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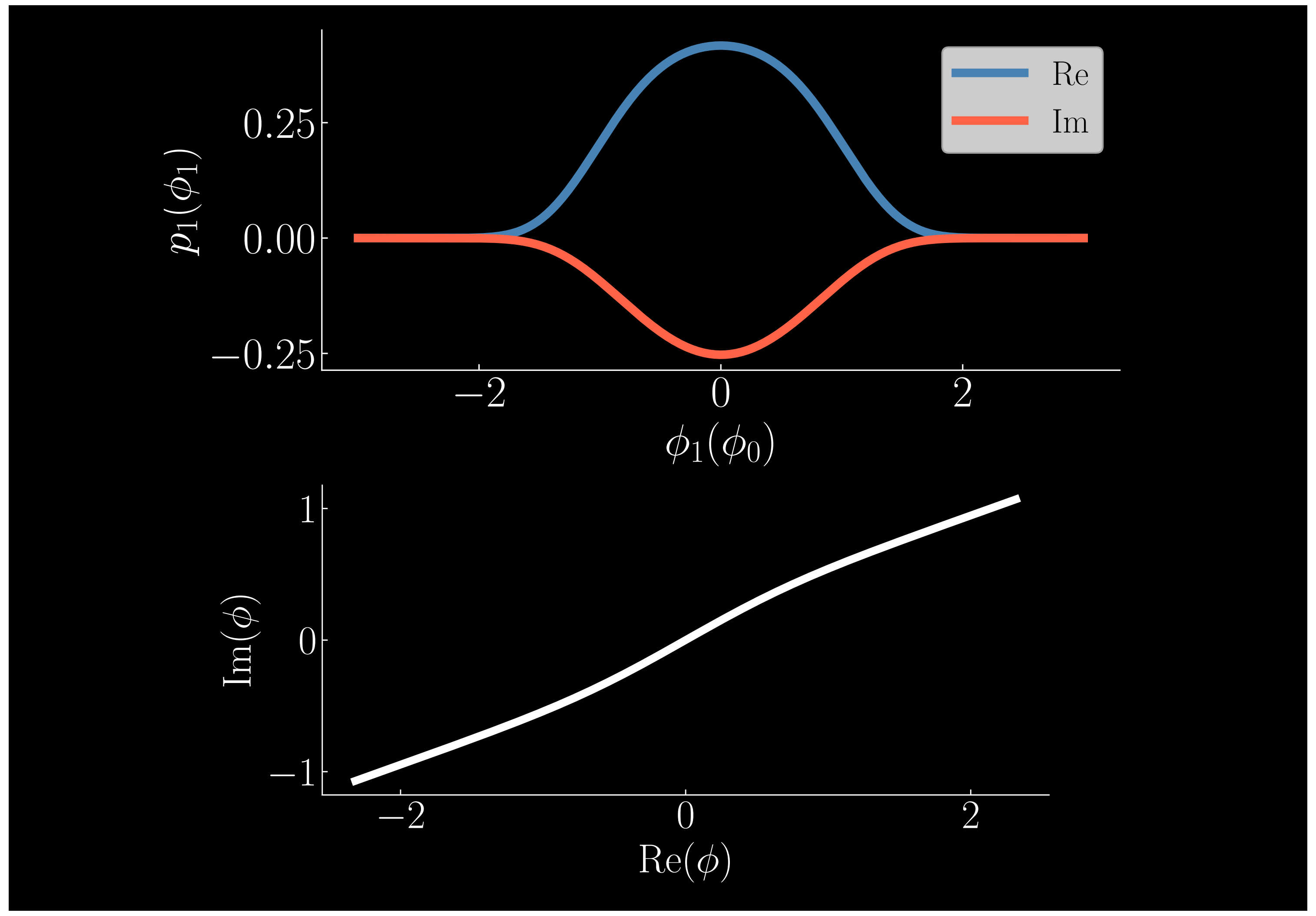


$(p_1, \mathcal{M}_1)$

Typically

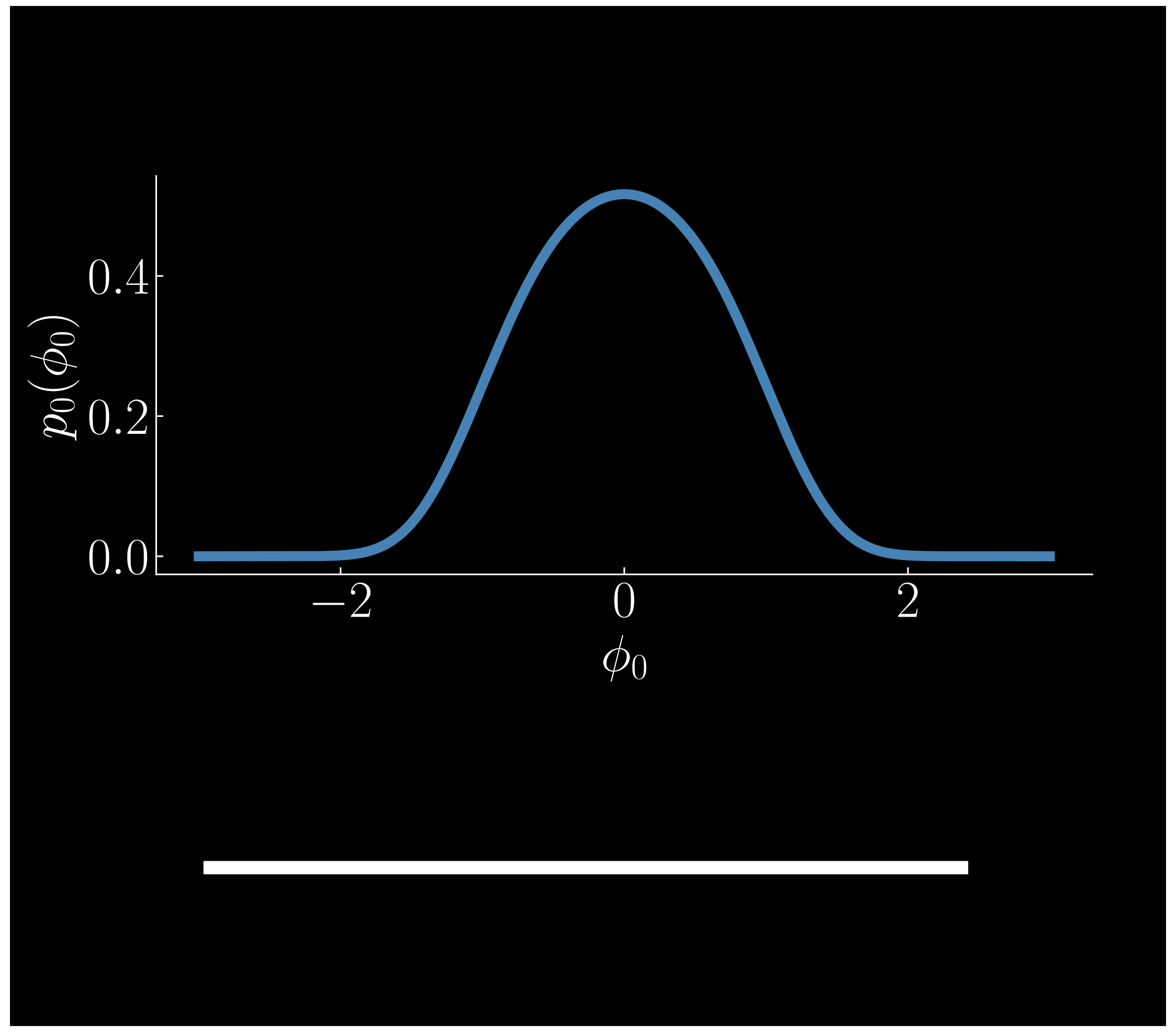
$$p_0(\phi_0) \in \mathbb{R}$$
$$\mathcal{M}_0 = \mathbb{R}^{\mathcal{D}}$$

$$p_1 = p$$
$$\mathcal{M} \subset \mathbb{C}^{\mathcal{D}}$$

PIKfolds: Taming the Sign Problem

$$\frac{d\phi_t}{dt} = \dot{\phi}_t(\phi) \qquad \frac{dS_t(\phi)}{dt} = \left[\frac{\partial}{\partial \phi_i} - \frac{\partial S_t(\phi)}{\partial \phi_i}\right] \dot{\phi}_{t,i}(\phi)$$

$(p_t, \mathcal{M}_t)$

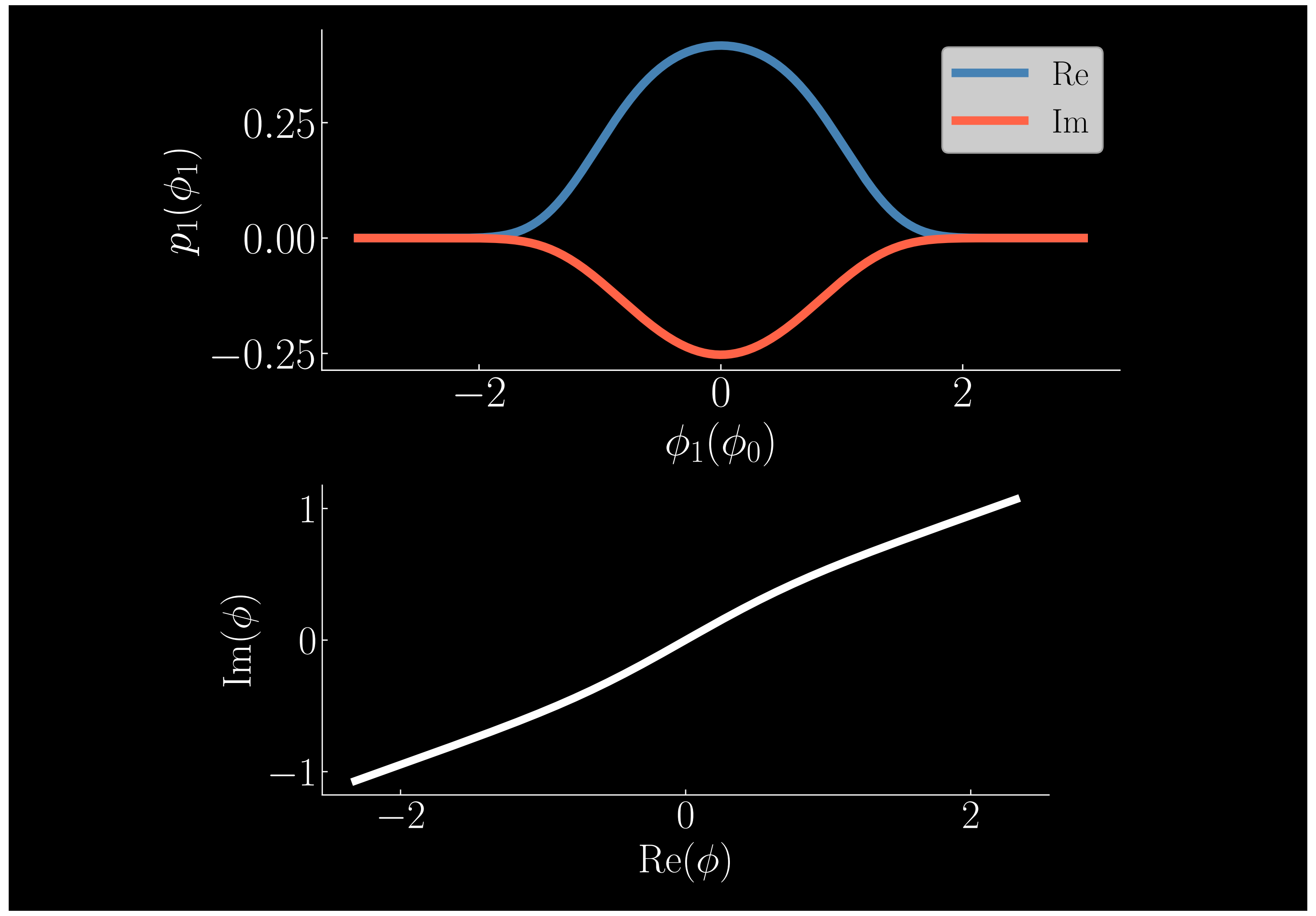


$(p_0, \mathcal{M}_0)$

Typically

$p_0(\phi_0) \in \mathbb{R}$

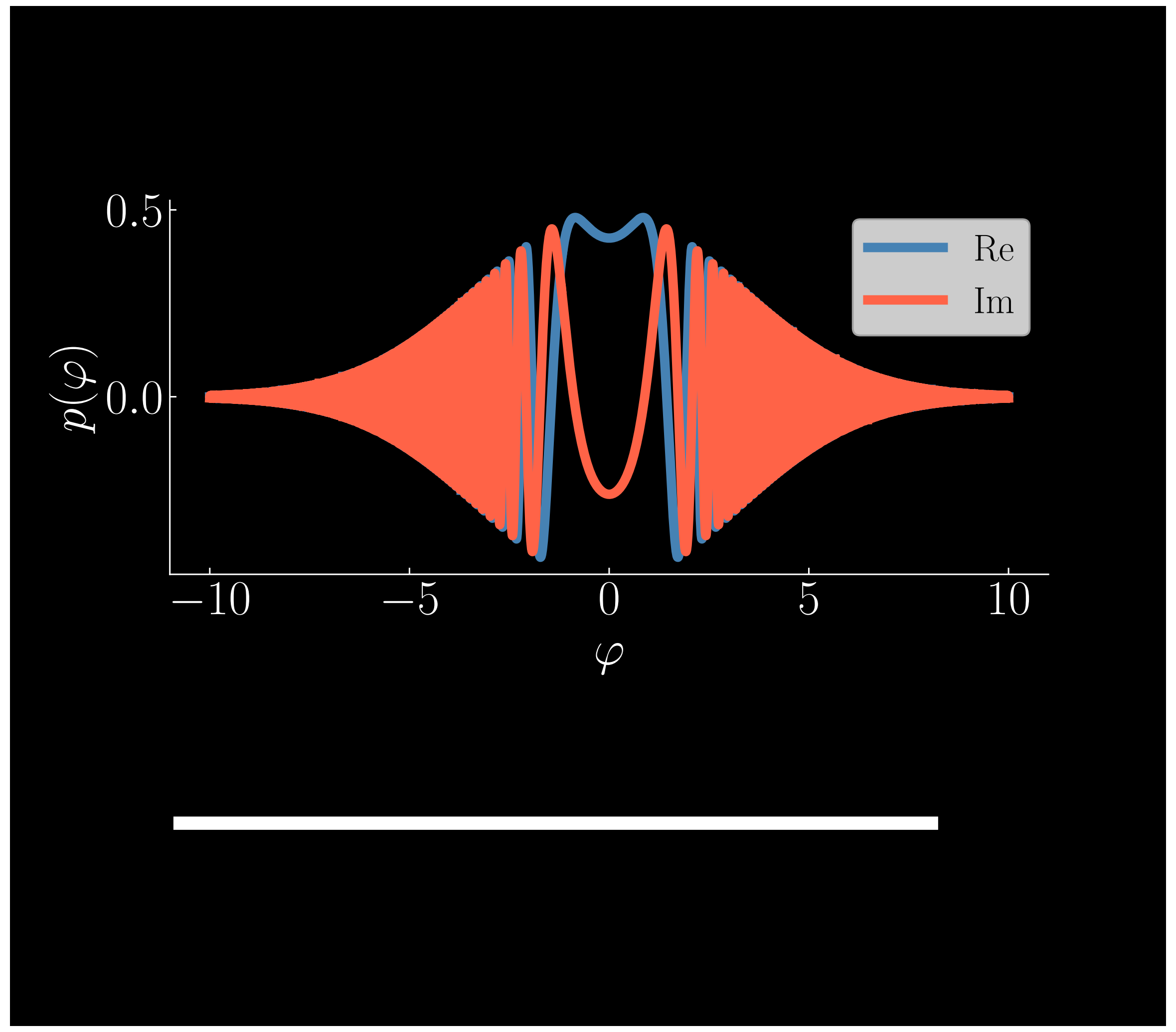
$\mathcal{M}_0 = \mathbb{R}^{\mathcal{D}}$



$(p_1, \mathcal{M}_1)$

$p_1 = p$

$\mathcal{M} \subset \mathbb{C}^{\mathcal{D}}$



$(p, \mathcal{M})$

Typically

$p(\varphi) \in \mathbb{C}$

$\mathcal{M} = \mathbb{R}^{\mathcal{D}}$

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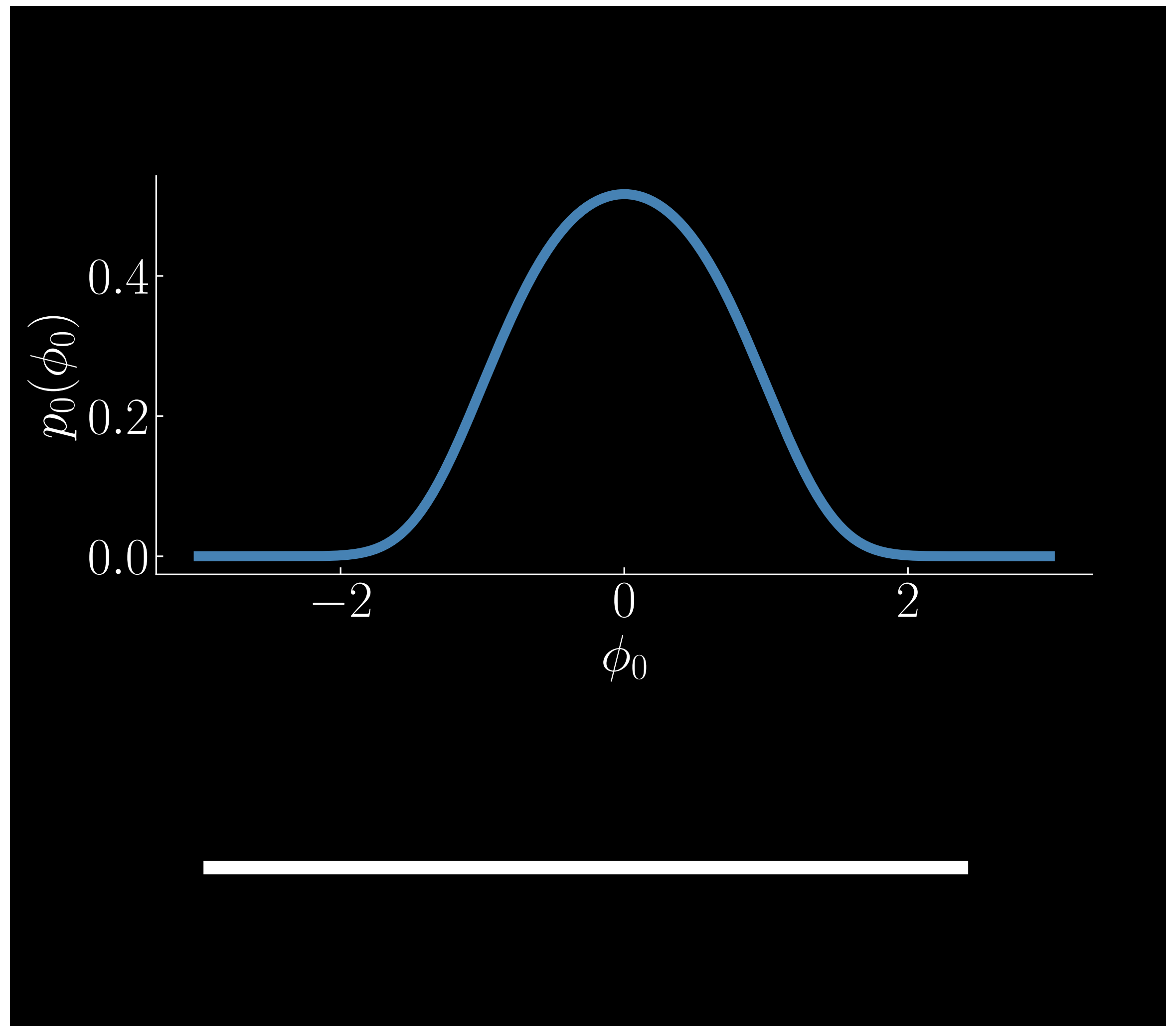

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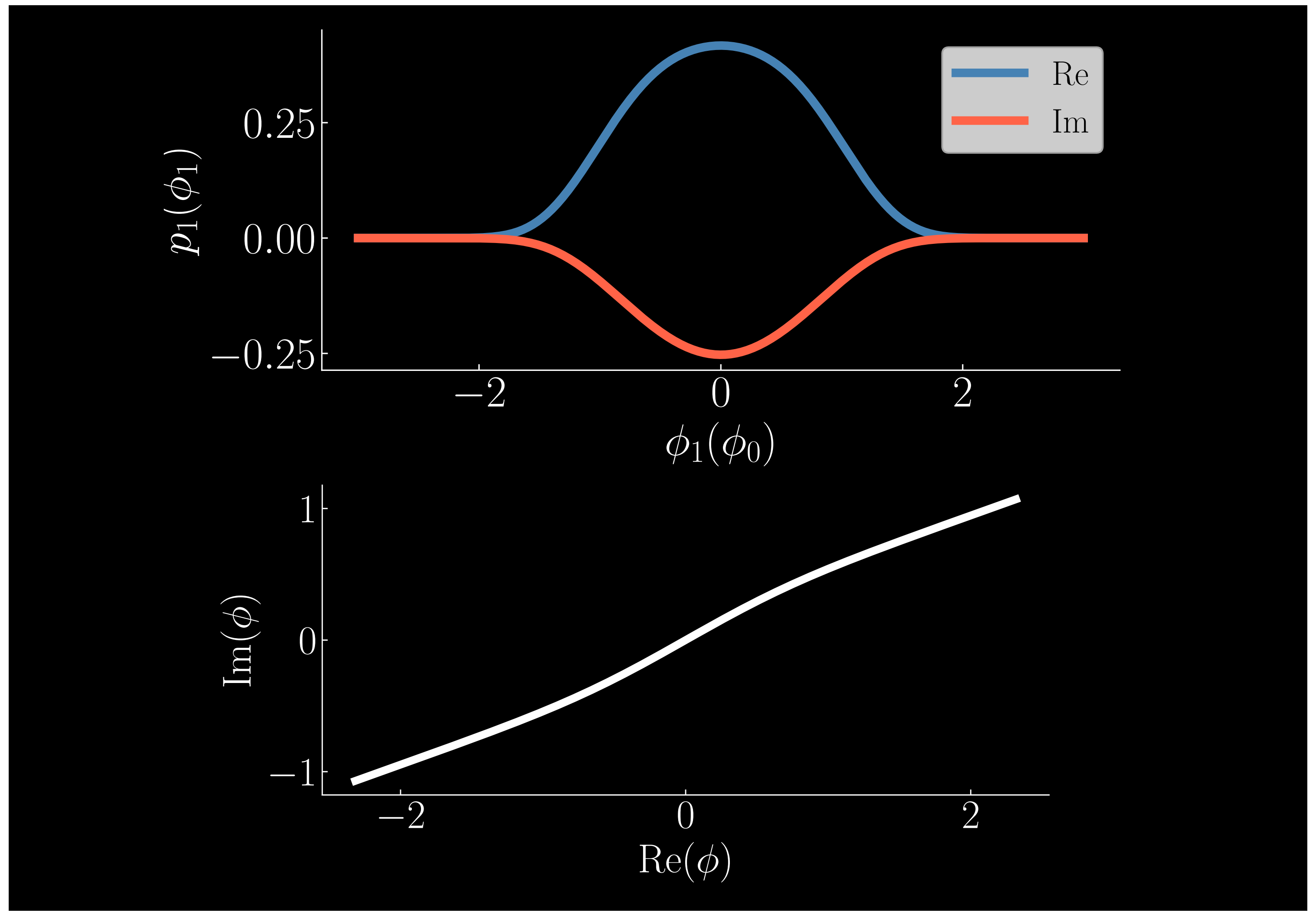

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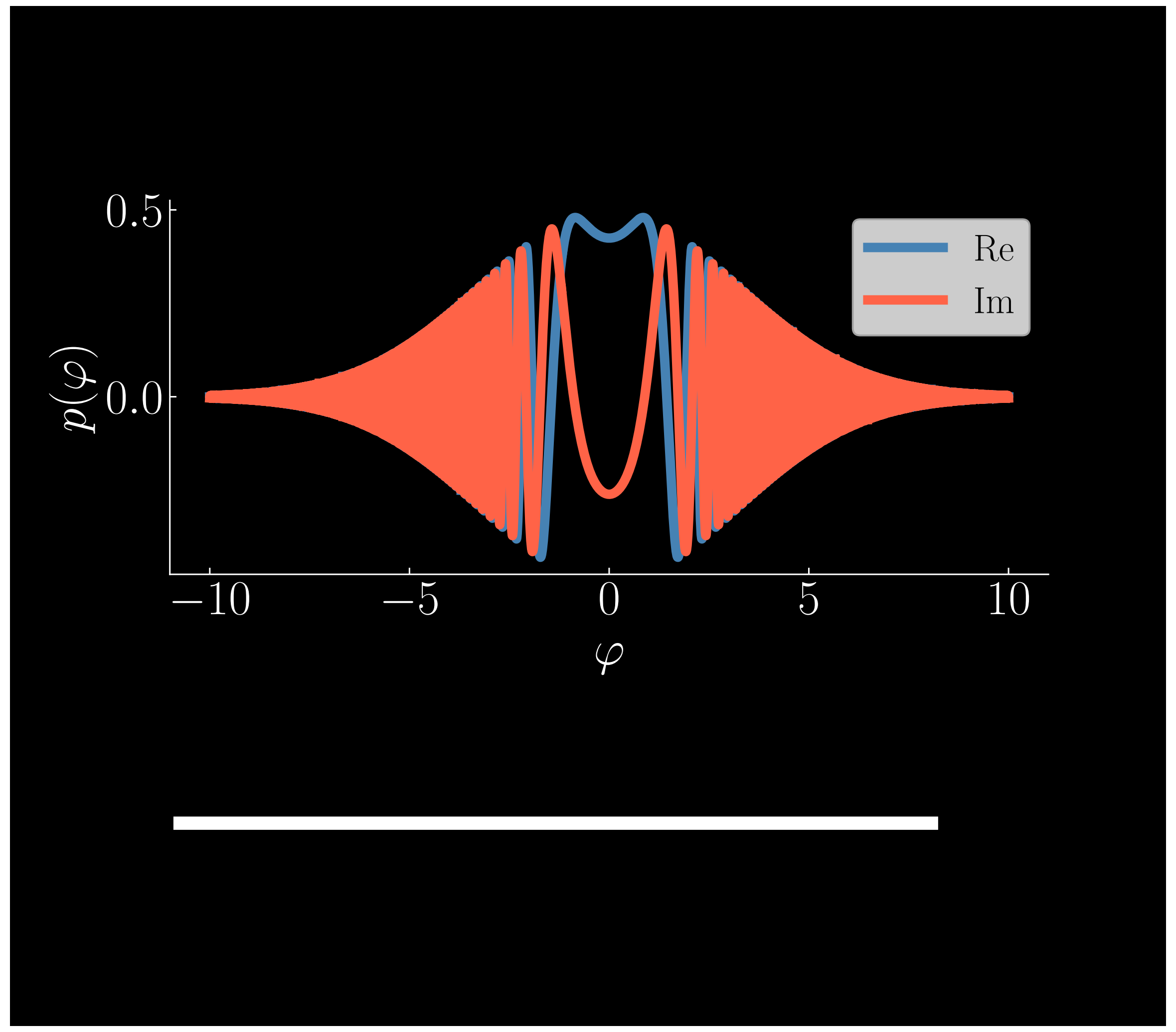

$(p, \mathcal{M})$

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Typically
$p(\varphi) \in \mathbb{C}$
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$$\int_{\mathcal{M}_0} d\mu_0\, p_0(\phi)\mathcal{O}(\,\phi_1(\phi)\,) \overset{\textbf{PIK}}{=} \int_{\mathcal{M}_1} d\mu_1\, p_1(\phi)\mathcal{O}(\phi) \overset{\textbf{Cauchy}}{=} \int_{\mathcal{M}} d\mu\, p(\varphi)\mathcal{O}(\varphi) = \langle \mathcal{O} \rangle$$

PIKfolds: Weight-preserving flows

$$P_t(\mathcal{T}_t) = \int_{\mathcal{T}_t} d\mu_t \, p_t(\phi)$$

For a subset $\mathcal{T}_t \subset \mathcal{M}_t$

$$\frac{dP_t(\mathcal{T}_t)}{dt} = 0$$

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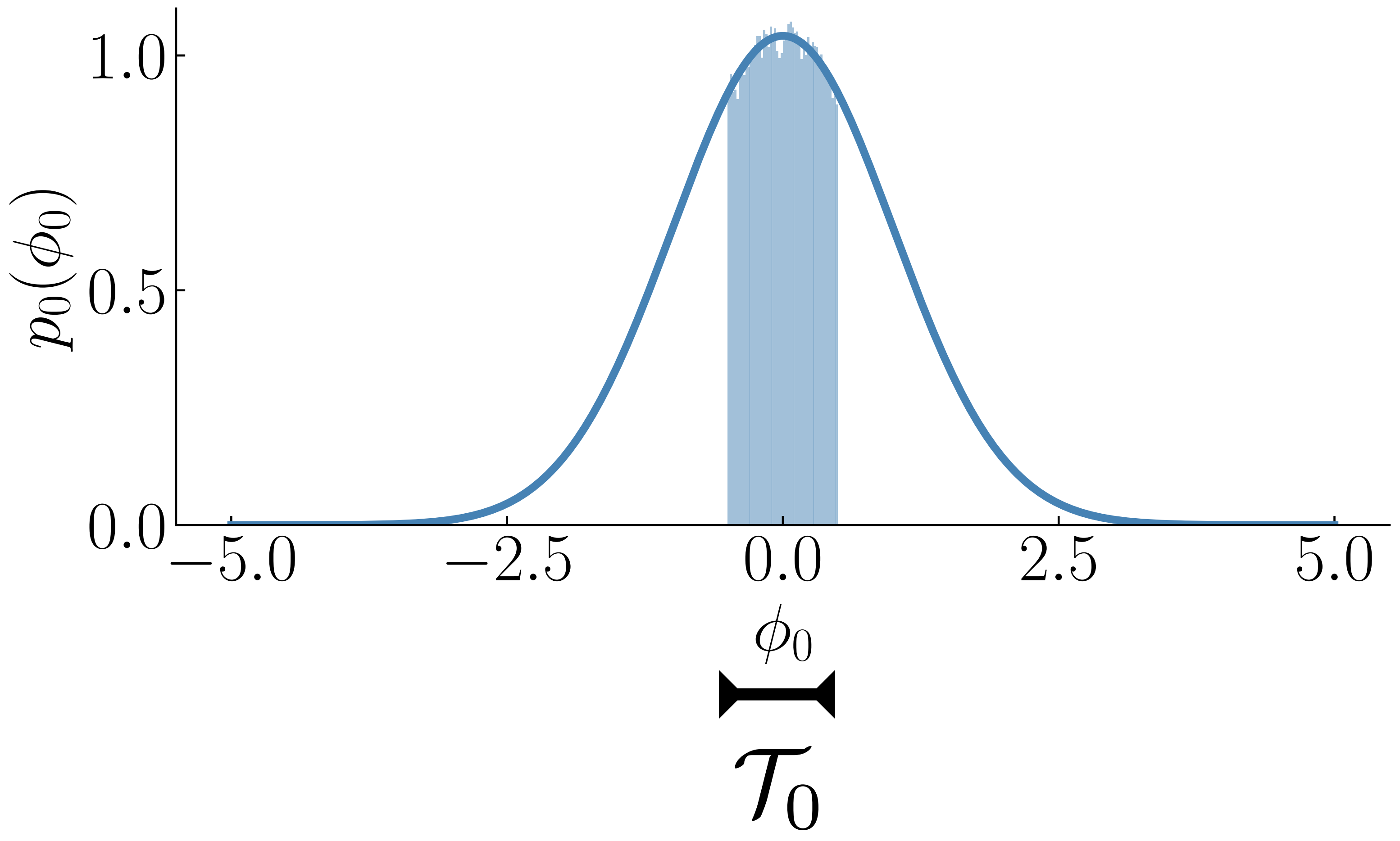

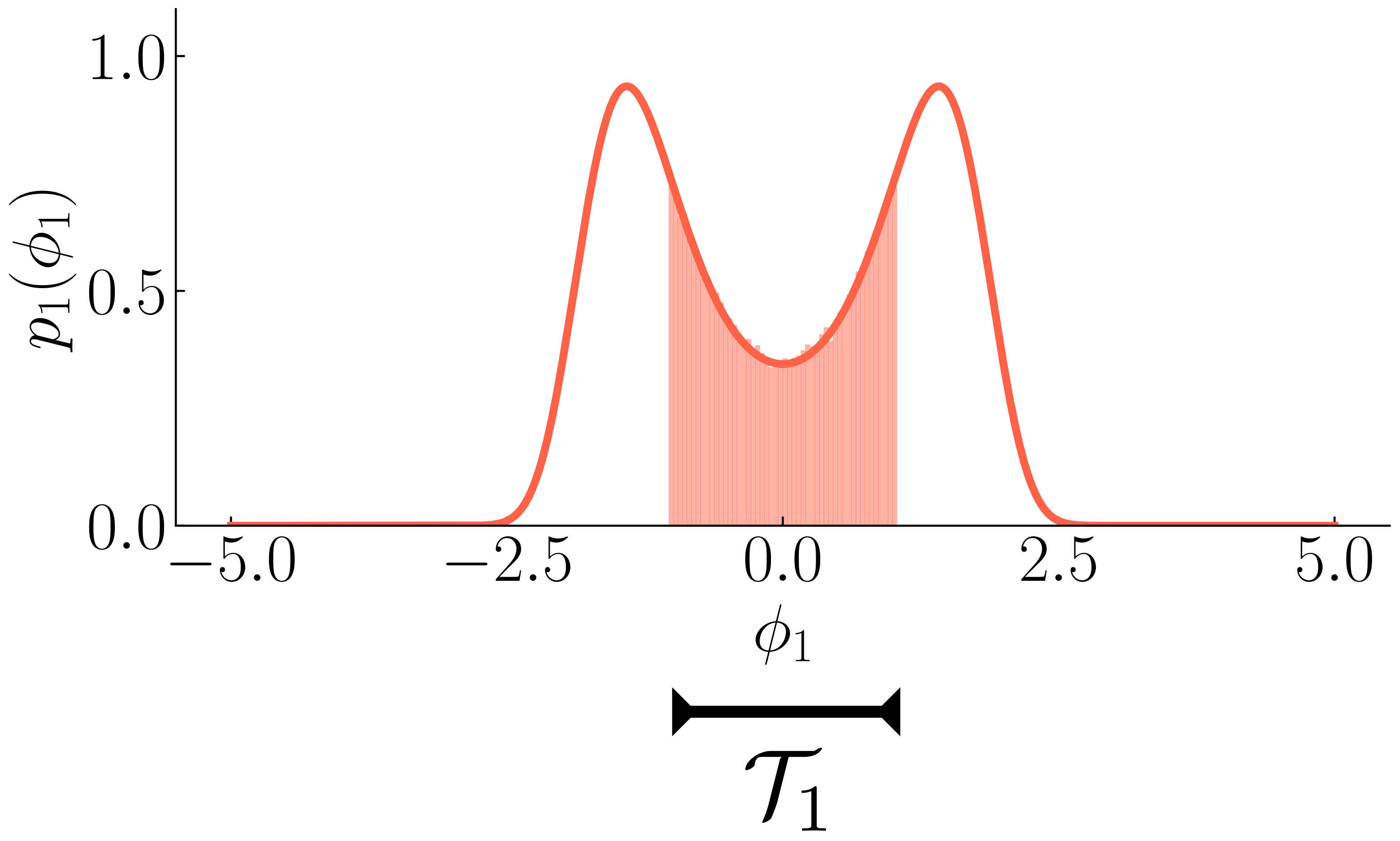

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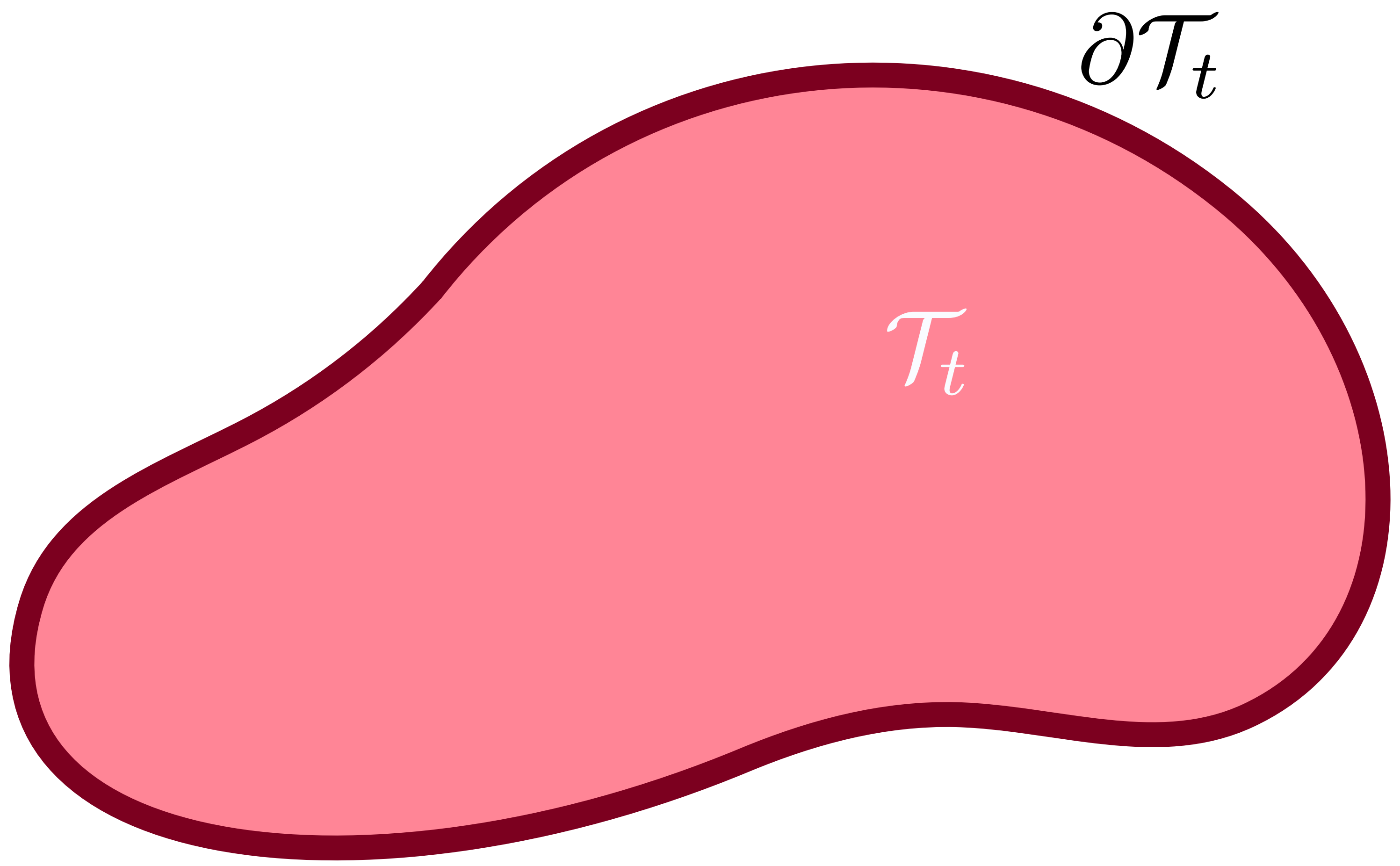

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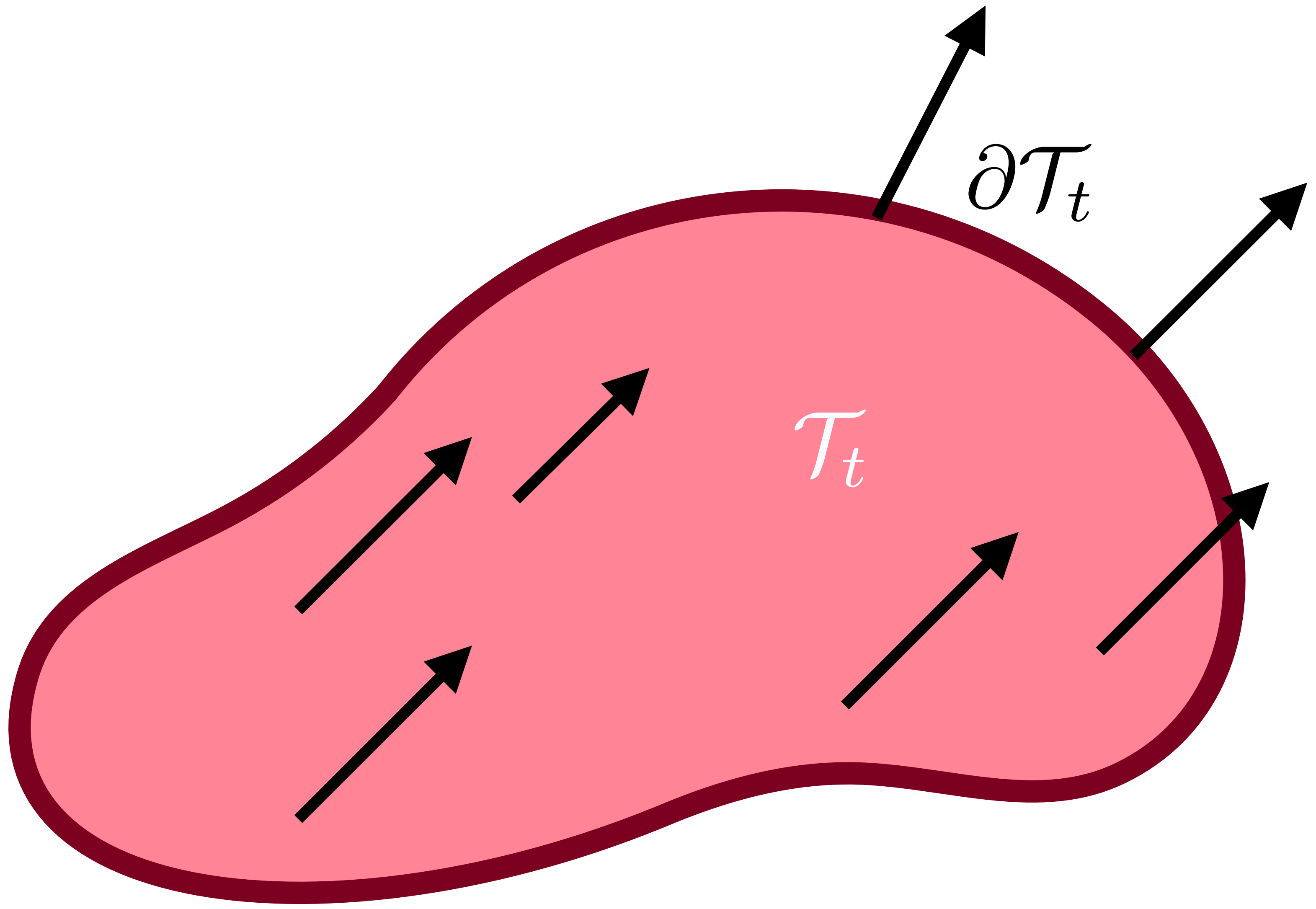

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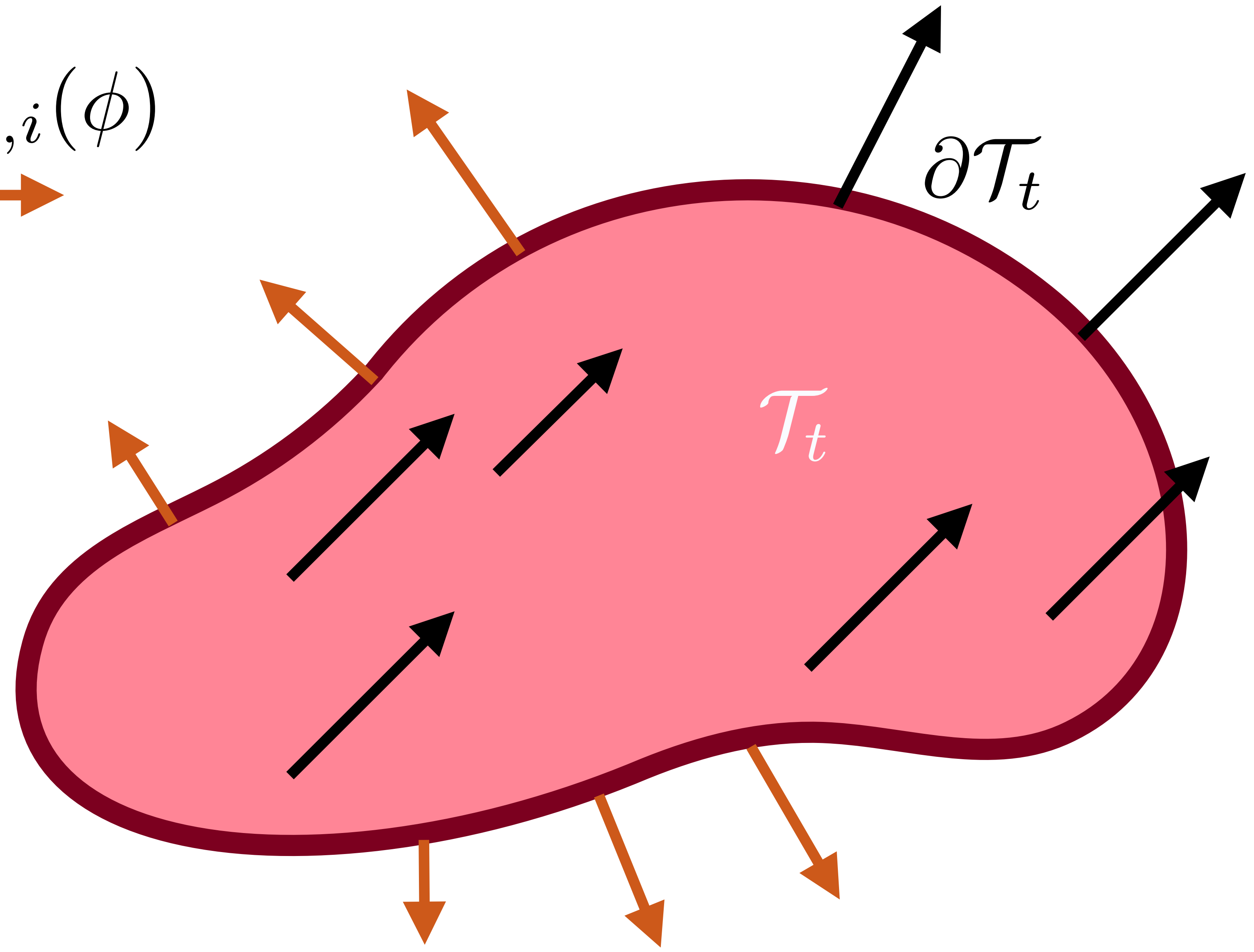
$$= \int_{\partial \mathcal{T}_t} d\mathcal{S}_i(\phi) \left[\sigma_{t,i}(\phi) - \dot{\phi}_{t,i}(\phi)\right] p_t(\phi)$$

$$\sigma_{t,i}(\phi) = \dot{\phi}_{t,i}(\phi) + \Delta\sigma_{t,i}(\phi)$$



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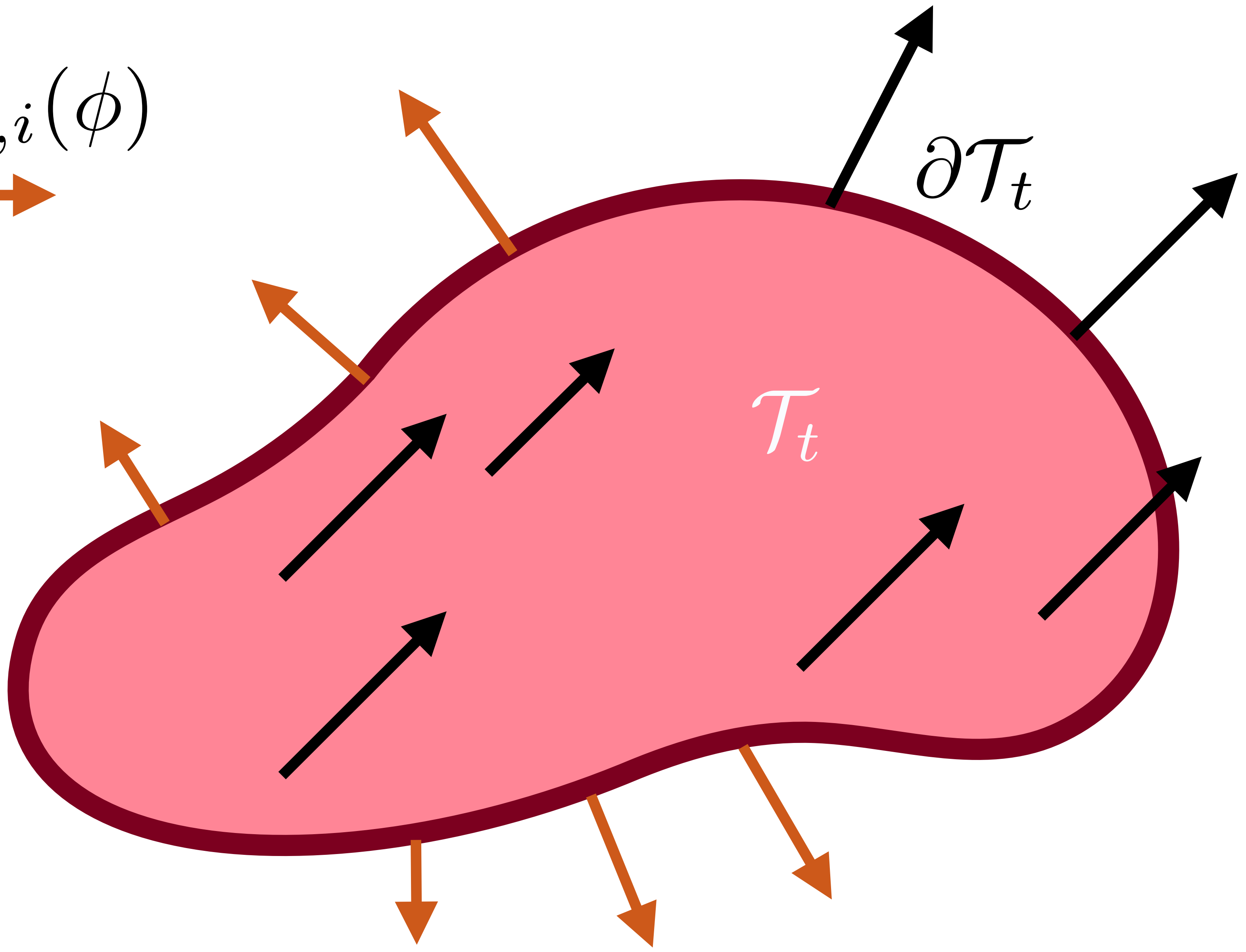

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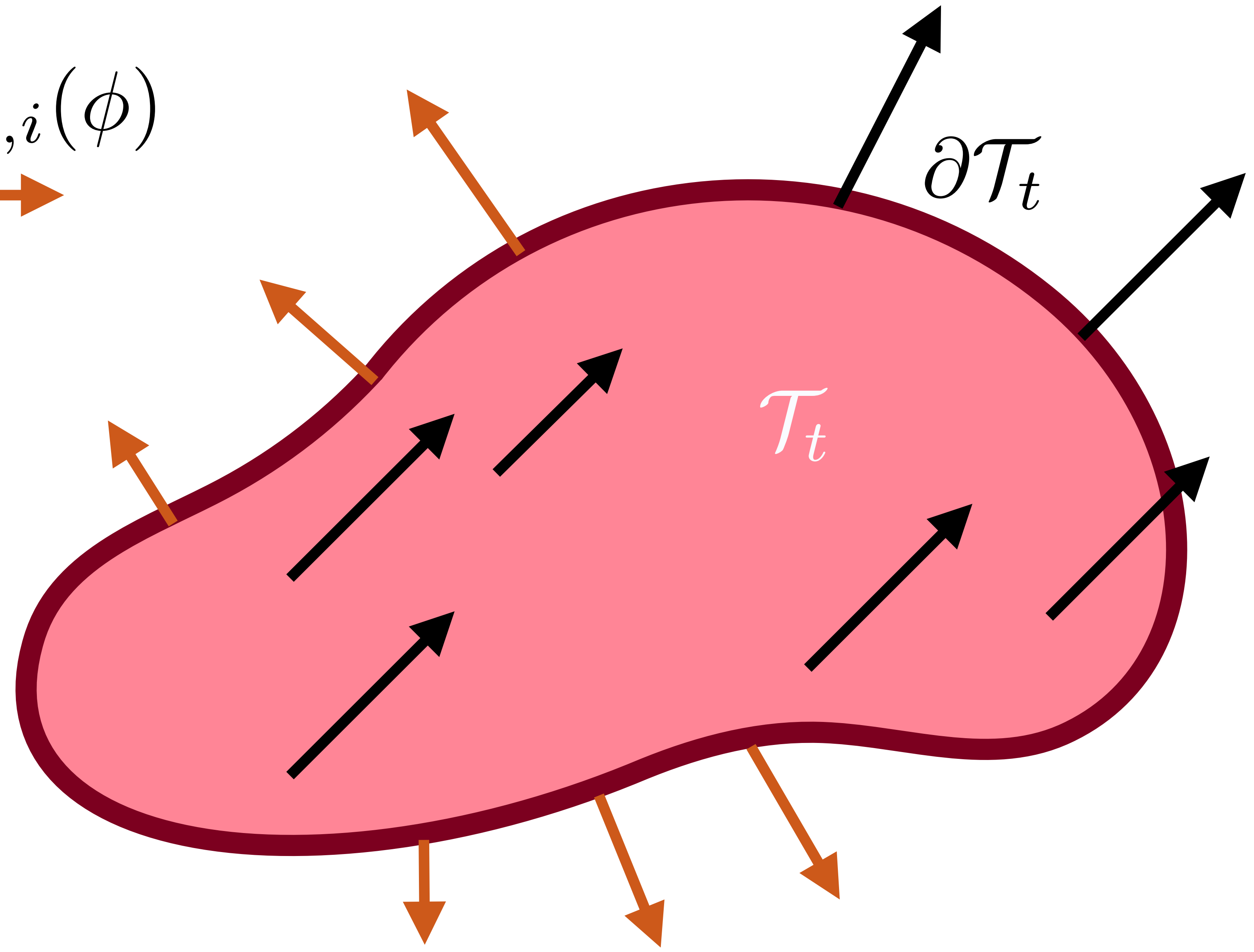

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$$\Big\downarrow$$

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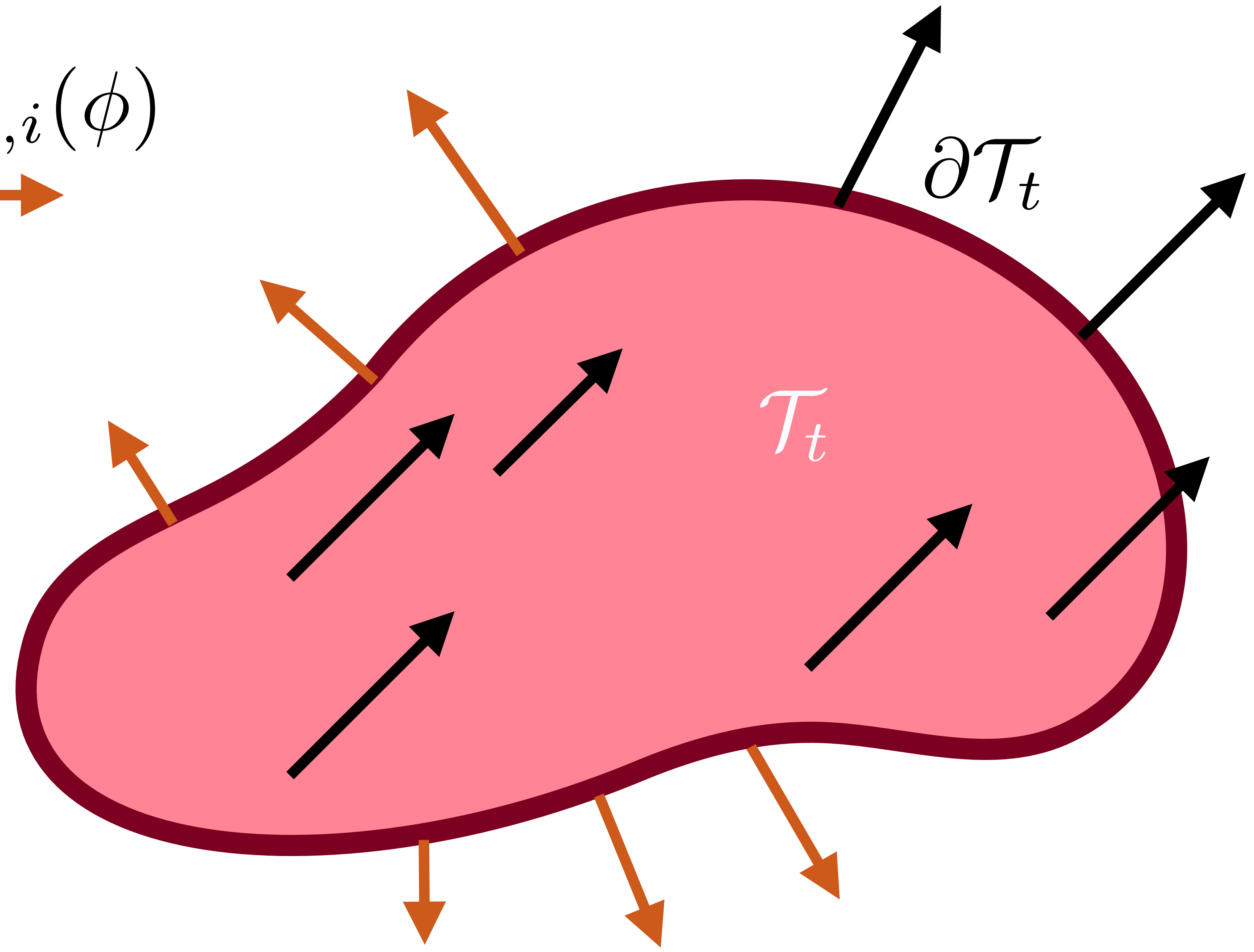

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$$\frac{d\phi_I}{d\phi_R} = -\frac{\mathrm{Im} p_t(\phi)}{\mathrm{Re} p_t(\phi)}$$

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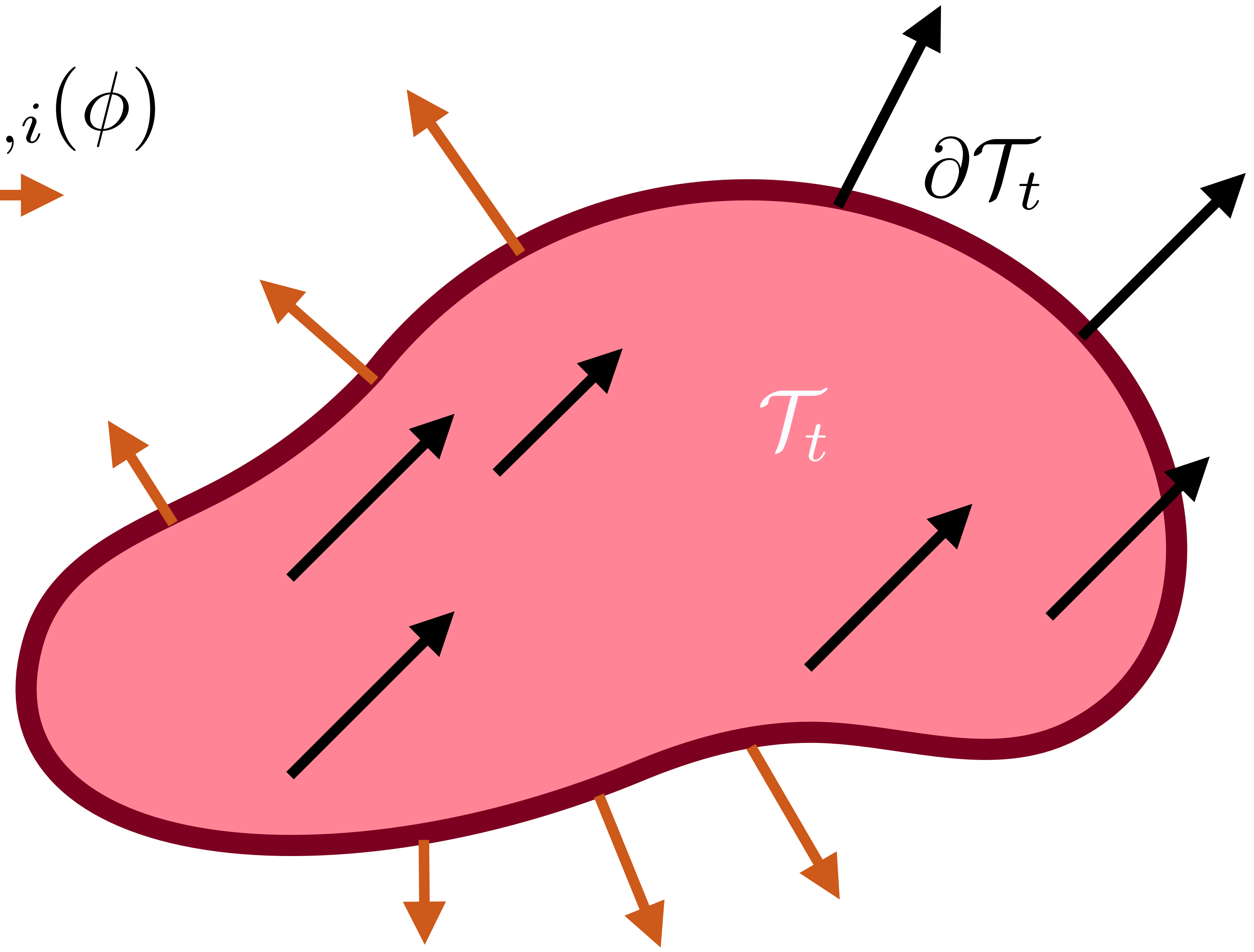
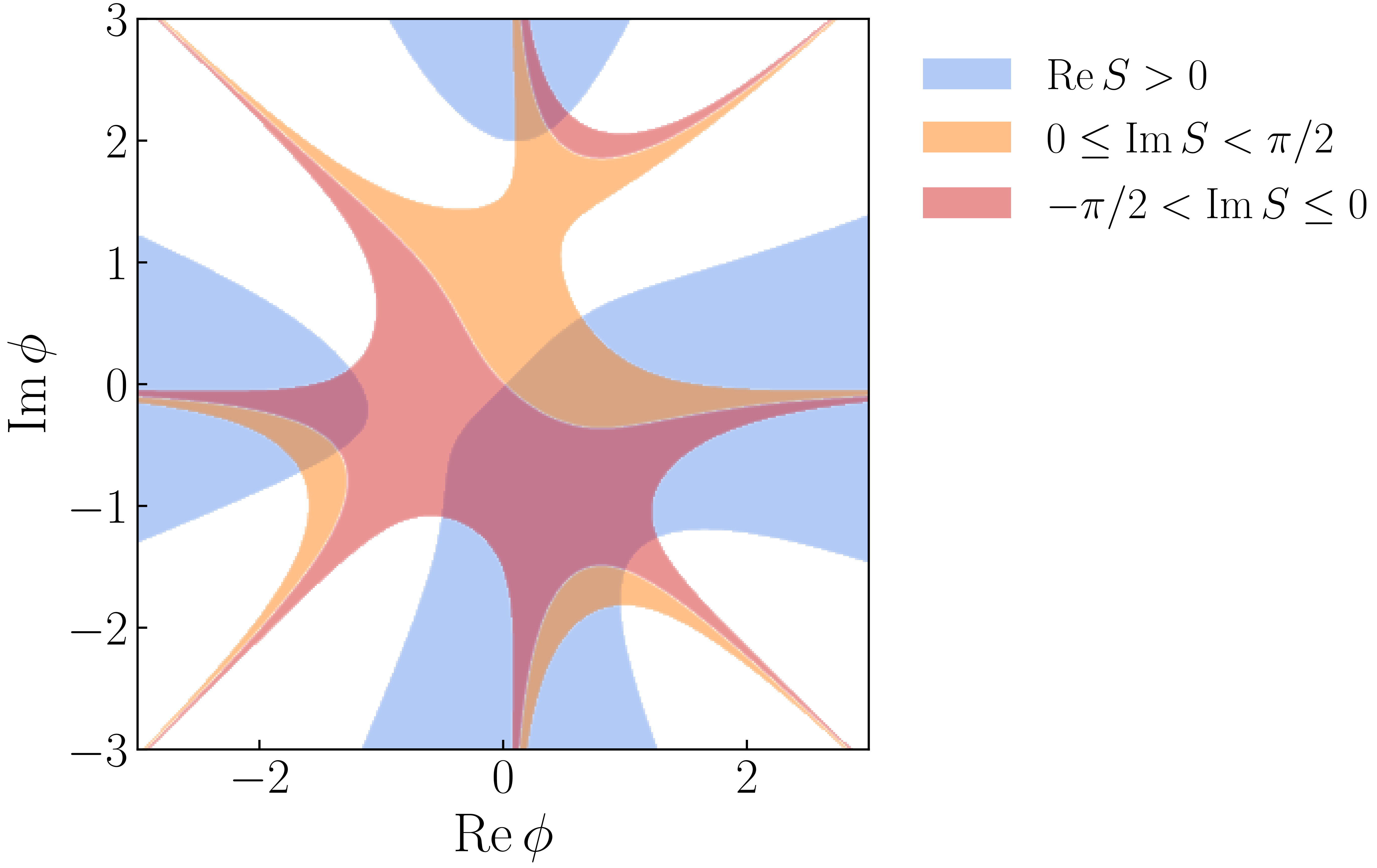


PIKfolds and Lefschetz Thimbles

Consider their approach to the same theory

$$\hat{S}_t(\phi) = \frac{1}{2}\phi^2 + \frac{1}{4}\phi^4 + (1+it)\phi$$



Ihssen, **RK**, Pawlowski, arXiv: 2603.03159
Aarts, Bongiovanni, Seiler, Sexty, JHEP Vol 2014(159), 2014.

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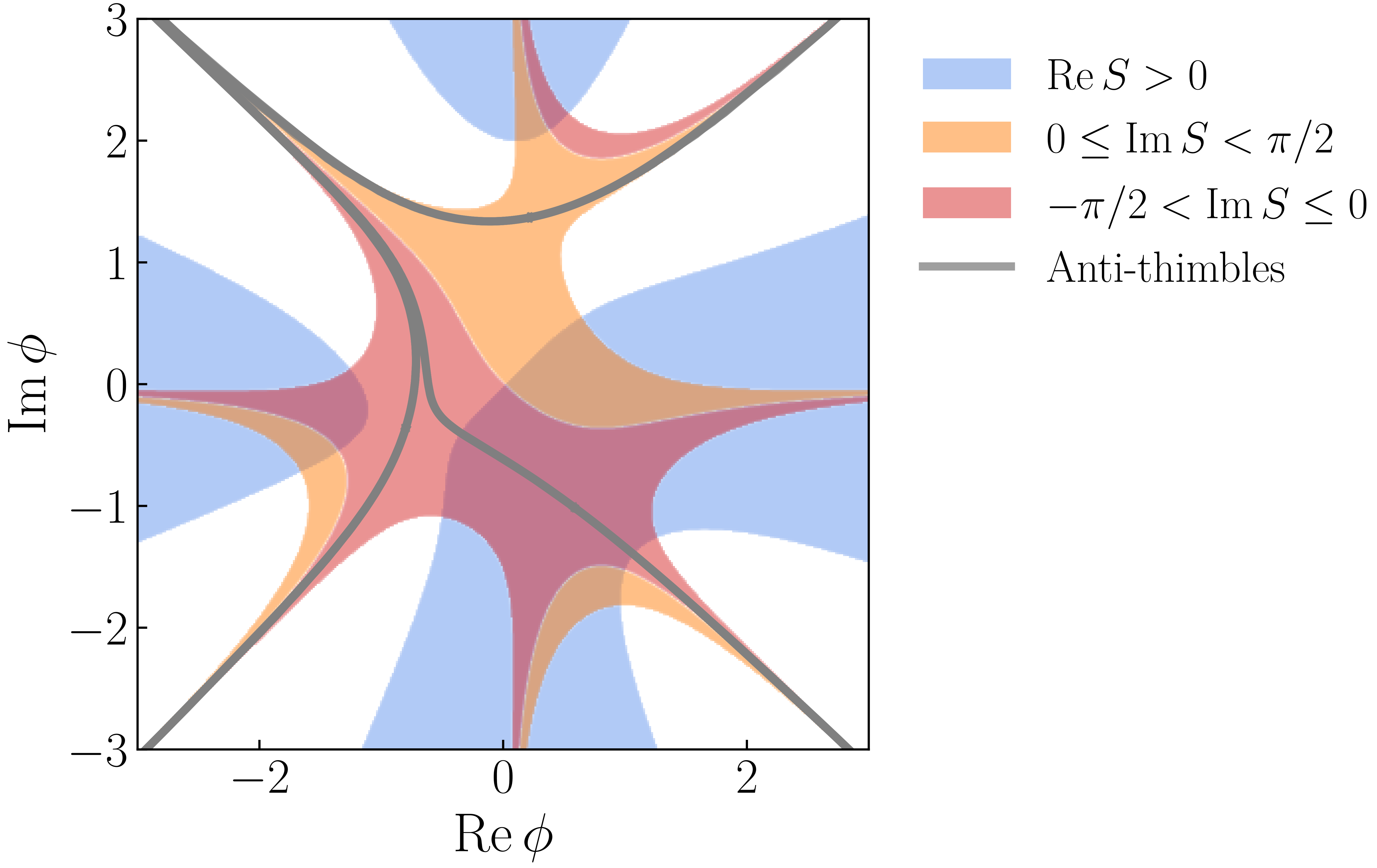

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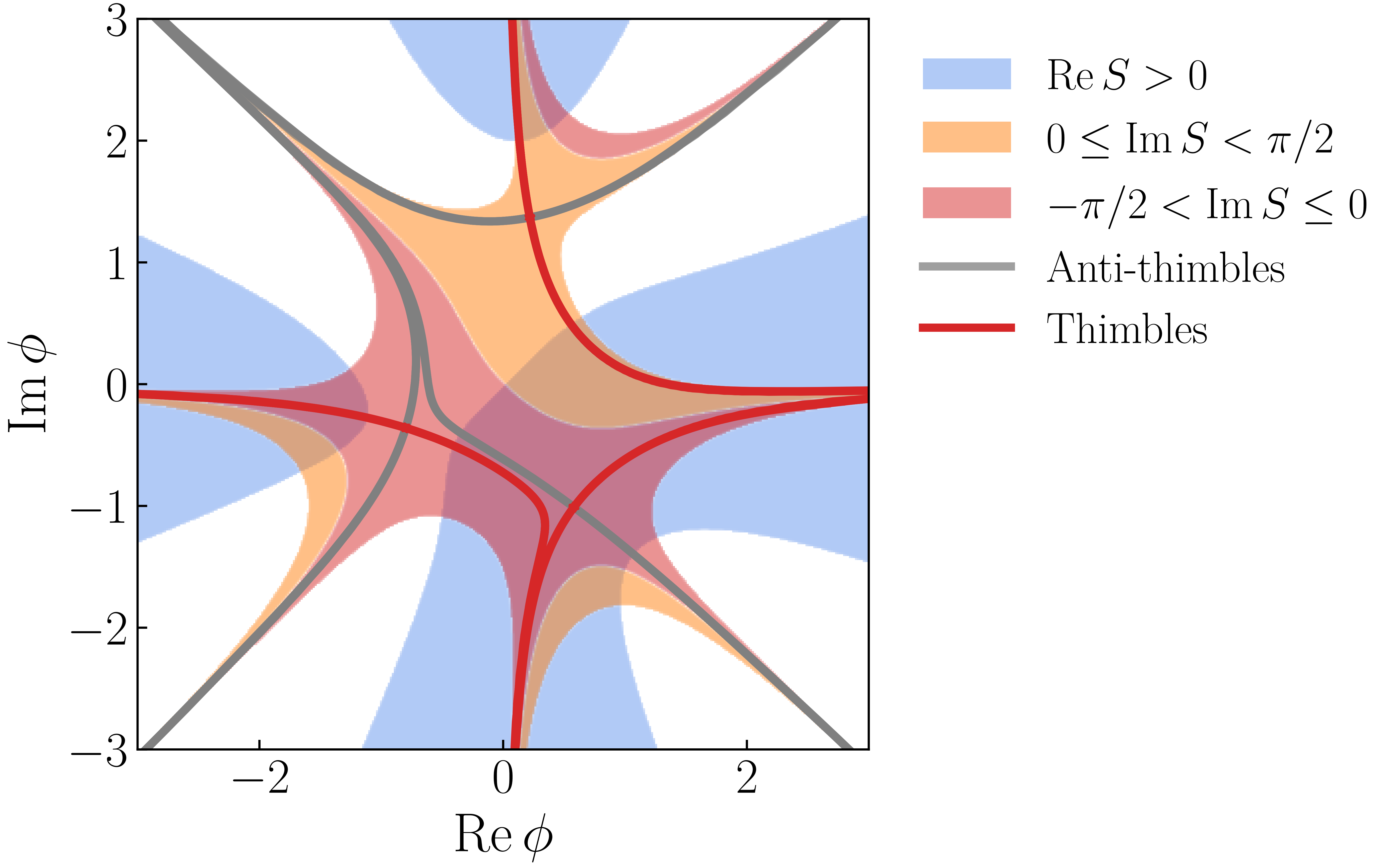

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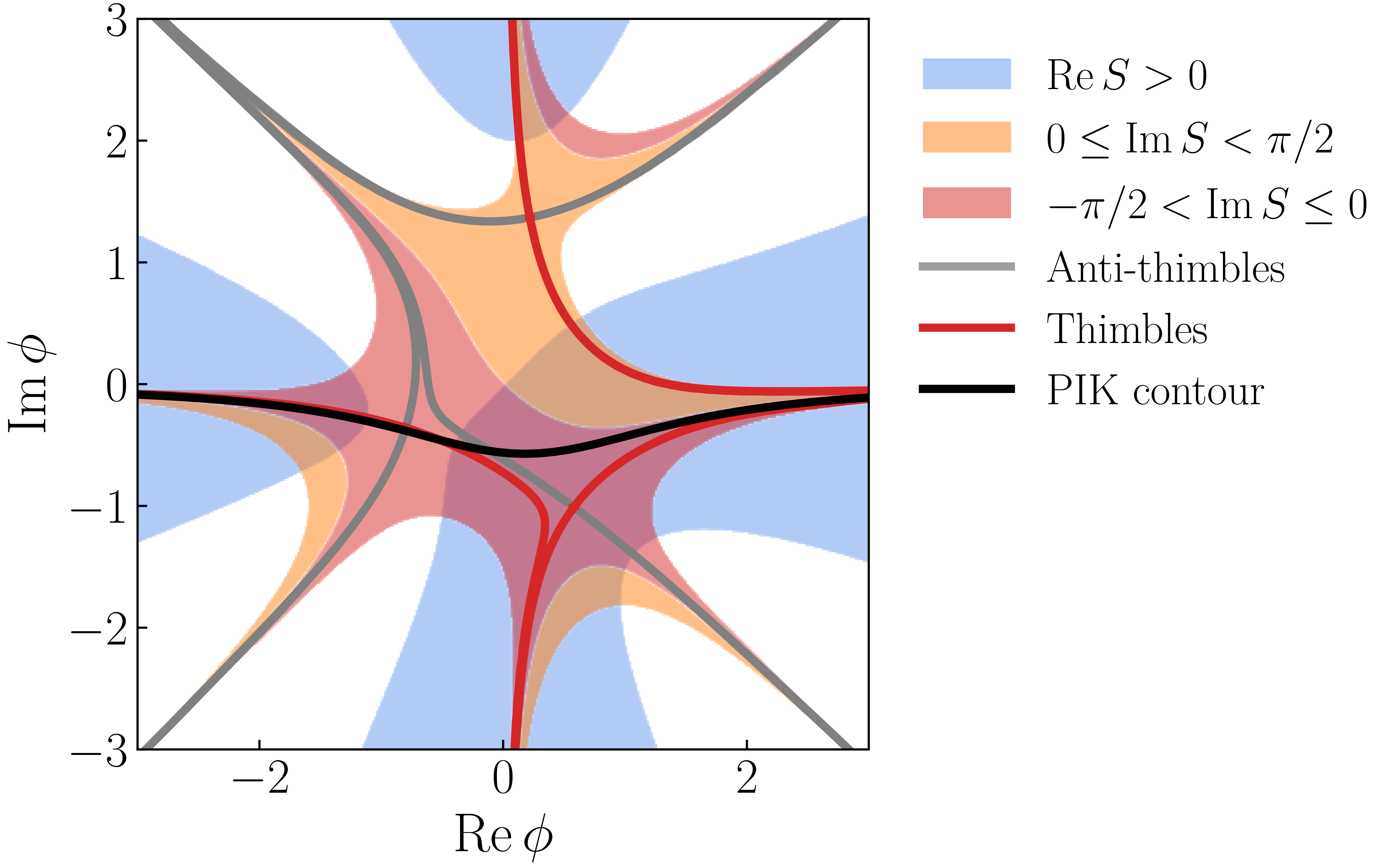

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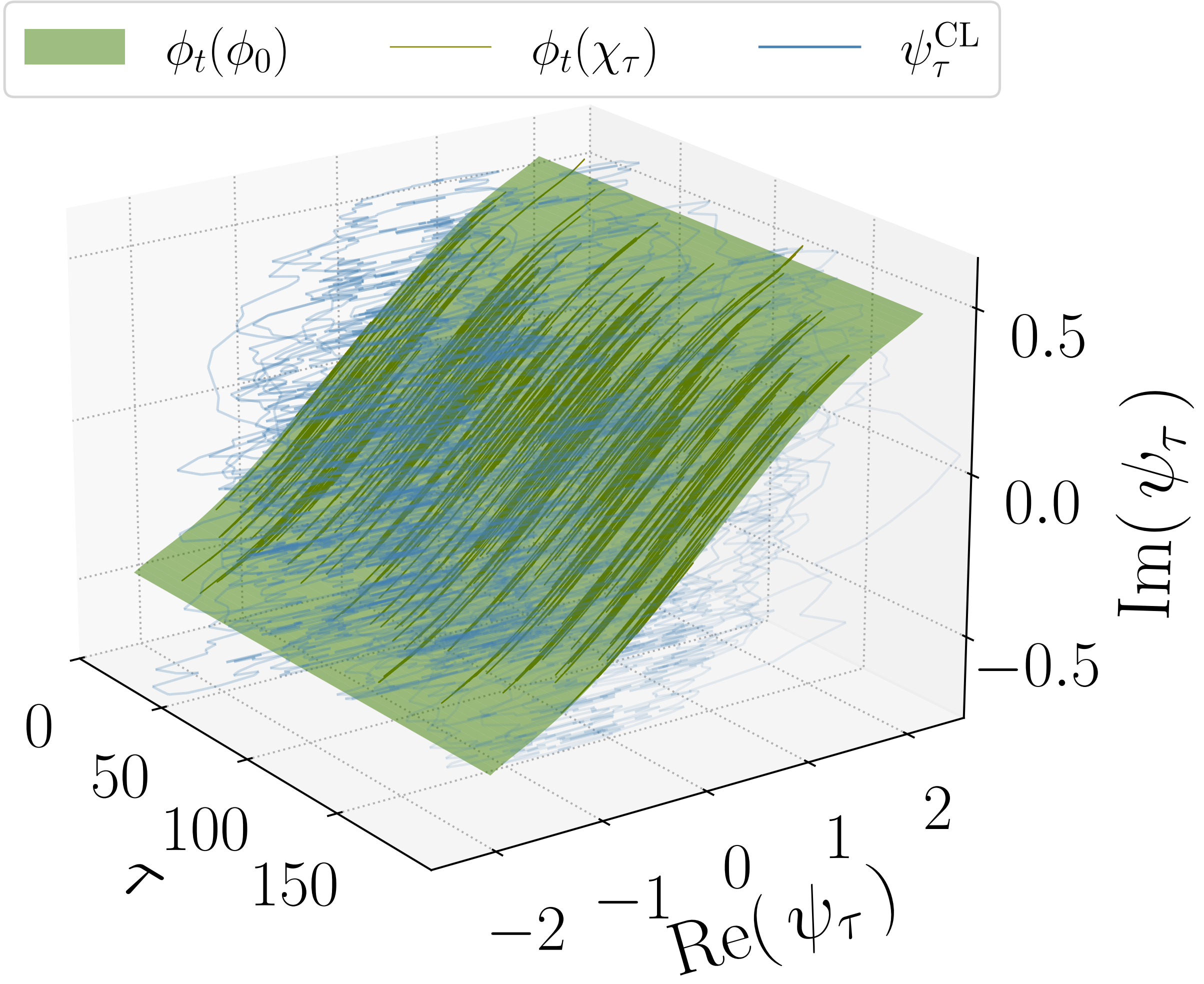
Aarts, Bongiovanni, Seiler, Sexty, JHEP Vol 2014(159), 2014.

Solving sign problems with physics-informed kernels

... things to look forward to

Application to higher-dimensional systems
(Stochastic PDE solvers & Tensor networks)

Application to fermionic theories
(Limits of contour deformations)



Application to gauge theories

Combination with existing sign problem methods

Thank you very much for your attention & questions

Solving sign problems with physics-informed kernels

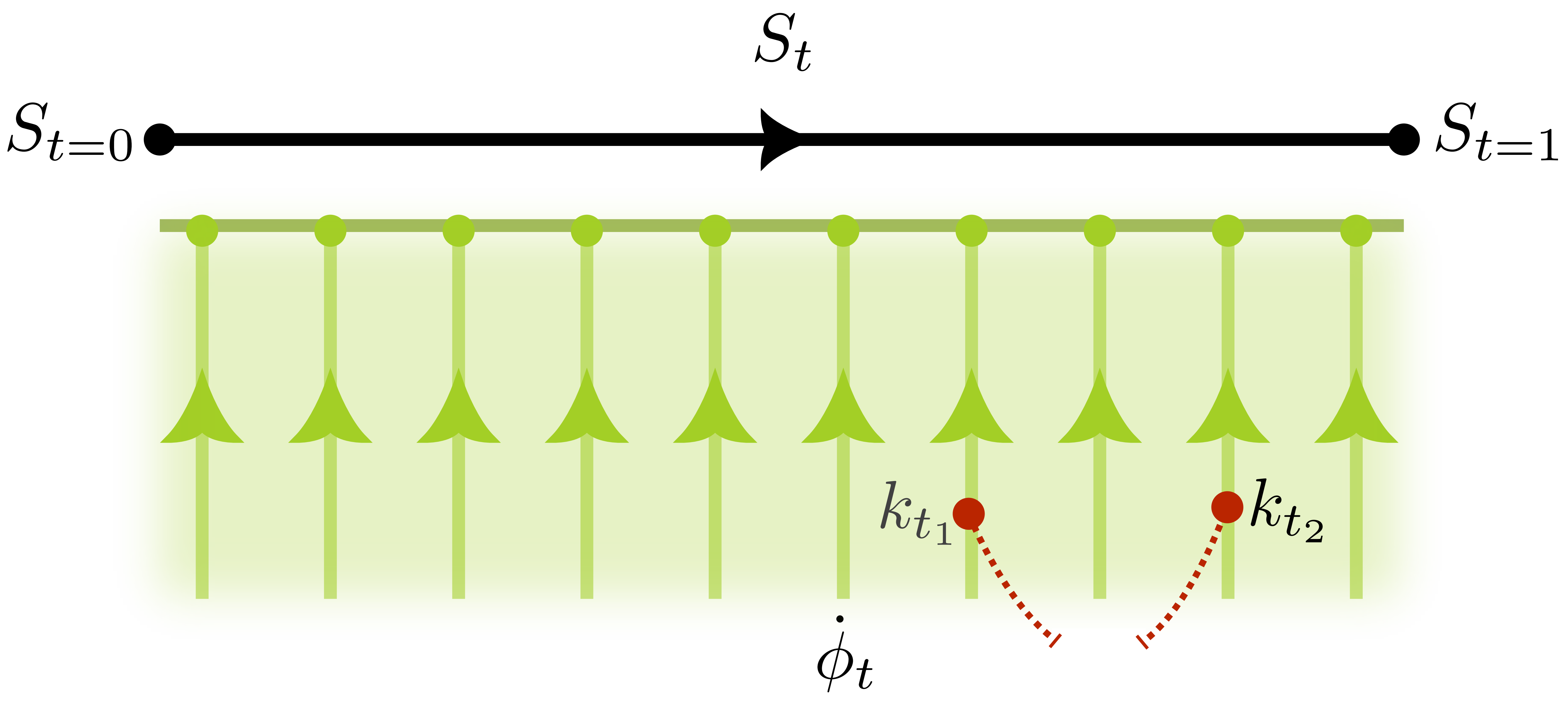
Friederike Ihssen, **Renzo Kapust**, Jan M. Pawlowski
University of Heidelberg

isoQuant SFB1225

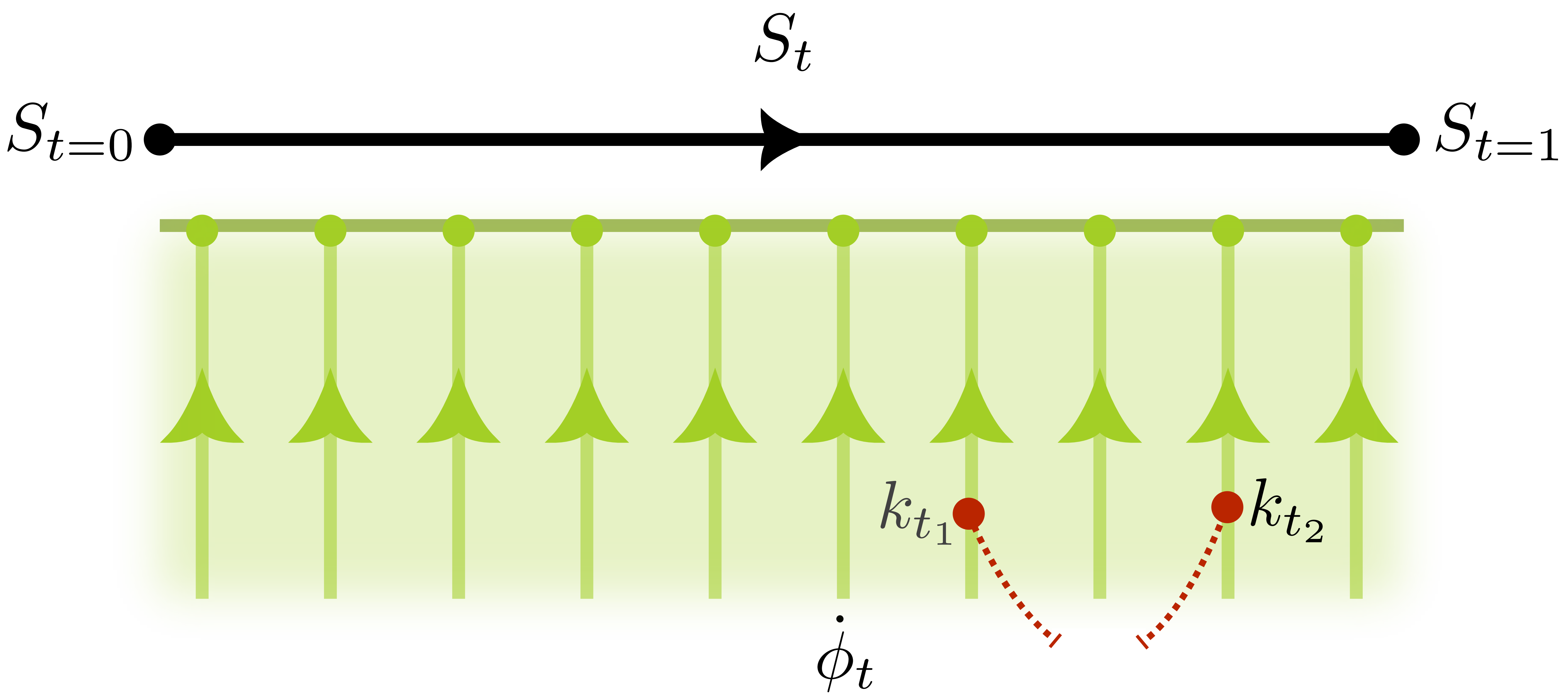
STRUCTURES CLUSTER OF EXCELLENCE

Backup Slides

Computing physics-informed kernels



Computing physics-informed kernels

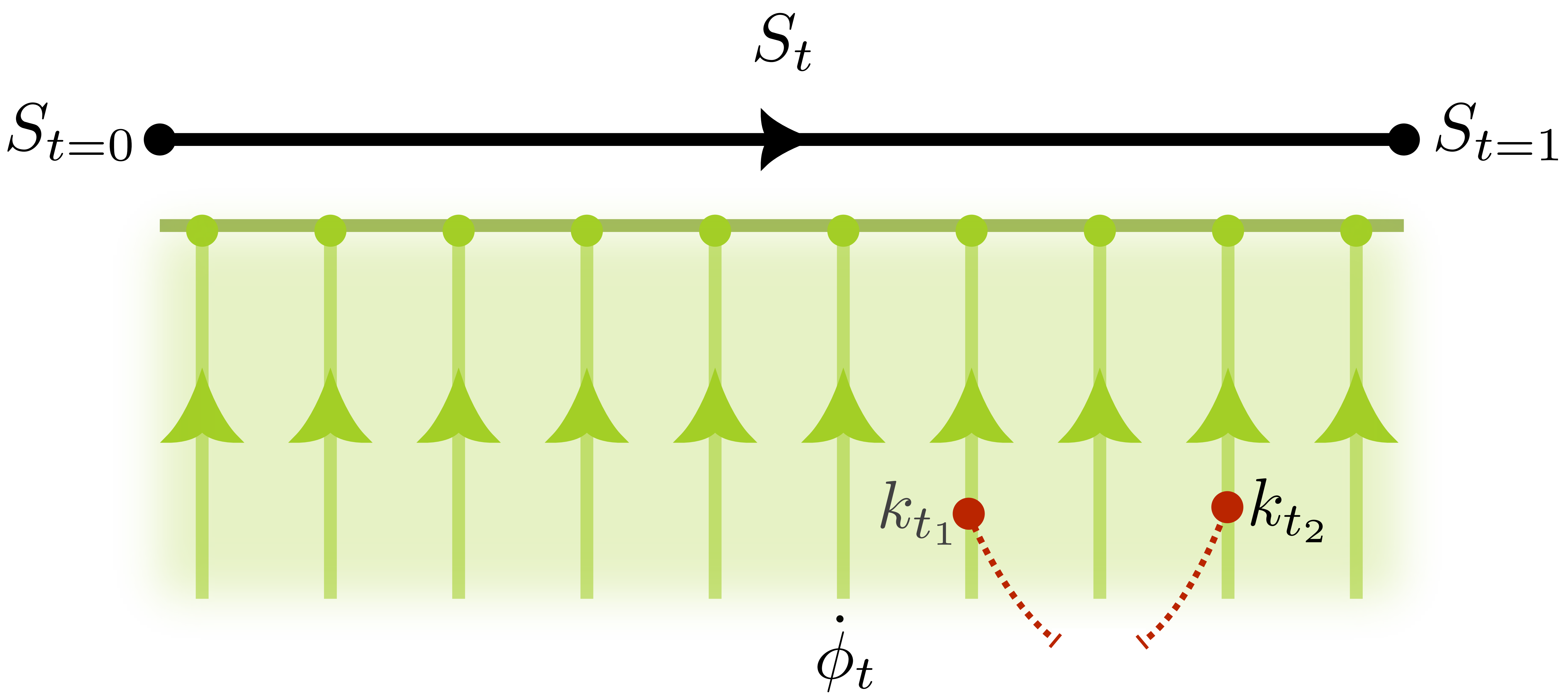


$$S_t(\phi) = \hat{S}_t(\phi) + \log \mathcal{N}_t$$

$$\hat{S}_t(\phi) = \sum_i c_{i,t} O_i(\phi)$$

$$\dot{\phi}_t(\phi) = \sum_i k_{i,t} K_i(\phi)$$

Computing physics-informed kernels



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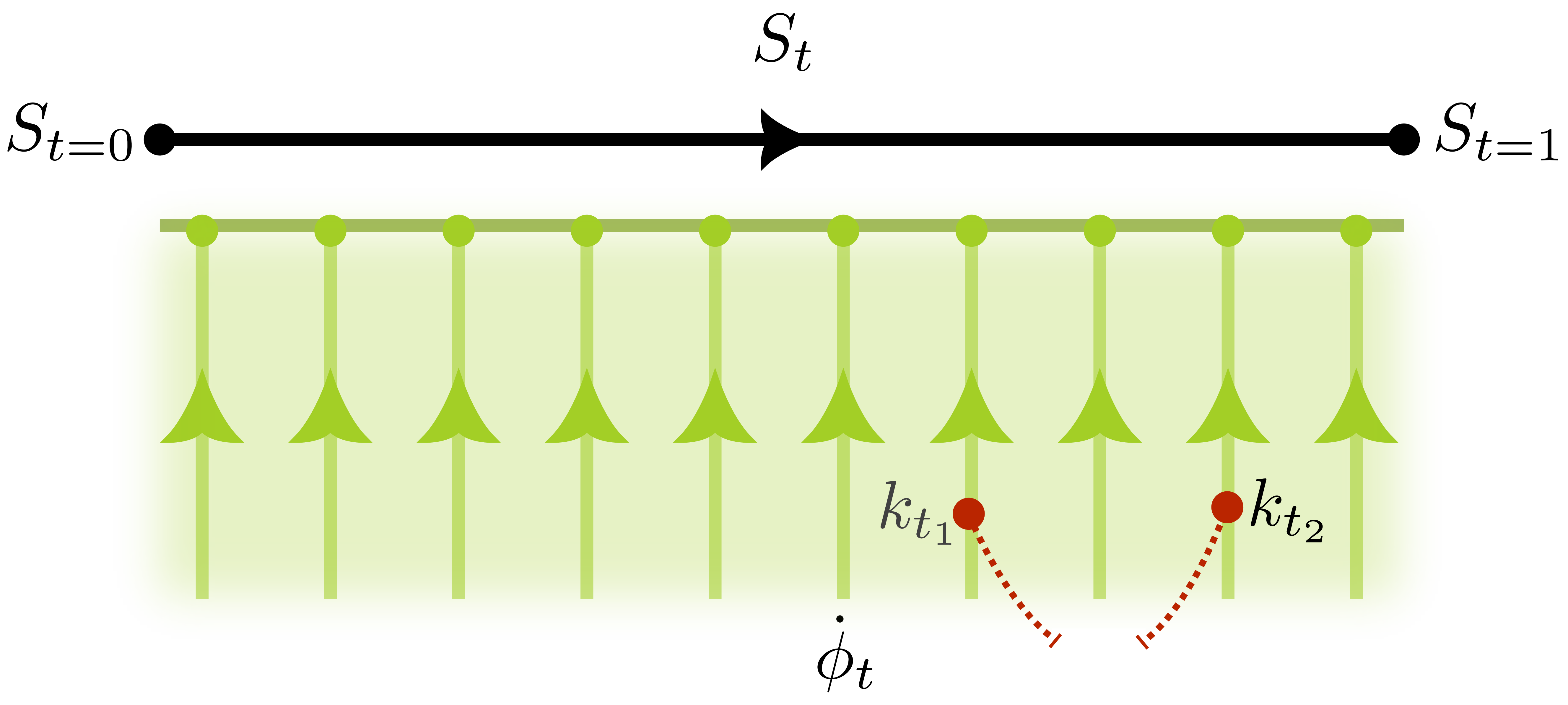
$$\frac{dS_t(\phi)}{dt} = \qquad \ell[\hat{S}_t] \qquad \dot{\phi}_t(\phi)$$

Computing physics-informed kernels



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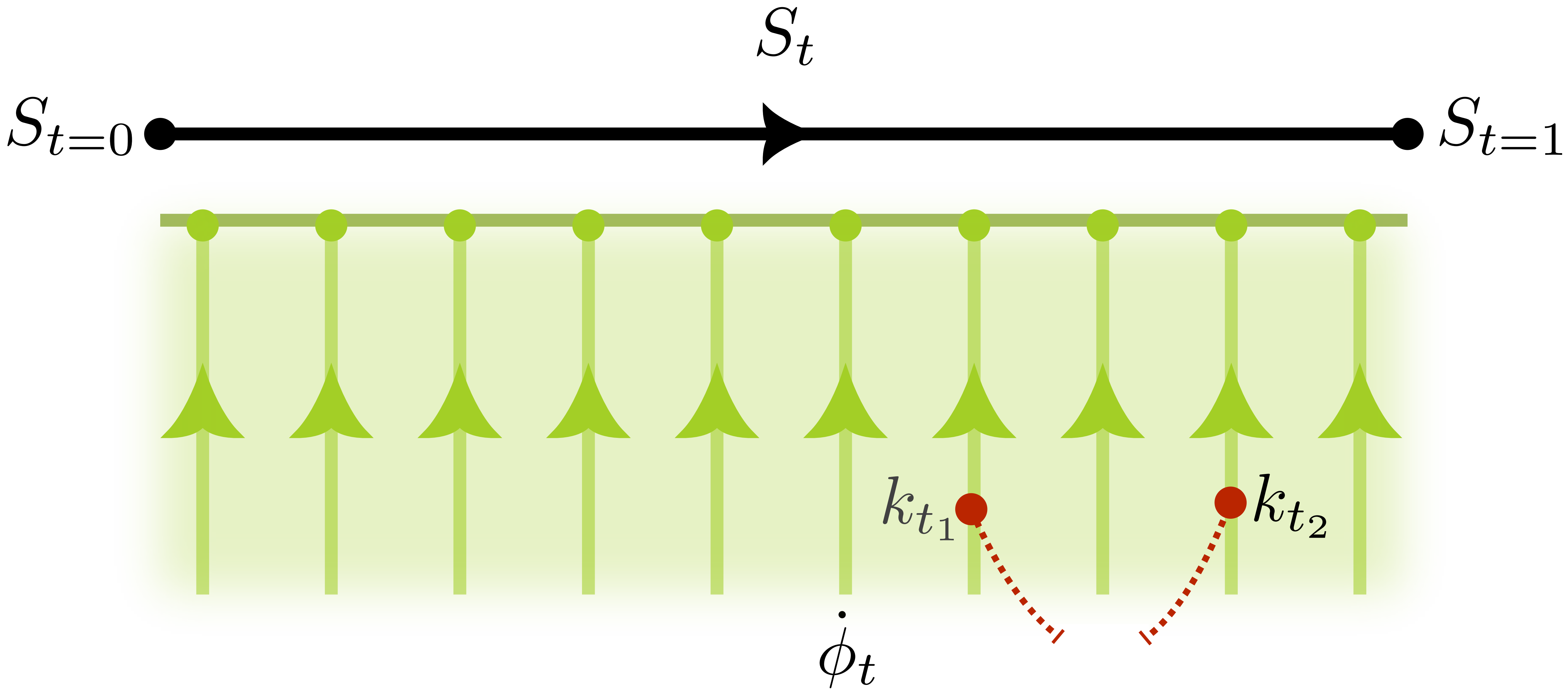
Field-Independence

$$\frac{d \log \mathcal{N}_t}{dt} = \ell[\hat{S}_t]\dot\phi_t(\phi) - \frac{d\hat{S}_t(\phi)}{dt}$$

Computing physics-informed kernels



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Field-Independence

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Cheap to compute

$$\mathscr{L}(\phi, \chi) = \frac{d\hat S_t(\chi)}{dt} - \frac{d\hat S_t(\phi)}{dt} + \ell[\hat S_t]\dot\phi_t(\phi) - \ell[\hat S_t]\dot\phi_t(\chi)$$

$$A_t(\phi) k_t = b_t(\phi)$$

Real-valued case

Computing physics-informed kernels

Preliminary

$$\frac{dS_t(\phi)}{dt} = \left[\frac{\partial}{\partial \phi_i} - \frac{\partial S_t(\phi)}{\partial \phi_i} \right] \dot{\phi}_{t,i}(\phi)$$

Real-valued case

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$$\Omega_t(\phi) : \mathbb{R}^{\mathcal{D}} \to \mathbb{R}$$

$$\frac{dS_t(\phi)}{dt} = \left[\frac{\partial^2}{\partial \phi_i^2} - \frac{\partial S_t(\phi)}{\partial \phi_i} \frac{\partial}{\partial \phi_i} \right] \Omega_t(\phi)$$

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Induces a stochastic process

$$d\psi_\tau = -\frac{\partial S_t(\psi_\tau)}{\partial \phi} d\tau + \sqrt{2} dW_\tau$$

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Feynman-Kac

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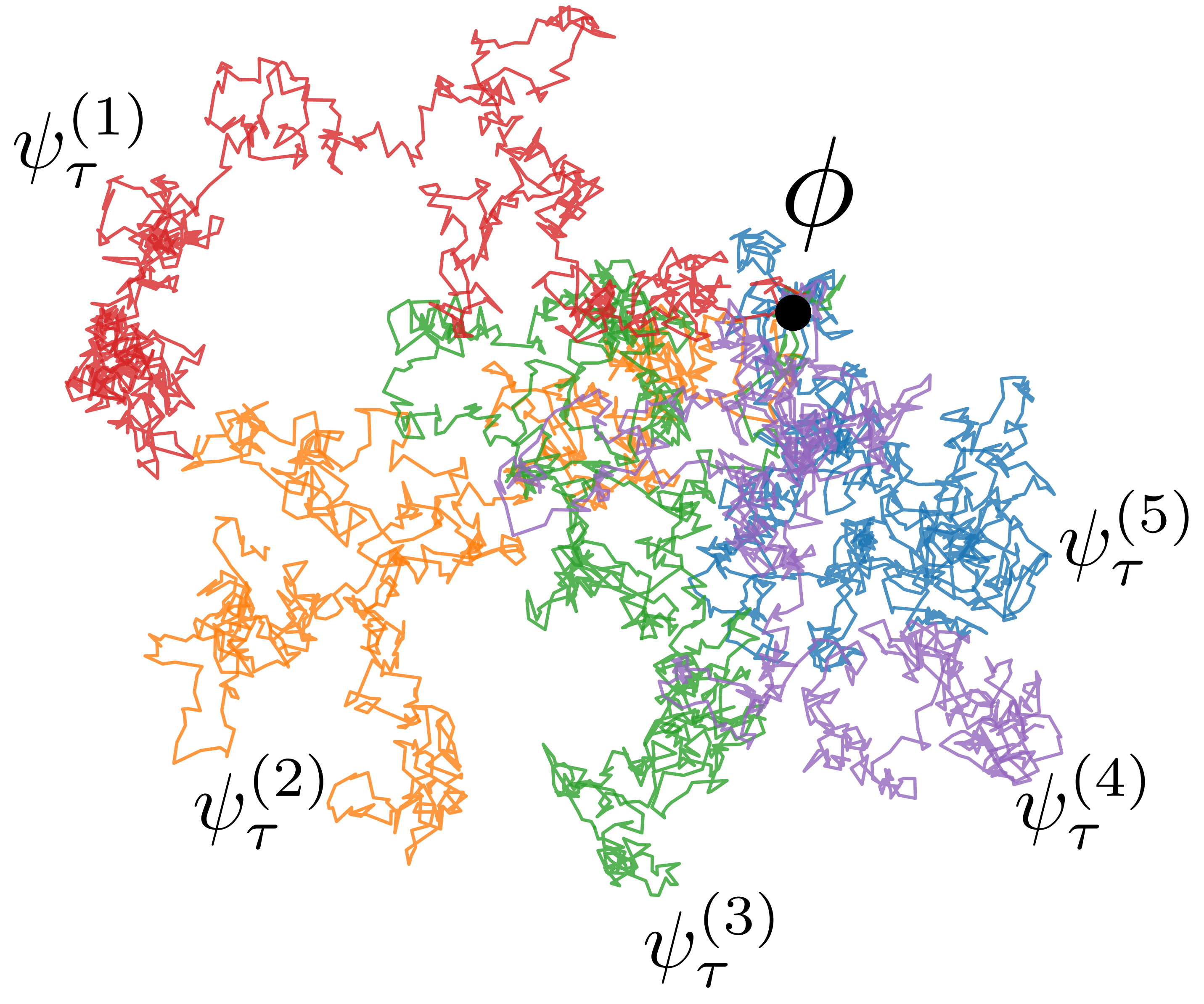
e.g. Albergo, Kanwar, arXiv:2603.00252



Real-valued case

Computing physics-informed kernels

Preliminary

$$\frac{dS_t(\phi)}{dt} = \left[\frac{\partial}{\partial\phi_i} - \frac{\partial S_t(\phi)}{\partial\phi_i}\right]\dot{\phi}_{t,i}(\phi)$$

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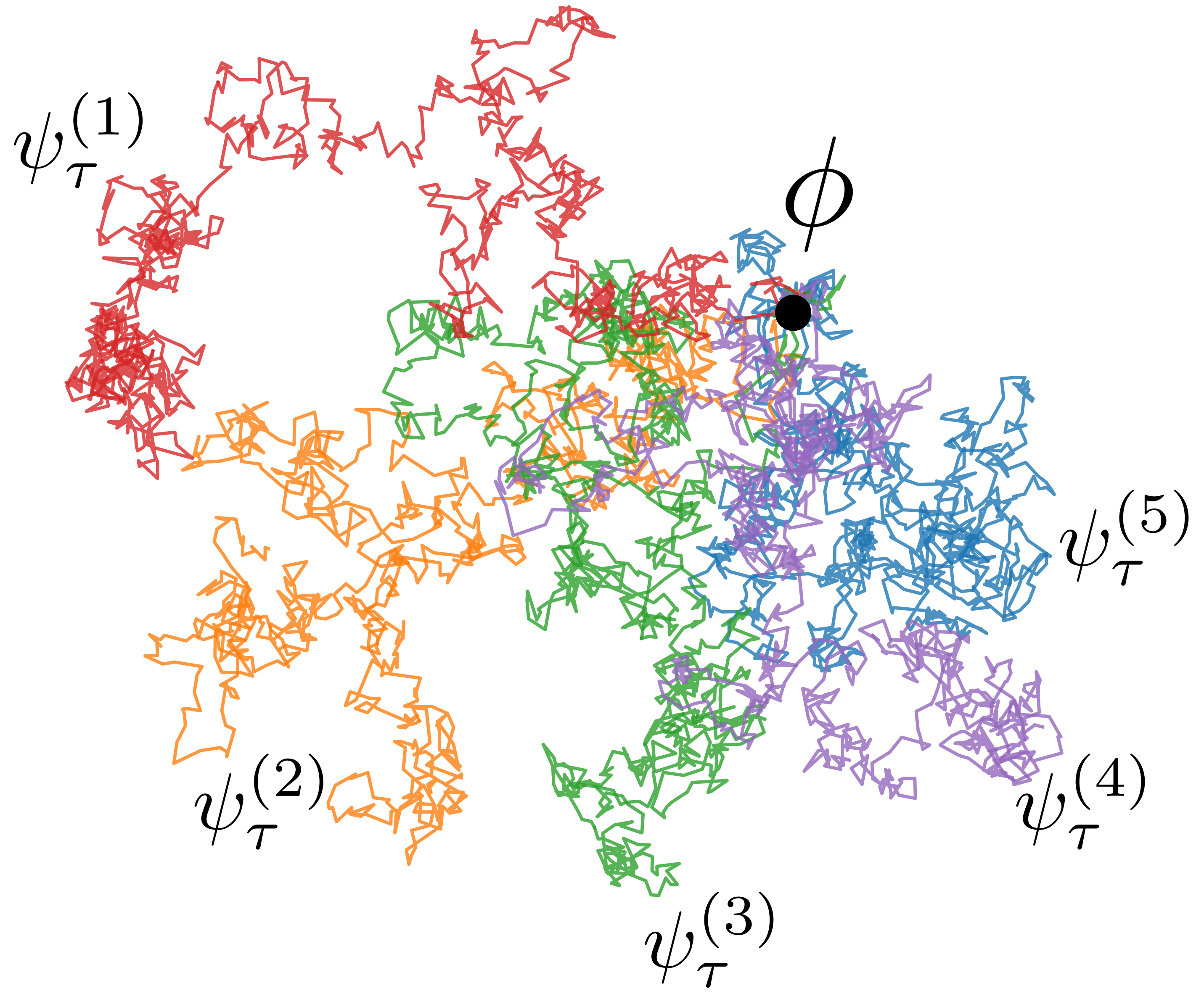

Extension to the

Complex-valued case ?

Computing physics-informed kernels

$$\frac{dS_t(\phi)}{dt} = \left[\frac{\partial}{\partial \phi_i} - \frac{\partial S_t(\phi)}{\partial \phi_i} \right] \dot{\phi}_{t,i}(\phi)$$

Preliminary

Computing physics-informed kernels

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Complex-valued case

Preliminary

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Complex-valued case

(I) **(II)** **(III)**

Preliminary

Computing physics-informed kernels

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Complex-valued case

(I)

$$\dot{\phi}_{t,i}(\,\phi_t(\phi_0)\,)$$

We are only interested in transformations on the manifold

(II)

(III)

Computing physics-informed kernels

Preliminary

$$\frac{dS_t(\phi)}{dt} = \left[\frac{\partial}{\partial \phi_i} - \frac{\partial S_t(\phi)}{\partial \phi_i} \right] \dot{\phi}_{t,i}(\phi)$$

Complex-valued case

(I)

$$\dot{\phi}_{t,i}(\,\phi_t(\phi_0)\,)$$

We are only interested in transformations on the manifold

(II)

$$\frac{\partial}{\partial \phi_{t,i}} = \frac{\partial \phi_{0,j}}{\partial \phi_{t,i}} \frac{\partial}{\partial \phi_{0,j}}$$

Rewrite derivatives in terms of the initial field

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Use the freedom to parametrise the kernel

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$$M_t(\,\phi_t(\phi_0)\,) = J_t(\phi_0) J_t^T(\phi_0)$$

$$d\chi_\tau = -\frac{\partial S_0}{\partial \phi}(\chi_\tau) d\tau + \sqrt{2} dW_\tau$$

$$\omega_t(\phi_0) = -\int_0^\infty \mathbb{E}\left[\frac{dS_t}{dt}(\chi_\tau) \,|\, \chi_0 = \phi_0 \right]$$