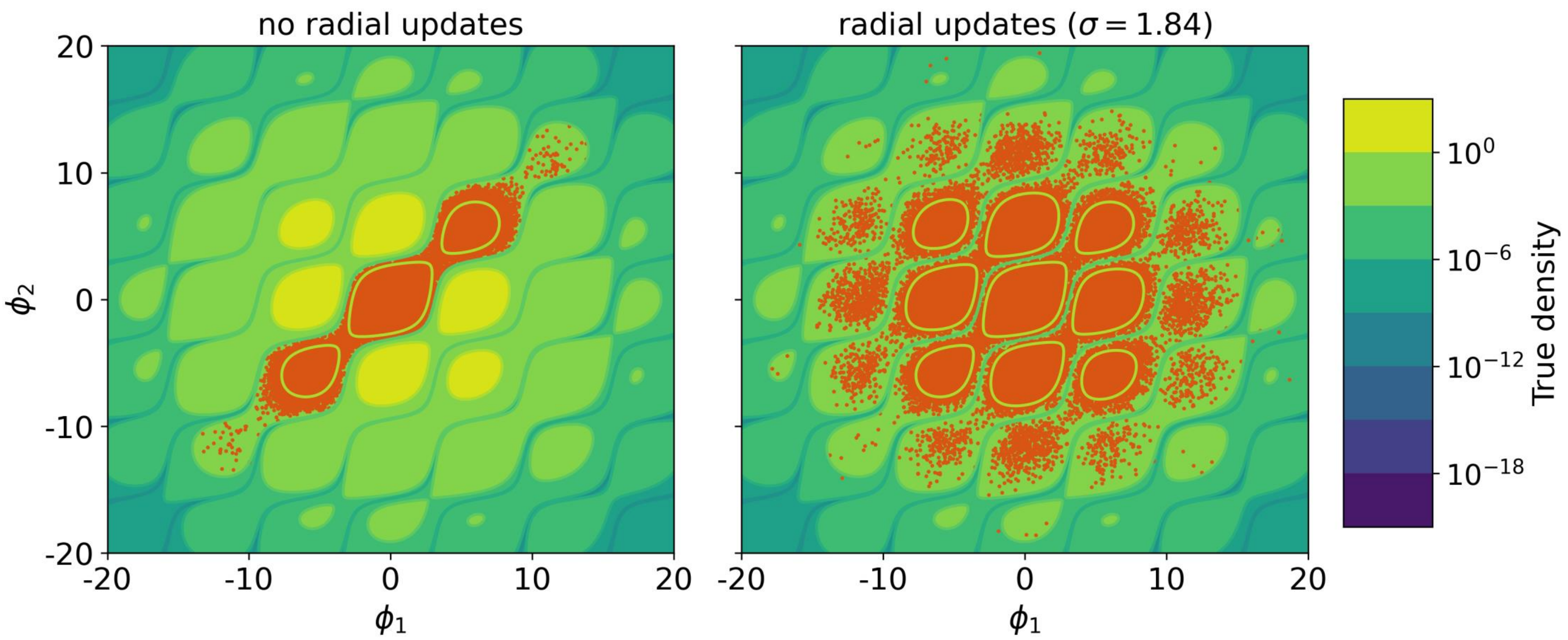

OVERCOMING ERGODICITY PROBLEMS OF THE HMC USING RADIAL UPDATES

JULY 30TH 2024 I FINN TEMMEN I FORSCHUNGSZENTRUM JÜLICH

OVERCOMING ERGODICITY PROBLEMS OF THE HMC USING RADIAL UPDATES

JULY 30TH 2024 I FINN TEMMEN I FORSCHUNGSZENTRUM JÜLICH

IN COLLABORATION WITH

JOHANN OSTMEYER (UNIVERSITY OF BONN)

ANTHONY KENNEDY (UNIVERSITY OF EDINBURGH)

XINHAO YU (UNIVERSITY OF EDINBURGH)

EVAN BERKOWITZ (FORSCHUNGSZENTRUM JÜLICH)

THOMAS LUU (FORSCHUNGSZENTRUM JÜLICH)

MOTIVATION

Ergodicity and convergence of HMC

Ergodicity violations due to potential barriers

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Ergodicity and convergence of HMC

Ergodicity violations due to potential barriers

- In-principle: infinite potential, e.g. vanishing fermion determinant
- In-practice: regions separated by exponentially large potential

[Wynen et al., arXiv:1812.09268]

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Convergence of HMC

- Proof for geometrical convergence of HMC on non-compact manifolds

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Augment HMC with Metropolis-Hastings update in radial direction

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Talk by Dominic Schuh at 4:15 PM
”Simulating the Hubbard Model
with Normalizing Flows”

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HUBBARD MODEL

Setting the stage

- Hubbard Hamiltonian in particle/hole basis

$$H = -\kappa \sum_{\langle x,y \rangle} \left(a_x^\dagger a_y - b_x^\dagger b_y \right) + \frac{U}{2} \sum_x \left(a_x^\dagger a_x - b_x^\dagger b_x \right)^2$$

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- Exponential discretization
- Hubbard-Stratonovich introduces non-compact auxiliary fields ϕ_{xt}
- Integrate out fermionic DoF

$$S[\phi] = \frac{N_t}{2U\beta} \sum_{x,t} \phi_{xt}^2 - \log\det \mathrm{M}[\mathrm{i}\phi] - \log\det \mathrm{M}[-\mathrm{i}\phi]$$

HUBBARD MODEL

Setting the stage

$$S[\phi] = \frac{N_t}{2U\beta}\sum_{x,t}\phi_{xt}^2 \underbrace{-\log\det \mathrm{M}[\mathrm{i}\phi] - \log\det \mathrm{M}[-\mathrm{i}\phi]}_{\text{Fermionic contribution}}$$

- Fermion matrix:
  - Manifolds of vanishing $\det M[i\phi]$ with codimension 1
  - Separated regions constitute problem for perfect Molecular Dynamics

Ulybyshev et al., arXiv:1712.02188

HUBBARD MODEL

Setting the stage

$$S[\phi] = \frac{N_t}{2U\beta} \underbrace{\sum_{x,t} \phi_{xt}^2}_{:= R^2} - \log\det \mathrm{M}[\mathrm{i}\phi] - \log\det \mathrm{M}[-\mathrm{i}\phi]$$

- Fermion matrix: Ulybyshev et al., arXiv:1712.02188
  - Manifolds of vanishing $\det M[i\phi]$ with codimension 1
  - Separated regions constitute problem for perfect Molecular Dynamics
- Define radius $R = \sqrt{\sum_{x,t} \phi_{xt}^2}$

RADIAL UPDATES

Initial configuration $\phi = (\phi_1, \phi_2, \ldots, \phi_d)$

- e.g. output of HMC

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Sample update $\gamma \sim \mathcal{N}\left(0, \sigma^2\right)$

- Tunable standard deviation σ

RADIAL UPDATES

Initial configuration $\phi = (\phi_1, \phi_2, \ldots, \phi_d)$

↓

Sample update $\gamma \sim \mathcal{N}(0, \sigma^2)$

↓

Propose new configuration

$\tilde{\phi} = e^{\gamma}\phi$

↓

- e.g. output of HMC
- Tunable standard deviation σ
- Scales radius $\tilde{R} = e^{\gamma} R$
- e^{γ} has median of 1

RADIAL UPDATES

Initial configuration $\phi = (\phi_1, \phi_2, \dots, \phi_d)$

- e.g. output of HMC

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- Tunable standard deviation σ

Propose new configuration

$$\tilde{\phi} = e^{\gamma} \phi$$

- Scales radius $\tilde{R} = e^{\gamma} R$
- e^{γ} has median of 1

Accept/reject with acceptance probability

$$\alpha(\phi, \tilde{\phi}) = \min(1, \exp\{-\Delta S + d\gamma\})$$

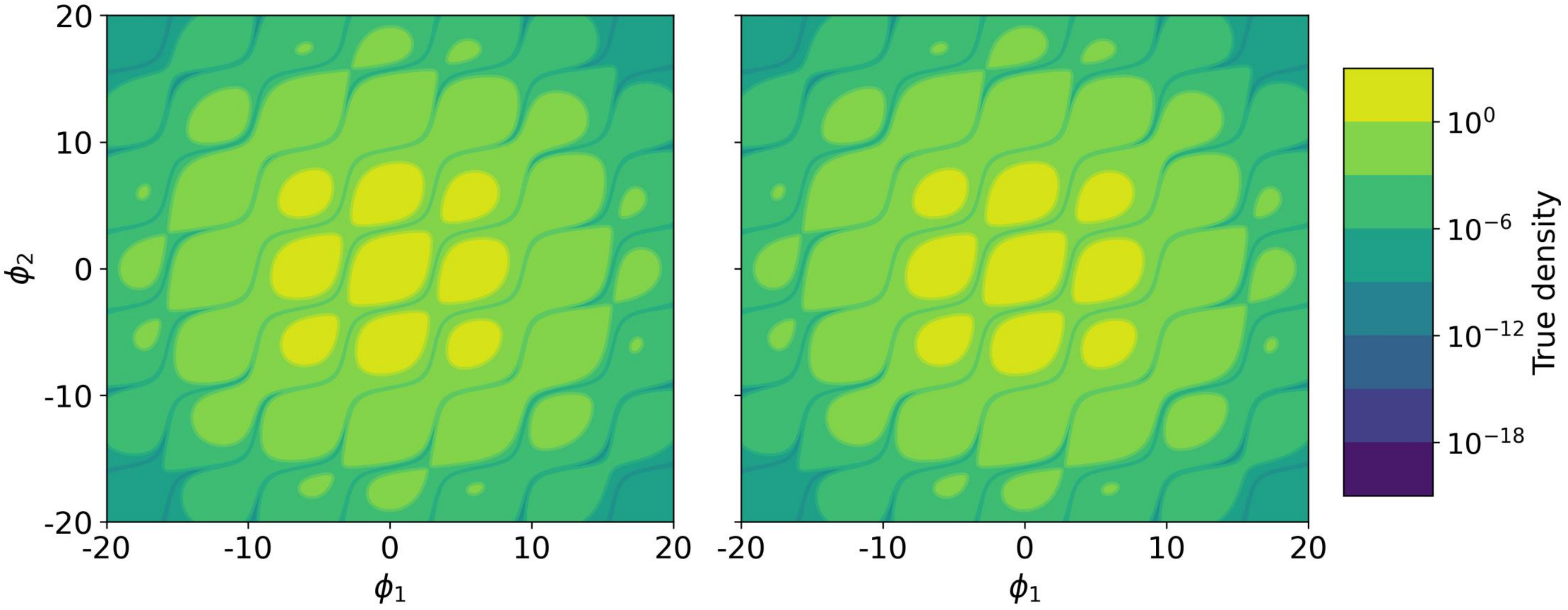
- Independent of proposal distribution
- Low computational cost
- Special case of RDMH or TMCMC
- Satisfies detailed balance

Dutta, arXiv:1008.5227v2 & Dutta et al., arXiv:1106.5850v3

RESULTS

Resolving ergodicity violations

$N_x = 2,\, N_t = 1,\, U = 18,\, \beta = \kappa = 1$



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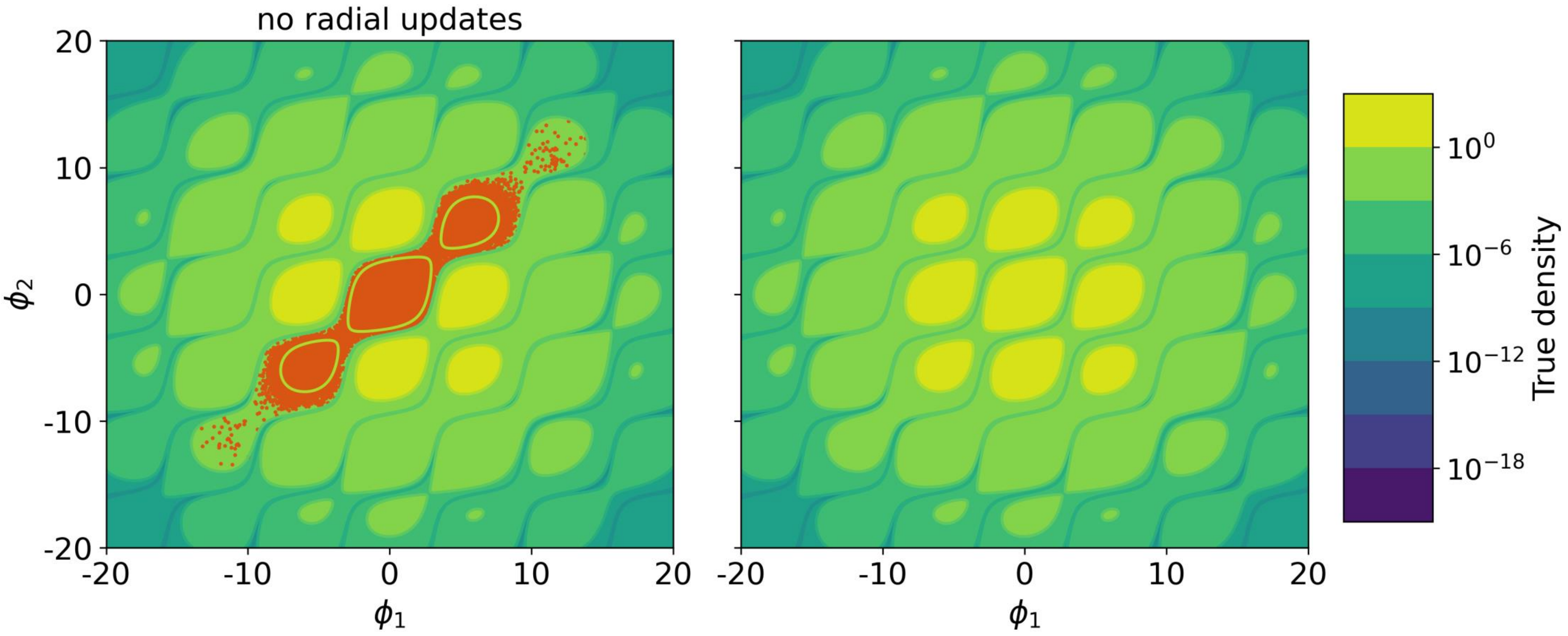

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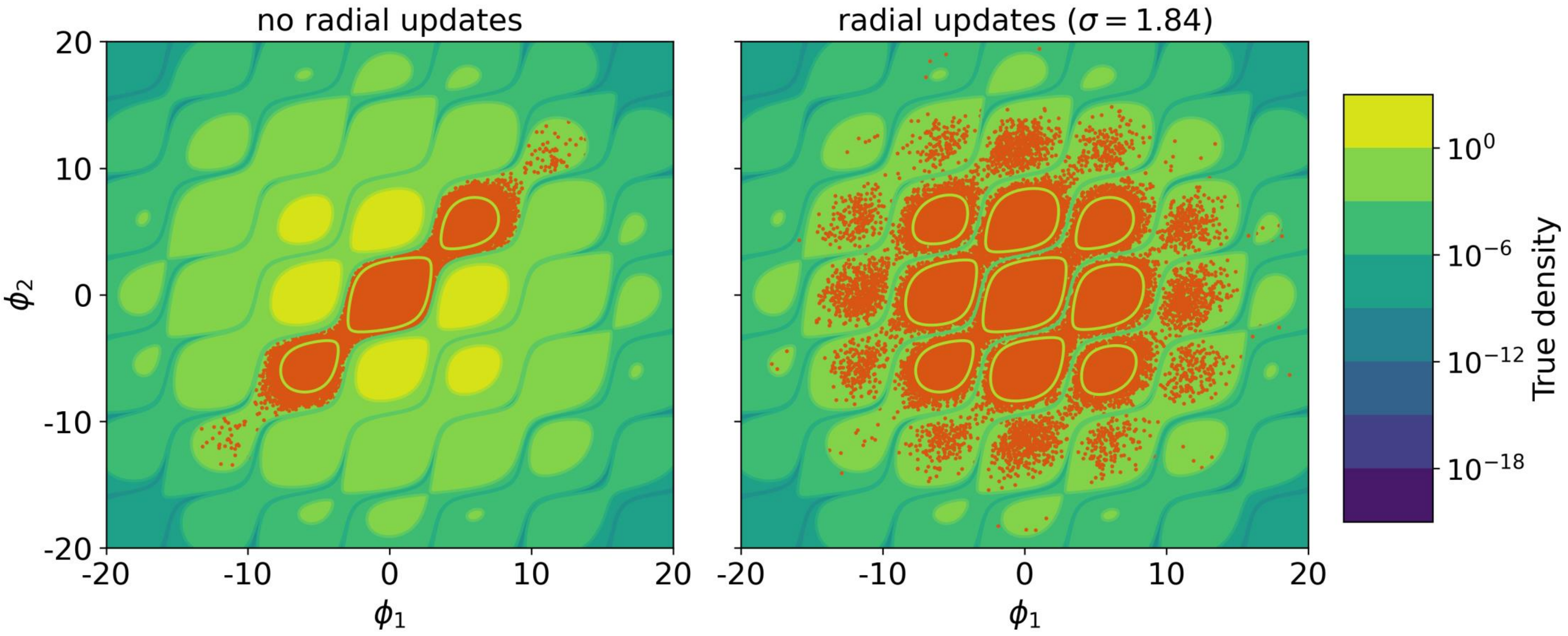

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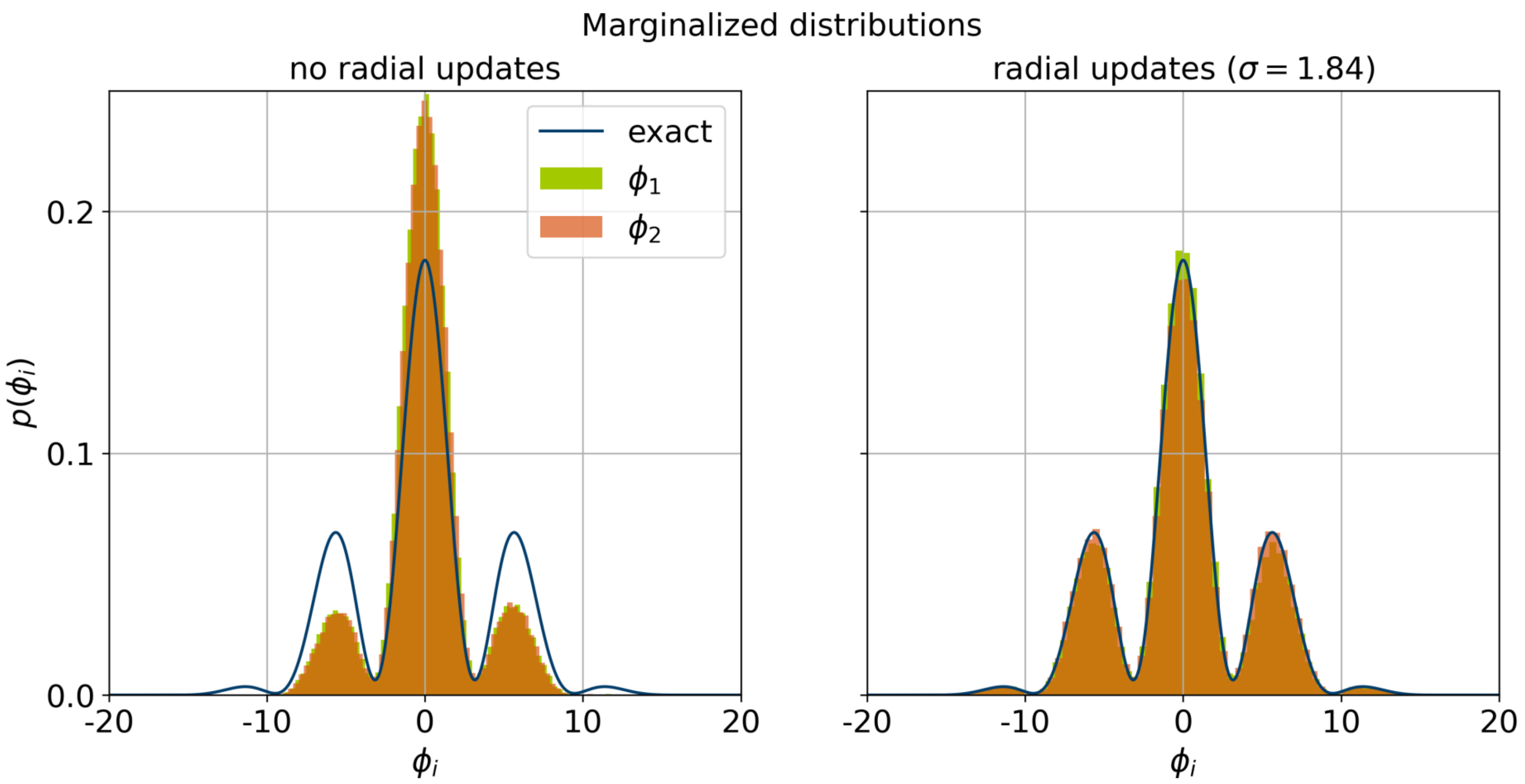

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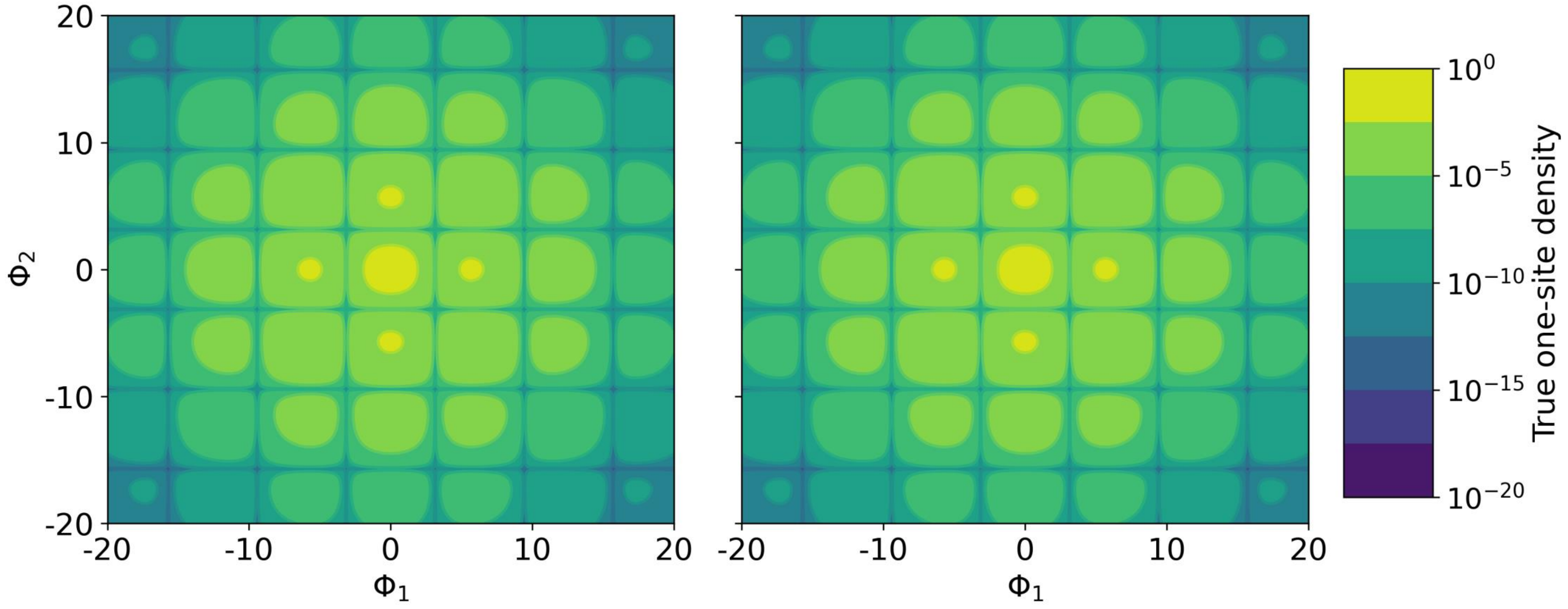
RESULTS

Resolving ergodicity violations

$$\Phi_x = \sum_t \phi_{xt}$$

$N_x = 2,\ N_t = 8,\ U = 18,\ \beta = \kappa = 1$



RESULTS

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$$\Phi_x = \sum_t \phi_{xt}$$

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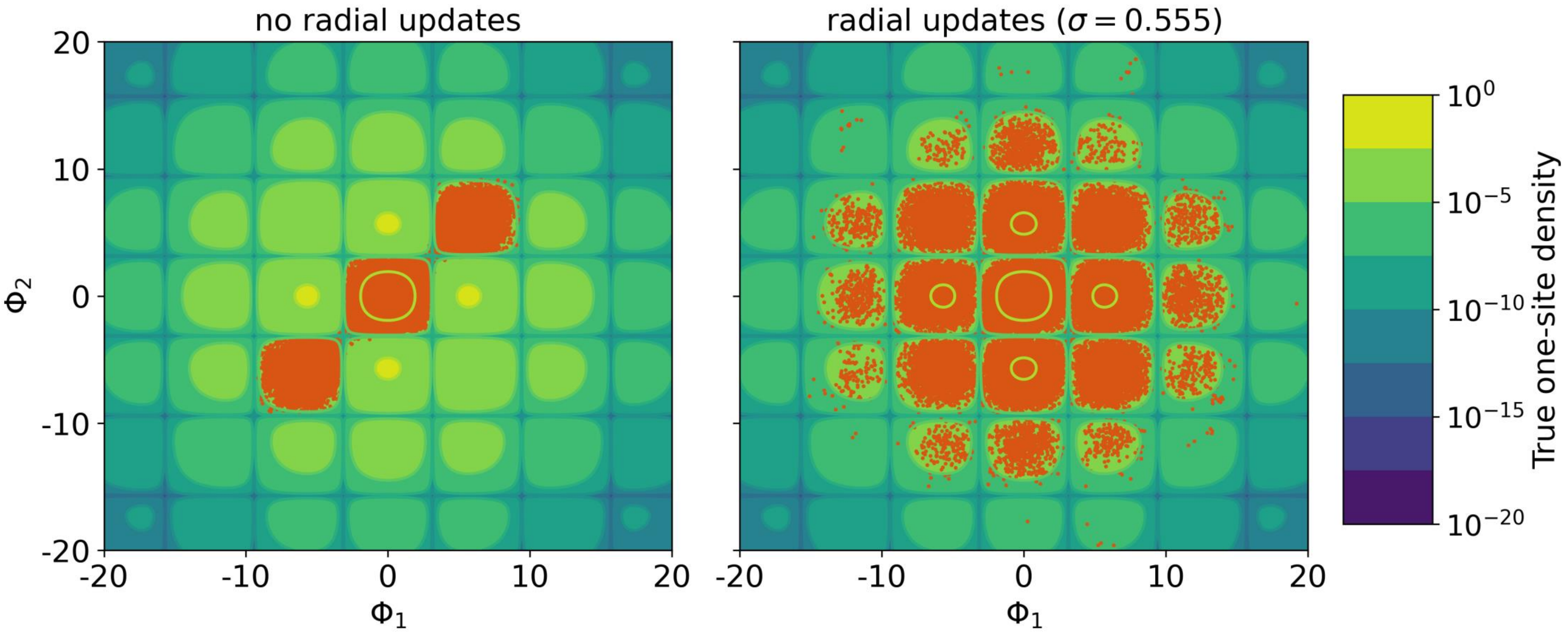


RESULTS

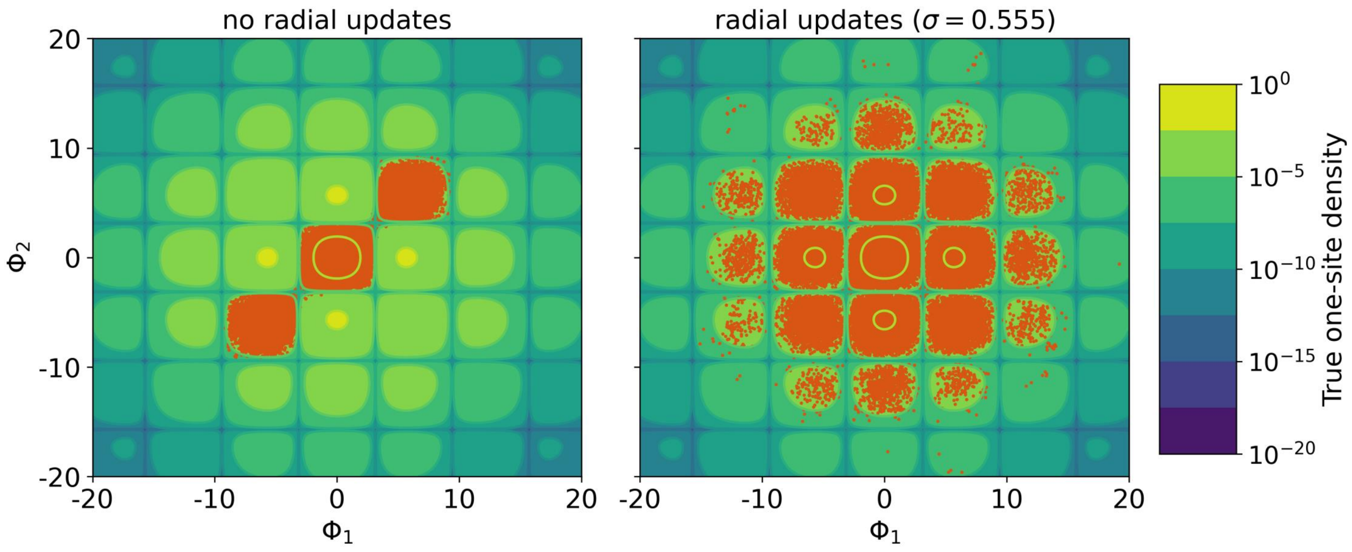
Autocorrelations, Scaling and Parameter Tuning

- Compute $\tau_{\mathcal{O},\mathrm{int}}$ as a function of σ for increasing N_t

RESULTS

Autocorrelations, Scaling and Parameter Tuning

- Compute $\tau_{\mathcal{O},\text{int}}$ as a function of σ for increasing N_t
- Consider two observables:
  - $\mathcal{O}_0 = \sqrt{\sum_x \Phi_x^2}$
  - $\mathcal{O}_1 = \sum_{xt} \phi_{xt}$ (charge)



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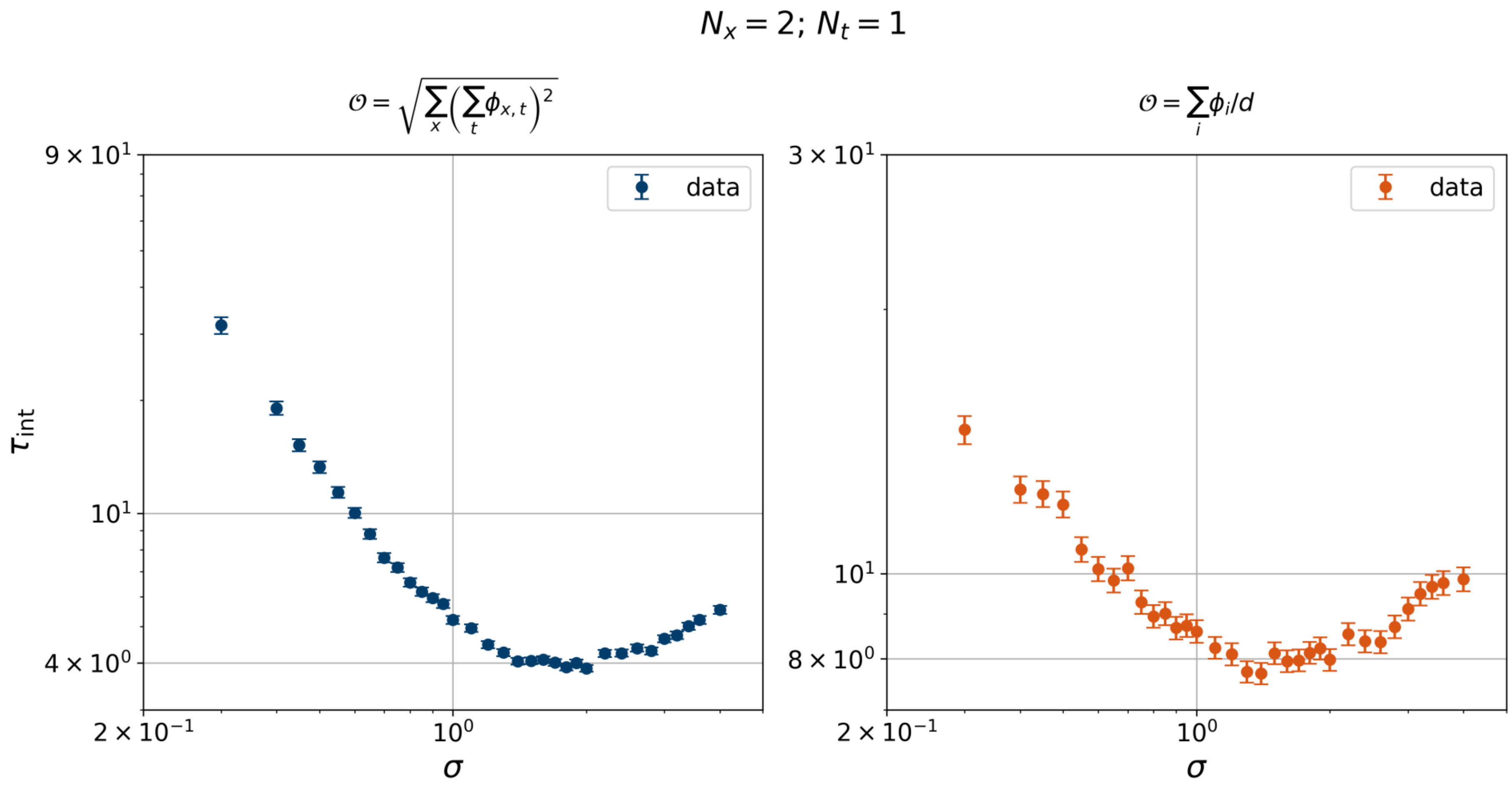

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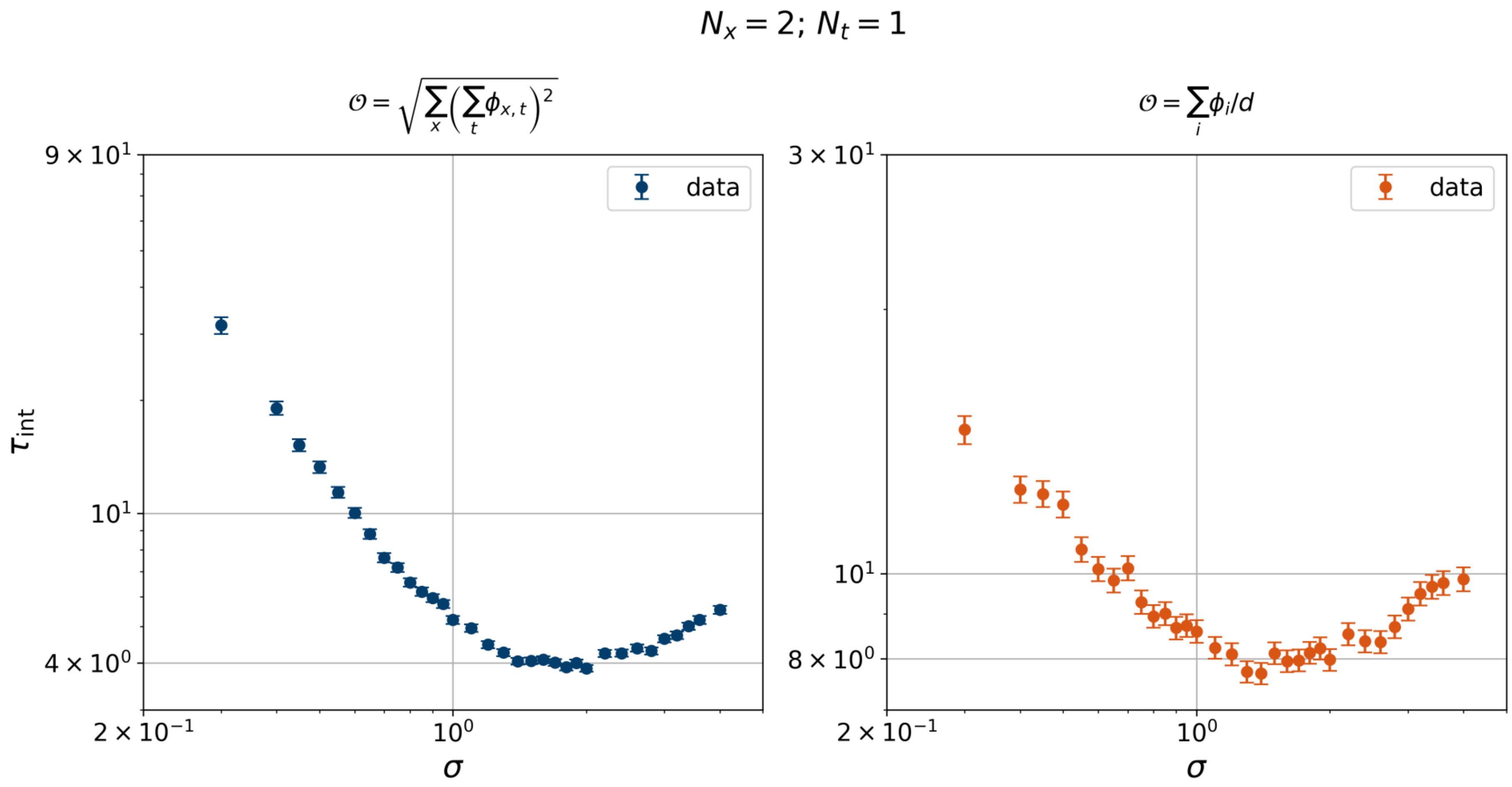
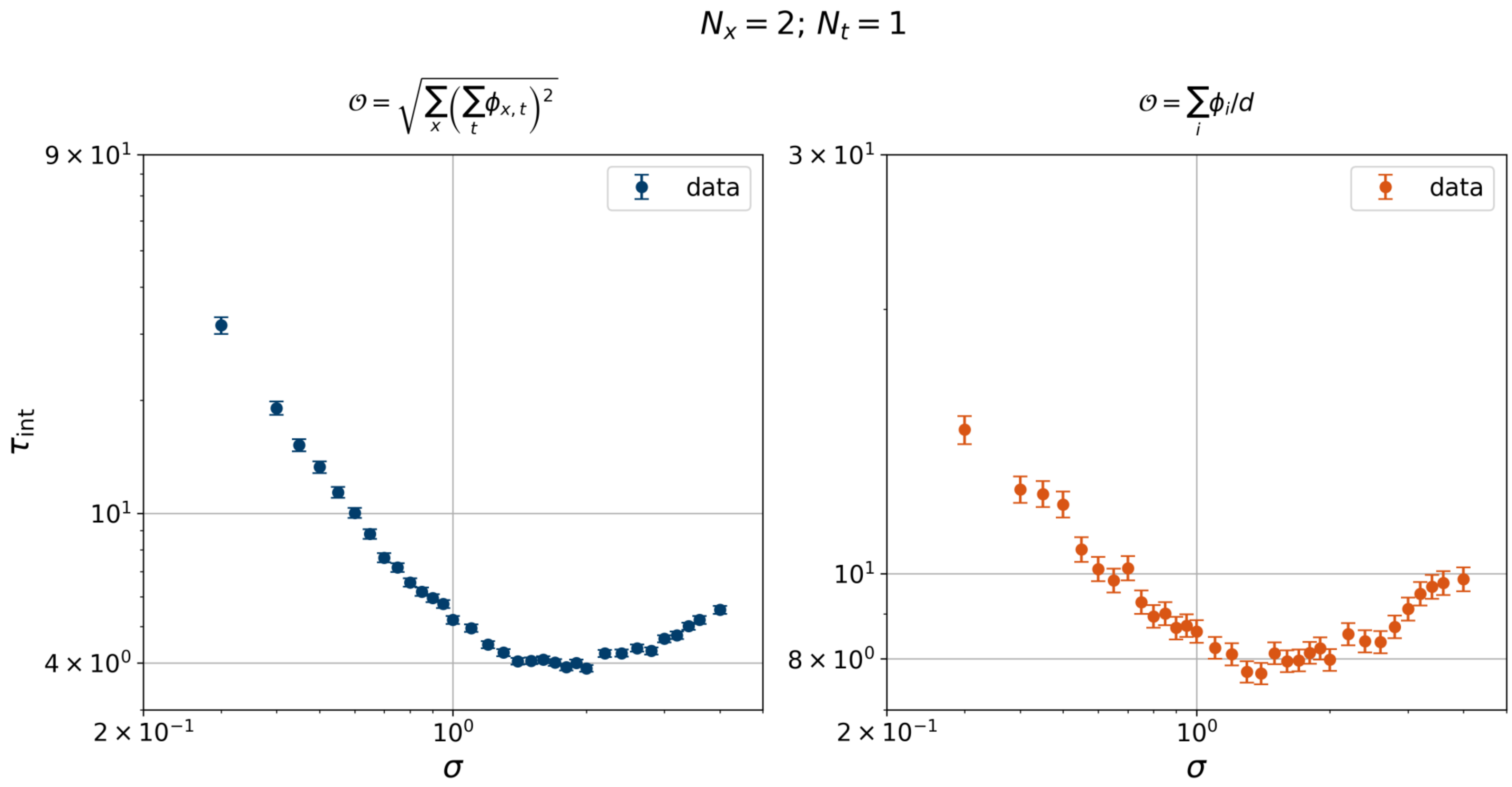


- Random walk and diffusive regime for small σ, i.e. $\tau_{\text{int}} \propto \sigma^{-2}$

RESULTS

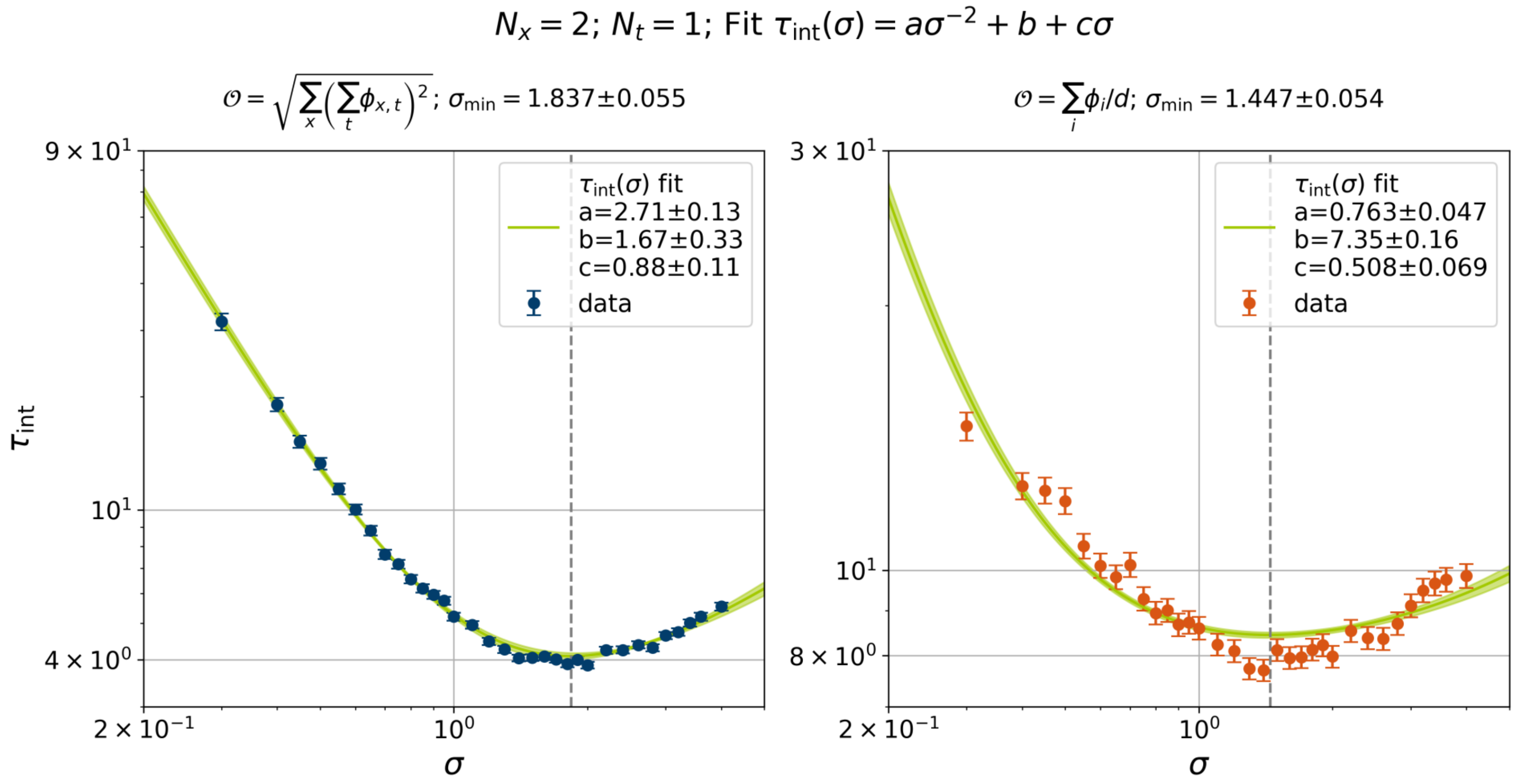
Autocorrelations, Scaling and Parameter Tuning



- Random walk and diffusive regime for small σ, i.e. $\tau_{\mathrm{int}} \propto \sigma^{-2}$
- Linear regime for large σ, i.e. $\tau_{\mathrm{int}} \propto \sigma$
- Fit function $\tau_{\mathrm{int}}(\sigma) = a\sigma^{-2} + b + c\sigma$

RESULTS

Autocorrelations, Scaling and Parameter Tuning



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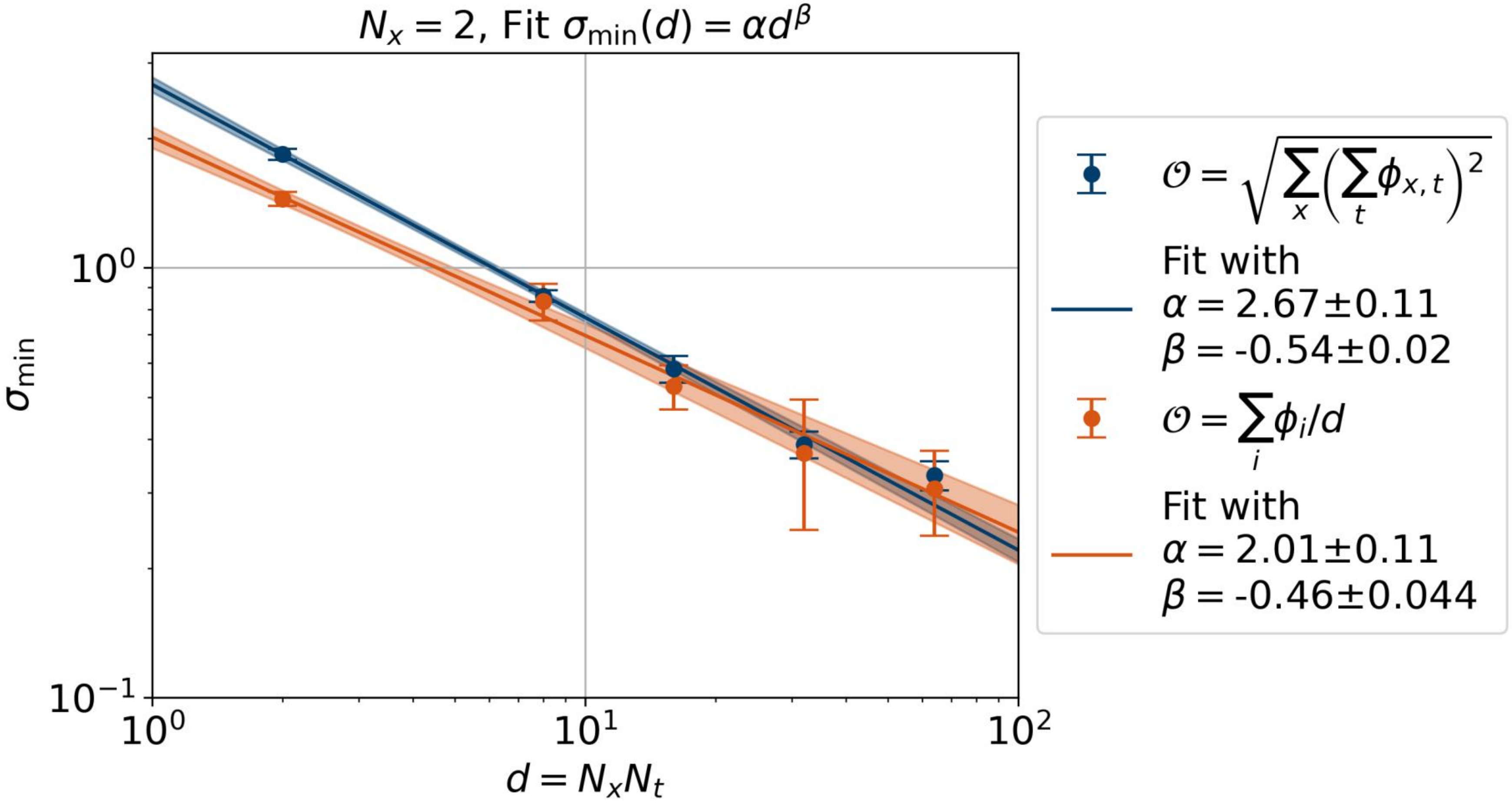
RESULTS

Autocorrelations, Scaling and Parameter Tuning



- From theoretical considerations

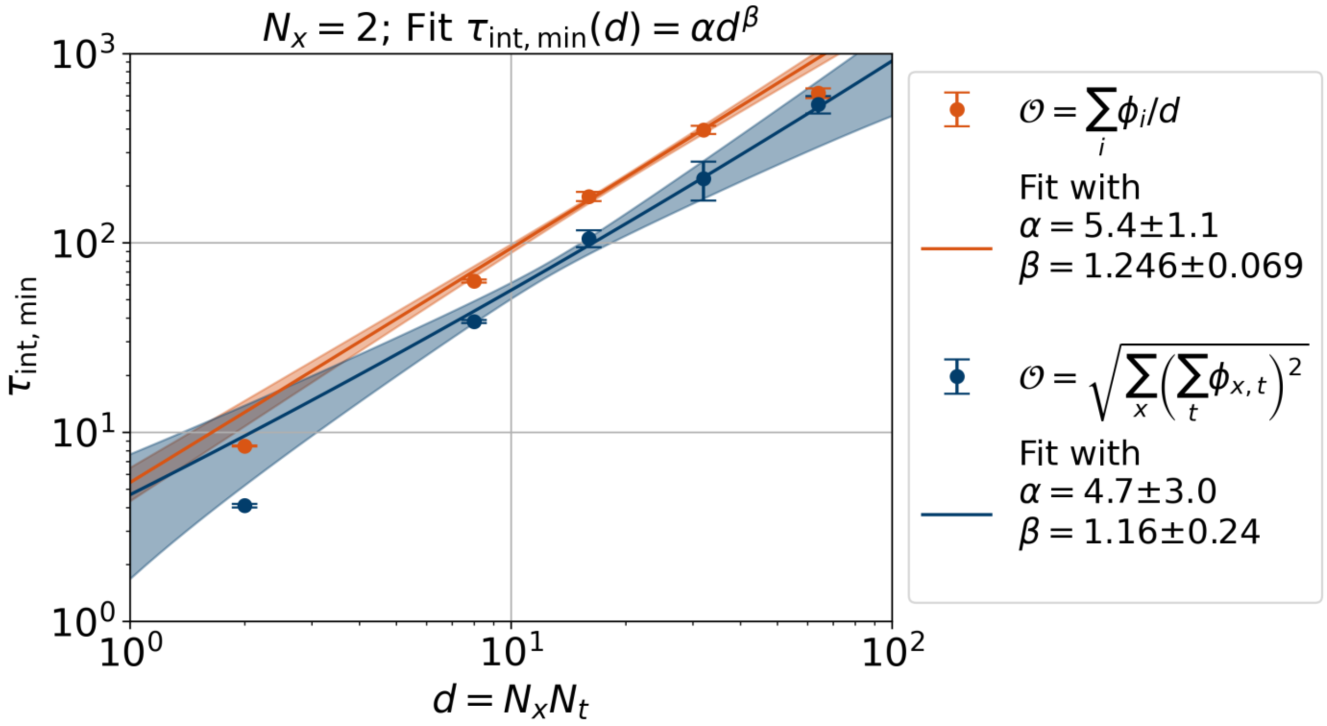
$$\sigma_{\min}(d) \propto d^{-0.5} + \mathcal{O}(d^{-1})$$

- Fit function

$$\sigma_{\min}(d) = \alpha d^{\beta}$$

RESULTS

Autocorrelations, Scaling and Parameter Tuning



- $\tau_{\text{int}}(\sigma_{\text{min}})$ scales almost linearly with d

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RESULTS

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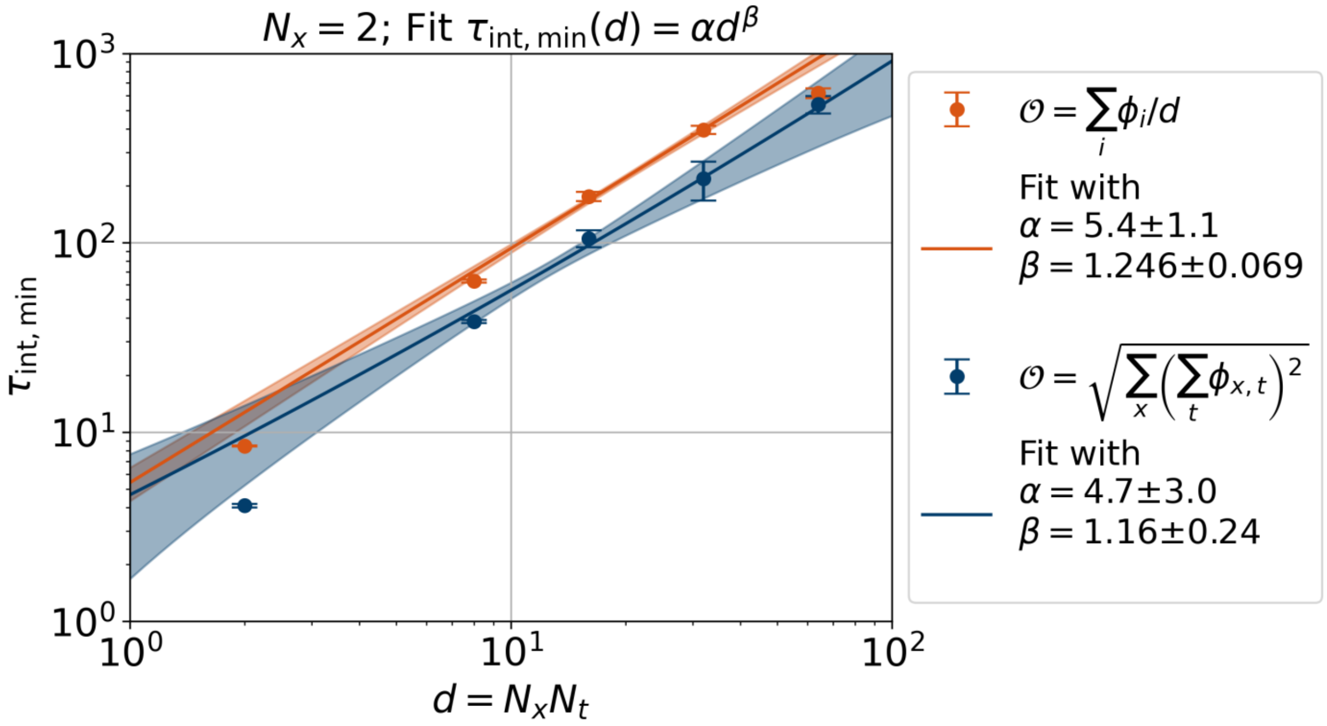

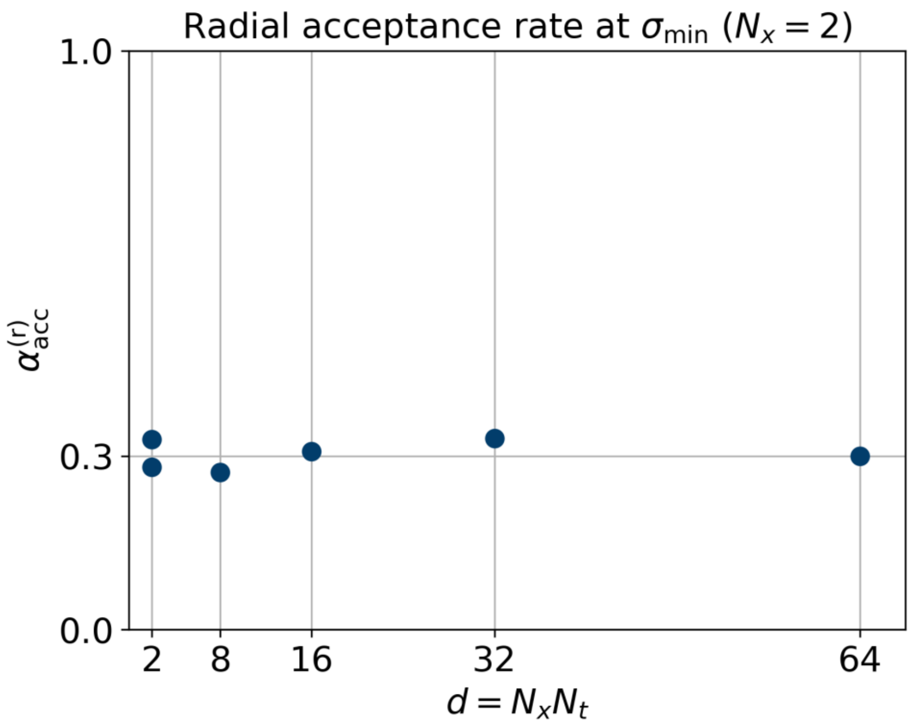

- $\tau_{\text{int}}(\sigma_{\text{min}})$ scales almost linearly with d

- At σ_{min} radial acceptance rate $\sim 30\%$

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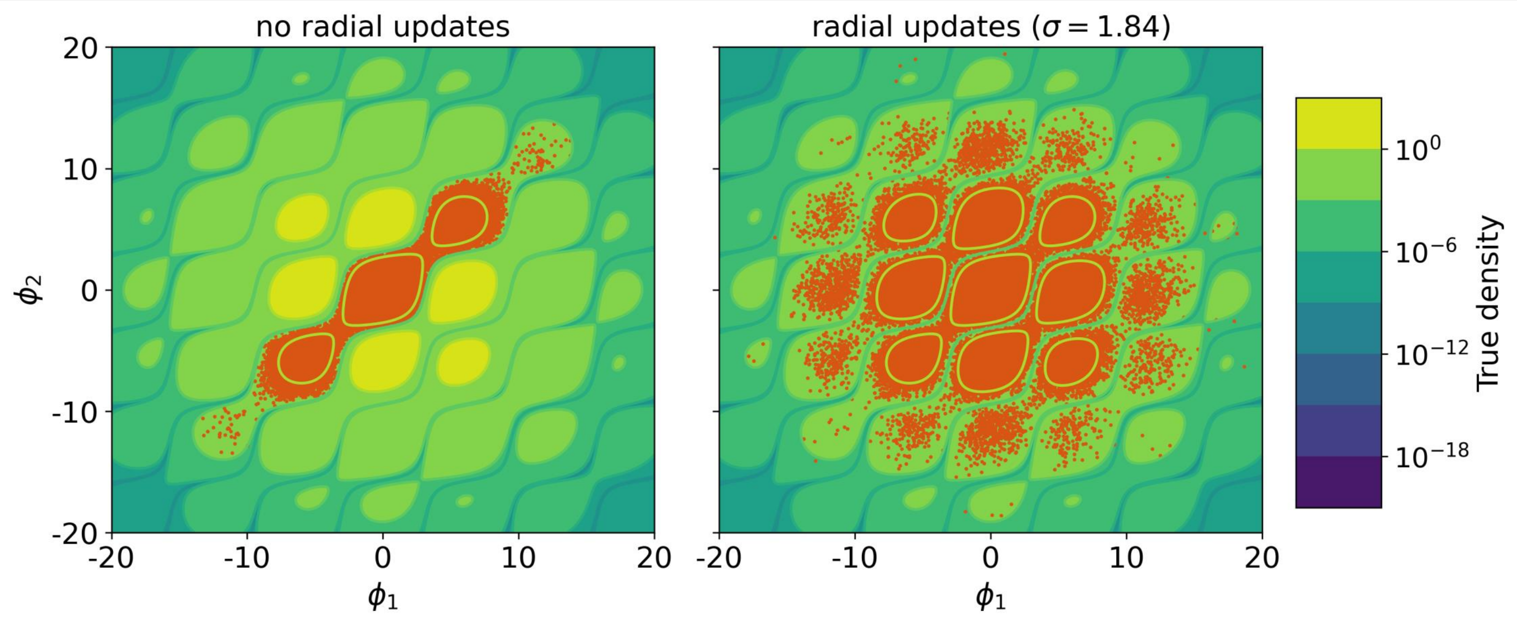
SUMMARY AND OUTLOOK

Take home message and future avenues

Radial updates successfully restore ergodicity in the Hubbard model

- Capability to jump over large or even infinite potential barriers



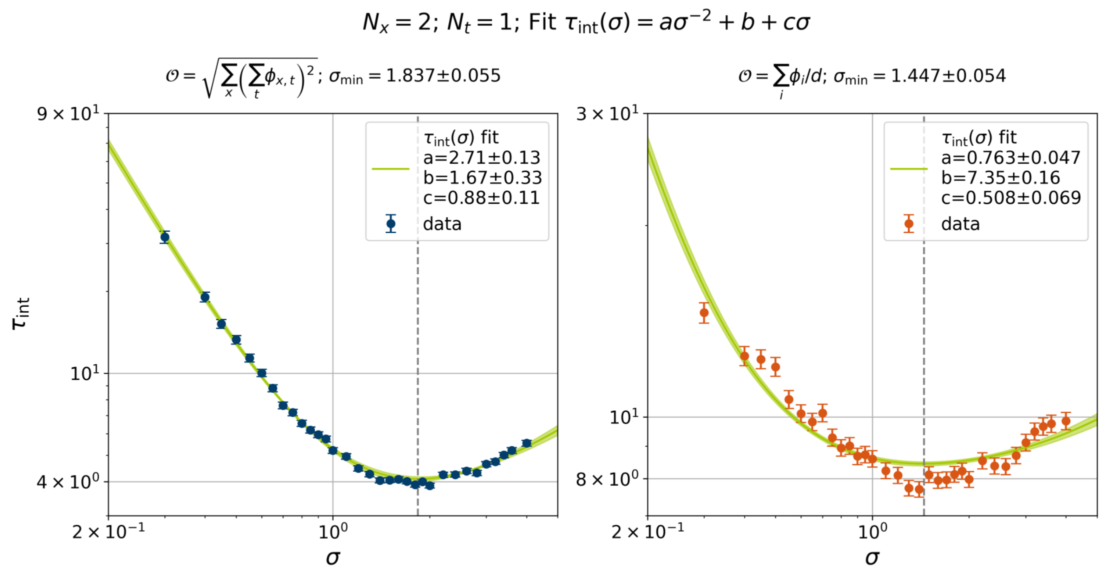
SUMMARY AND OUTLOOK

Take home message and future avenues

Radial updates successfully restore ergodicity in the Hubbard model

Radial updates reduce autocorrelations at low computational cost

- Can be used to tune additional parameter σ



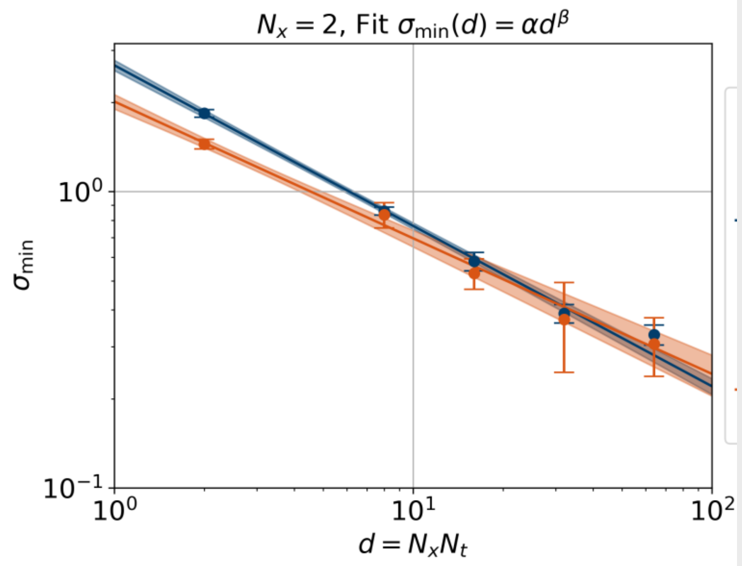
SUMMARY AND OUTLOOK

Take home message and future avenues

Radial updates successfully restore ergodicity in the Hubbard model

Radial updates reduce autocorrelations at low computational cost

- Can be used to tune additional parameter σ
- $\sigma_{\text{min}} \propto d^{-0.5}$ at leading order



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SUMMARY AND OUTLOOK

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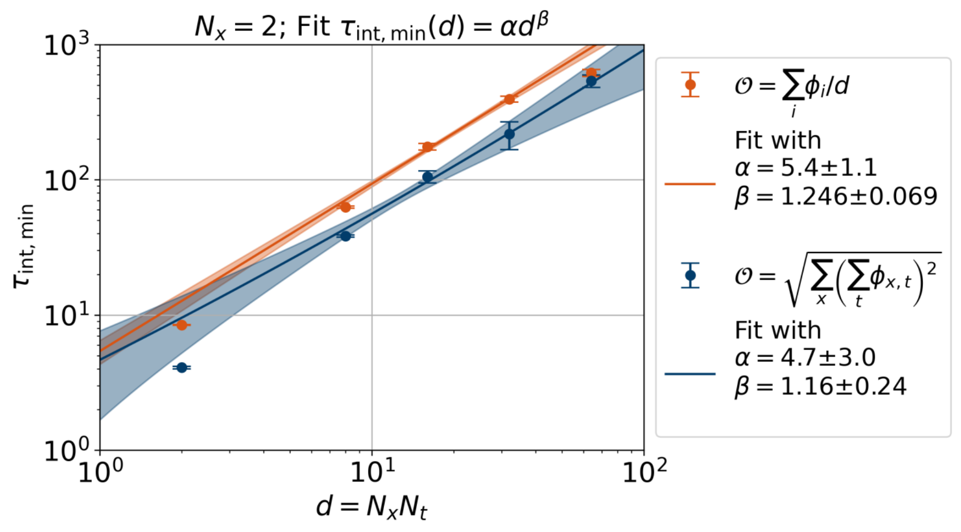
Radial updates successfully restore ergodicity in the Hubbard model

Radial updates reduce autocorrelations at low computational cost

- Can be used to tune additional parameter σ
- $\sigma_{\min} \propto d^{-0.5}$ at leading order
- τ_{int} scales almost linearly when employing radial updates



SUMMARY AND OUTLOOK

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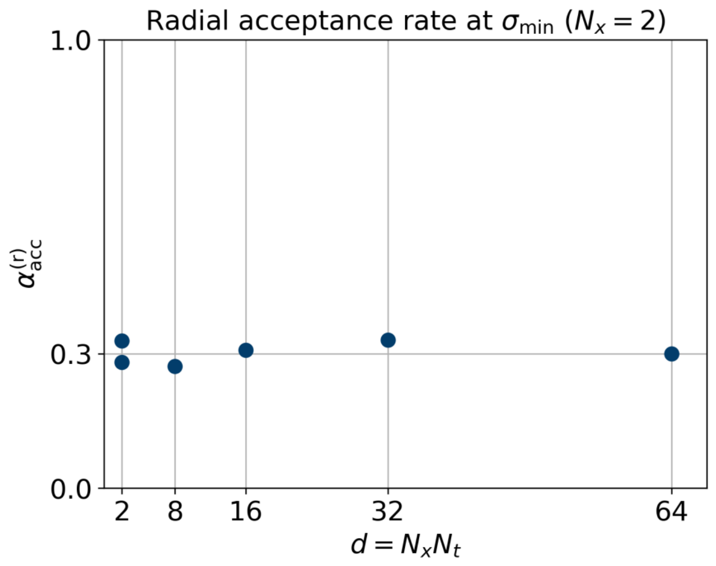
Radial updates successfully restore ergodicity in the Hubbard model

Radial updates reduce autocorrelations at low computational cost

- Can be used to tune additional parameter σ
- $\sigma_{\text{min}} \propto d^{-0.5}$ at leading order
- τ_{int} scales almost linearly when employing radial updates
- Optimal radial acceptance rate $\sim 30\%$



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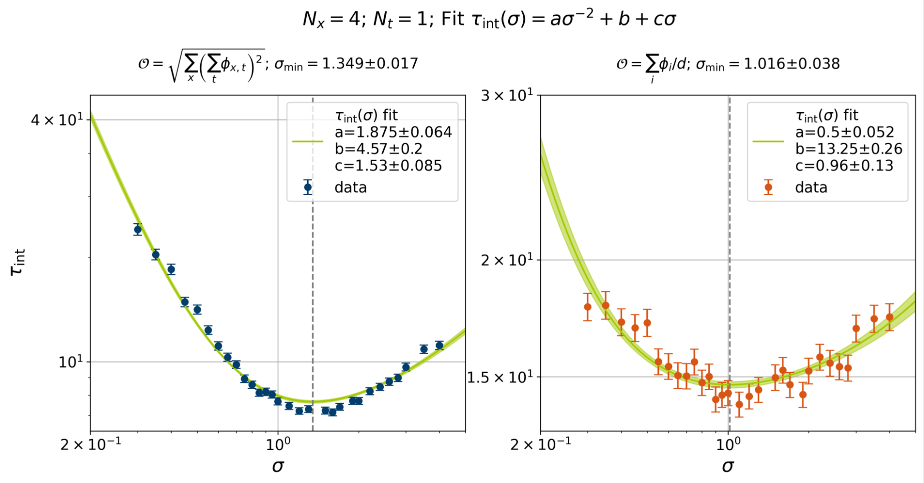
SUMMARY AND OUTLOOK

Take home message and future avenues

- **Radial updates successfully restore ergodicity in the Hubbard model**
- **Radial updates reduce autocorrelations at low computational cost**
- **Outlook: Scaling to larger systems and realistic simulation**
  - Increase N_x and add more spatial dimensions



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Radial updates reduce autocorrelations at low computational cost

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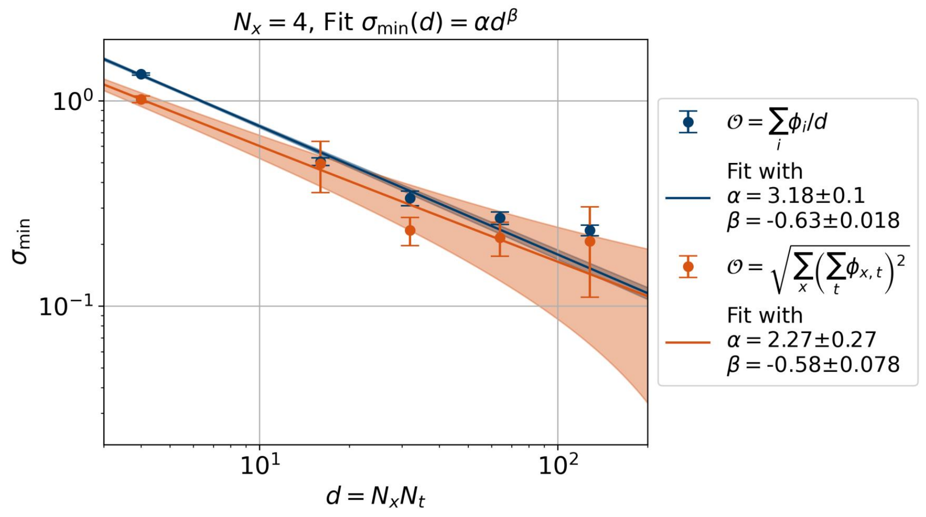

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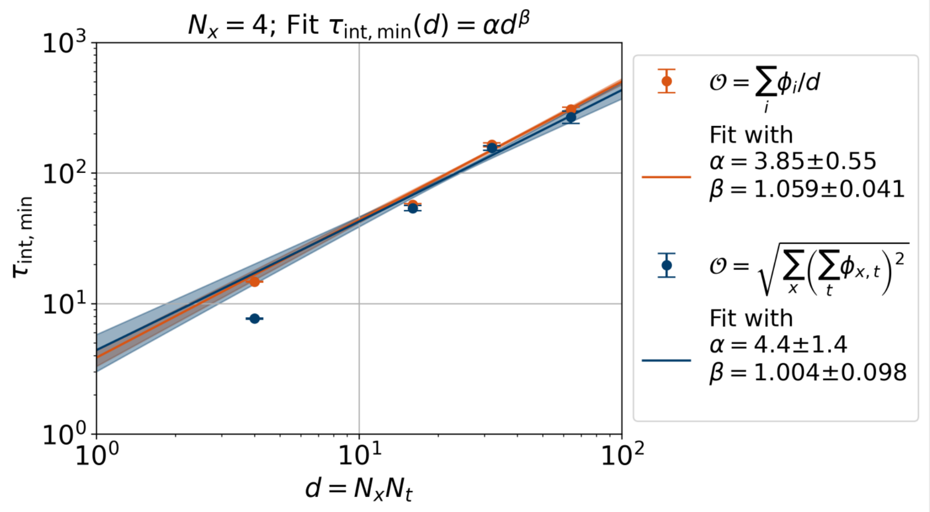

SUMMARY AND OUTLOOK

Take home message and future avenues

Radial updates successfully restore ergodicity in the Hubbard model

Radial updates reduce autocorrelations at low computational cost

Outlook: Scaling to larger systems and realistic simulation

- Increase N_x and add more spatial dimensions
- Perform realistic simulation with tuned acceptance rate, e.g. Perylene

Rodekamp et al., arXiv:2406.06711v1

SUMMARY AND OUTLOOK

Take home message and future avenues

Radial updates successfully restore ergodicity in the Hubbard model

Radial updates reduce autocorrelations at low computational cost

Outlook: Scaling to larger systems and realistic simulation

Bonus: Geometric convergence of HMC

- Talk by Xinhao Yu on Friday, August 2nd 2:55 PM

”On the geometric convergence of HMC on Riemannian manifolds.”

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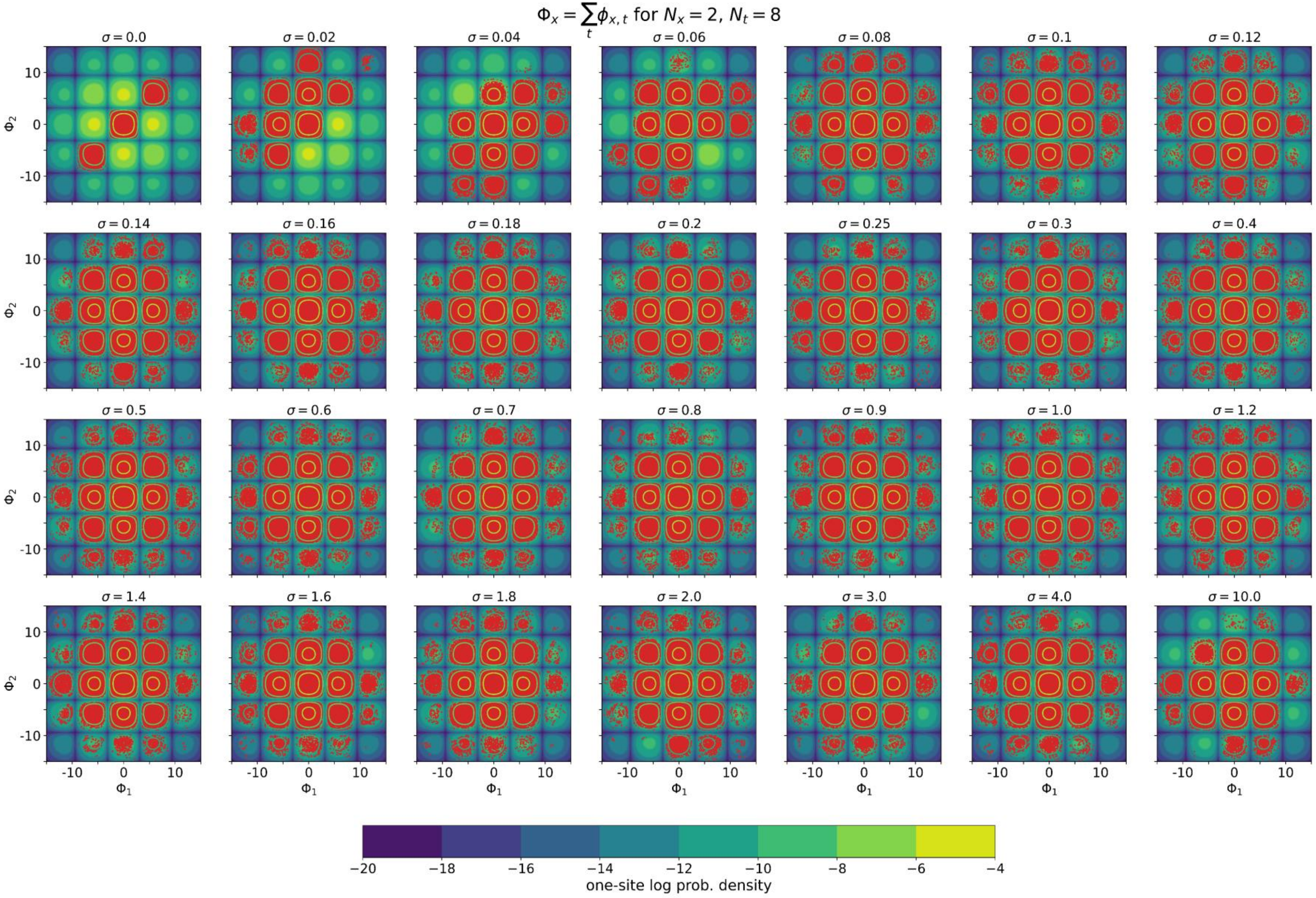
THANK YOU!

BACKUP SLIDES

RESULTS

Ergodicity for very small σ

- Strong ergodicity problem for $\sigma = 0$
- Reduced ergodicity problem for $\sigma \approx 0$ but slow exploration



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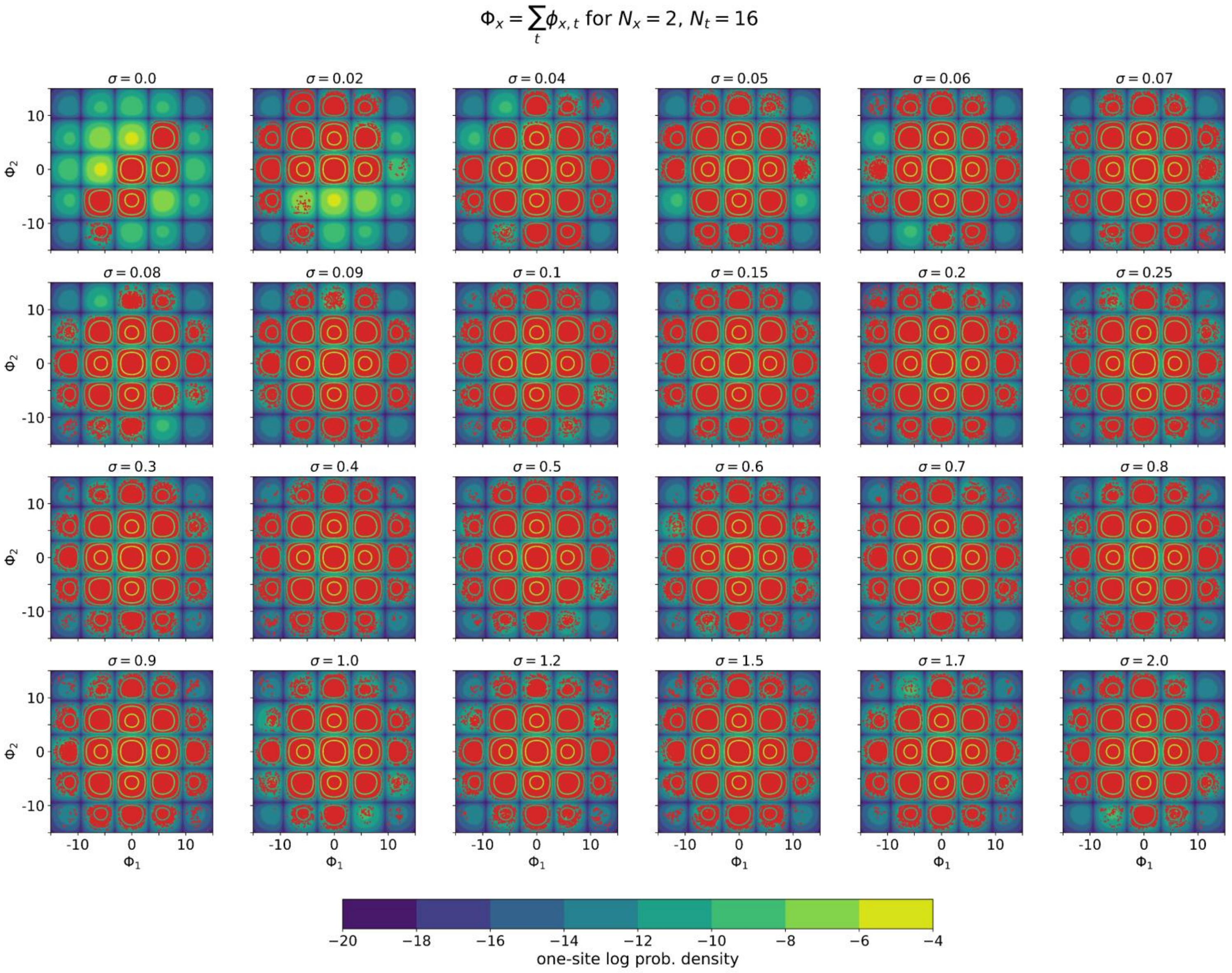
RESULTS

Tunneling of HMC

- In practice: energy violations due to imperfect MD
- HMC can tunnel through potential barriers
- Also happens at ∼99% acceptance rate for long trajectories



RADIAL UPDATES

The Algorithm - Pseudocode

```
function RADIAL_UPDATE(ϕ, σ)
    γ = SAMPLE_NORMAL(mean = 0, standard_deviation = σ^2)
    ϕ̃ = e^γ ϕ
    α = exp{−(S(ϕ̃) − S(ϕ)) + dγ}
    u = SAMPLE_UNIFORM(low = 0, high = 1)
    if u ≤ α then
        return ϕ̃
    else
        return ϕ
```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RADIAL UPDATES

The Algorithm - Pseudocode

for $i = 0$ to $\mathrm{N_{cfgs}}$ do

ϕ = HMC(ϕ)

if i % radial_frequency $==0$ then

for $j = 0$ to $\mathrm{N_{Radial}}$ do

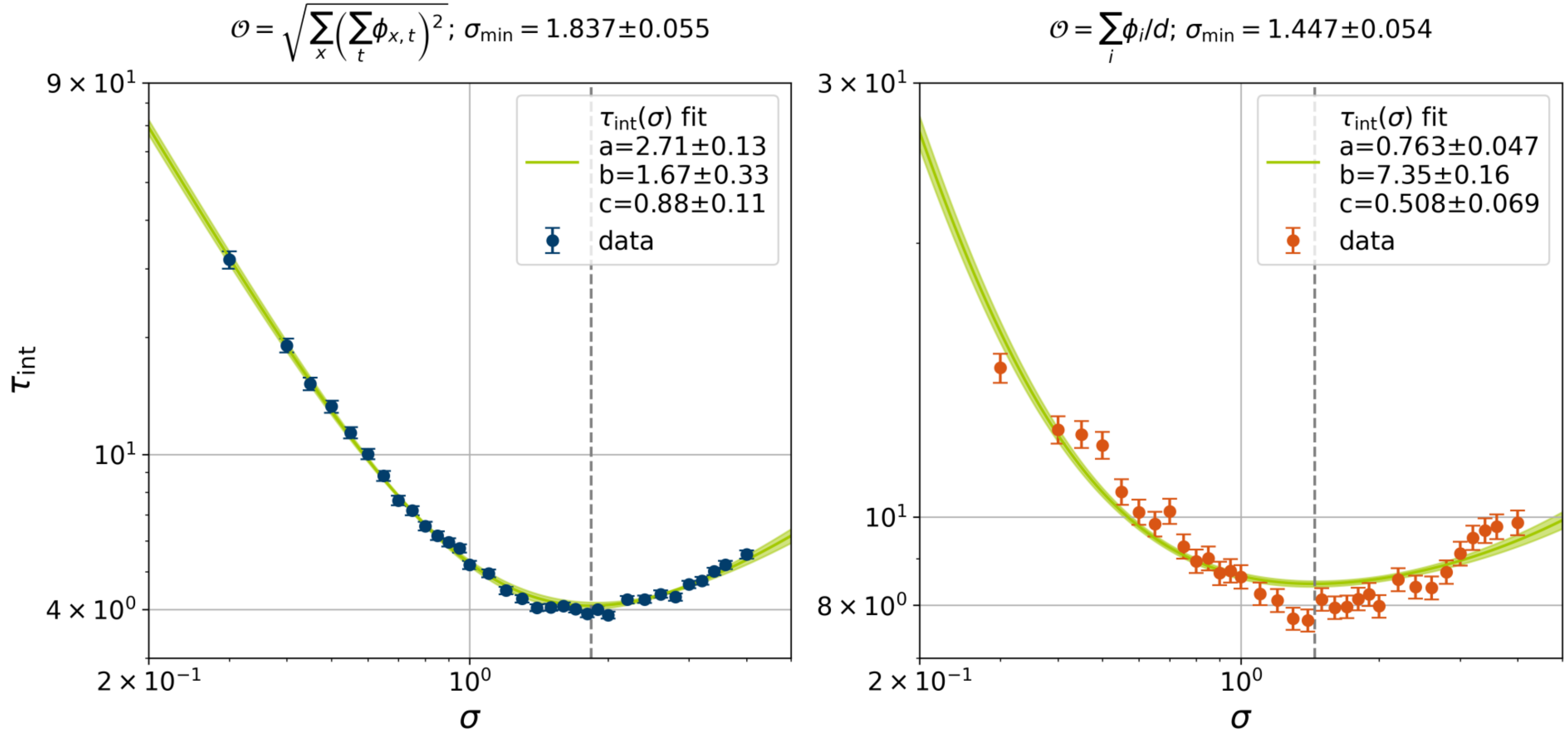
$\phi = \mathrm{RADIAL\_UPDATE}(\phi, \sigma)$

RESULTS
2-SITE MODEL

RESULTS

Autocorrelations, Scaling and Parameter Tuning

$N_x = 2;\ N_t = 1;$ Fit $\tau_{\mathrm{int}}(\sigma) = a\sigma^{-2} + b + c\sigma$

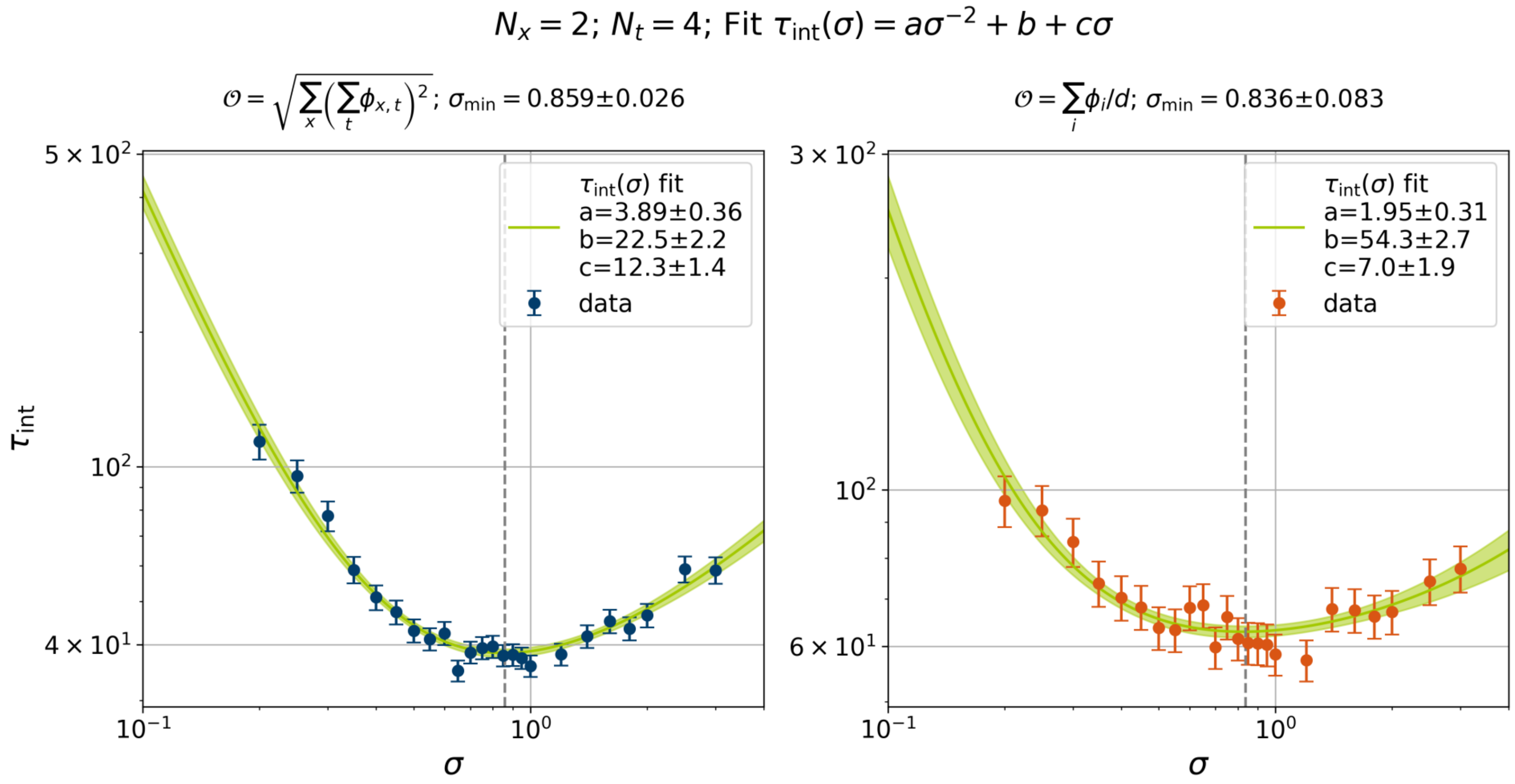


- Fit function

$$\tau_{\mathrm{int}}(\sigma) = a\sigma^{-2} + b + c\sigma$$

RESULTS

Autocorrelations, Scaling and Parameter Tuning



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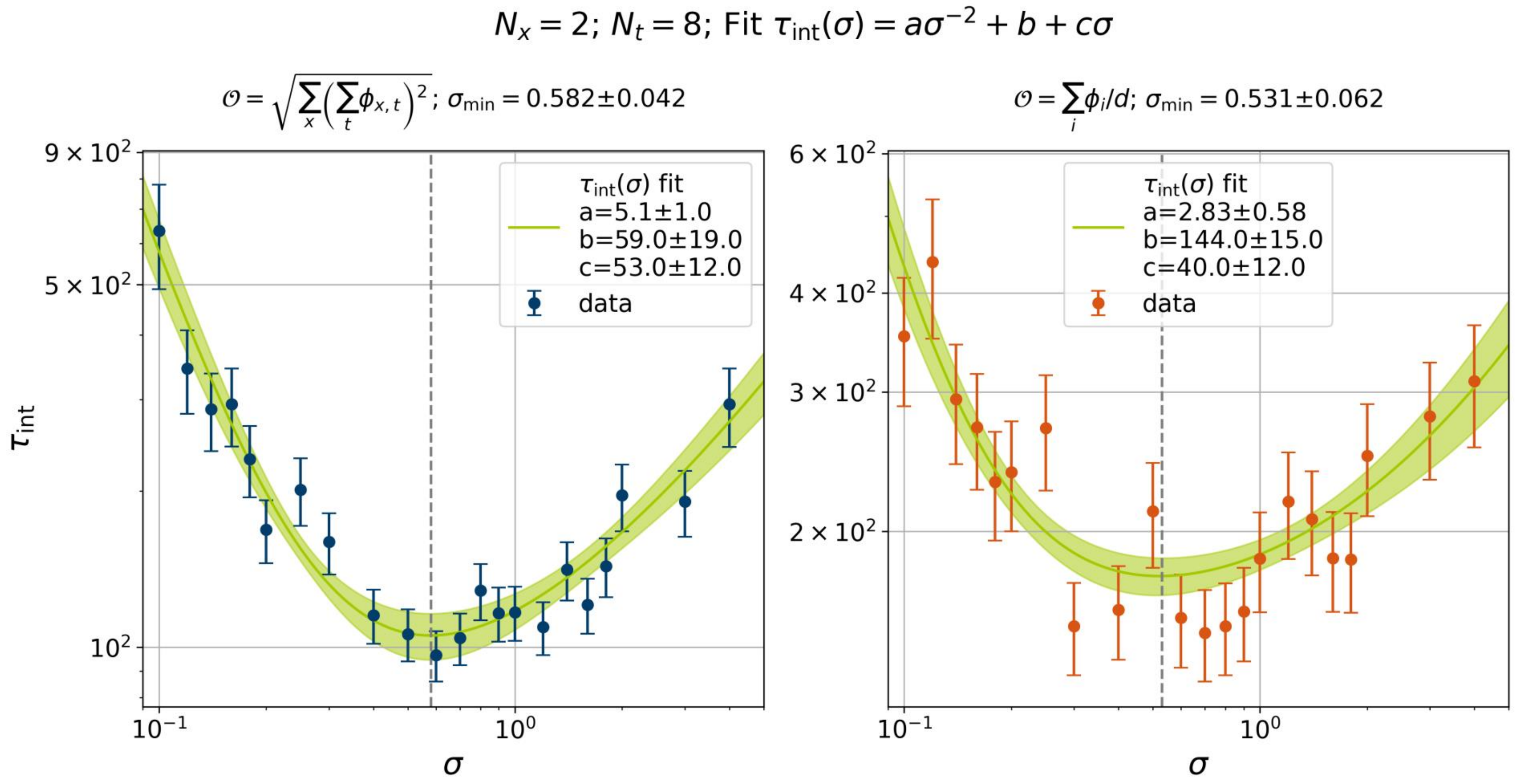

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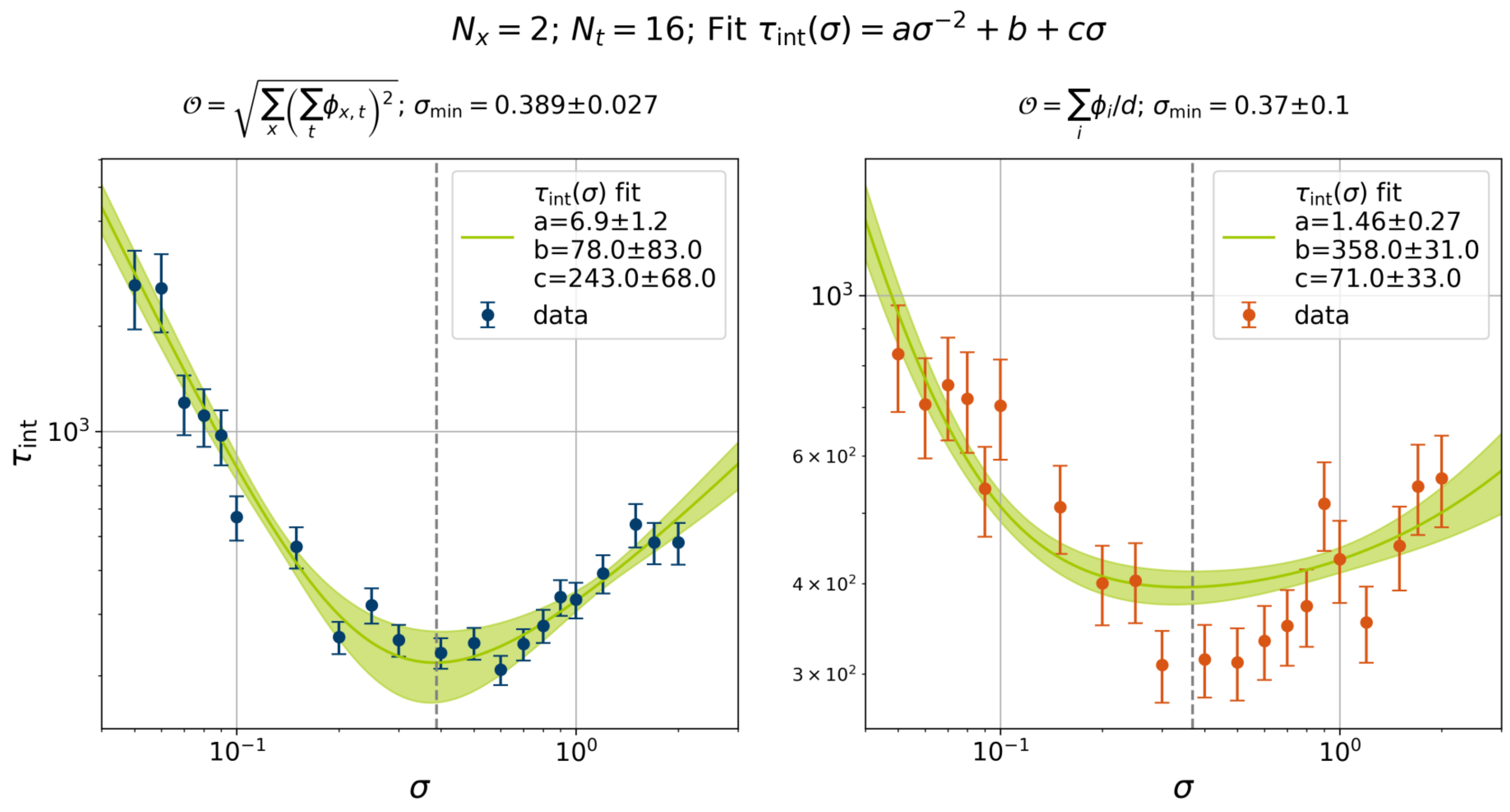

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RESULTS

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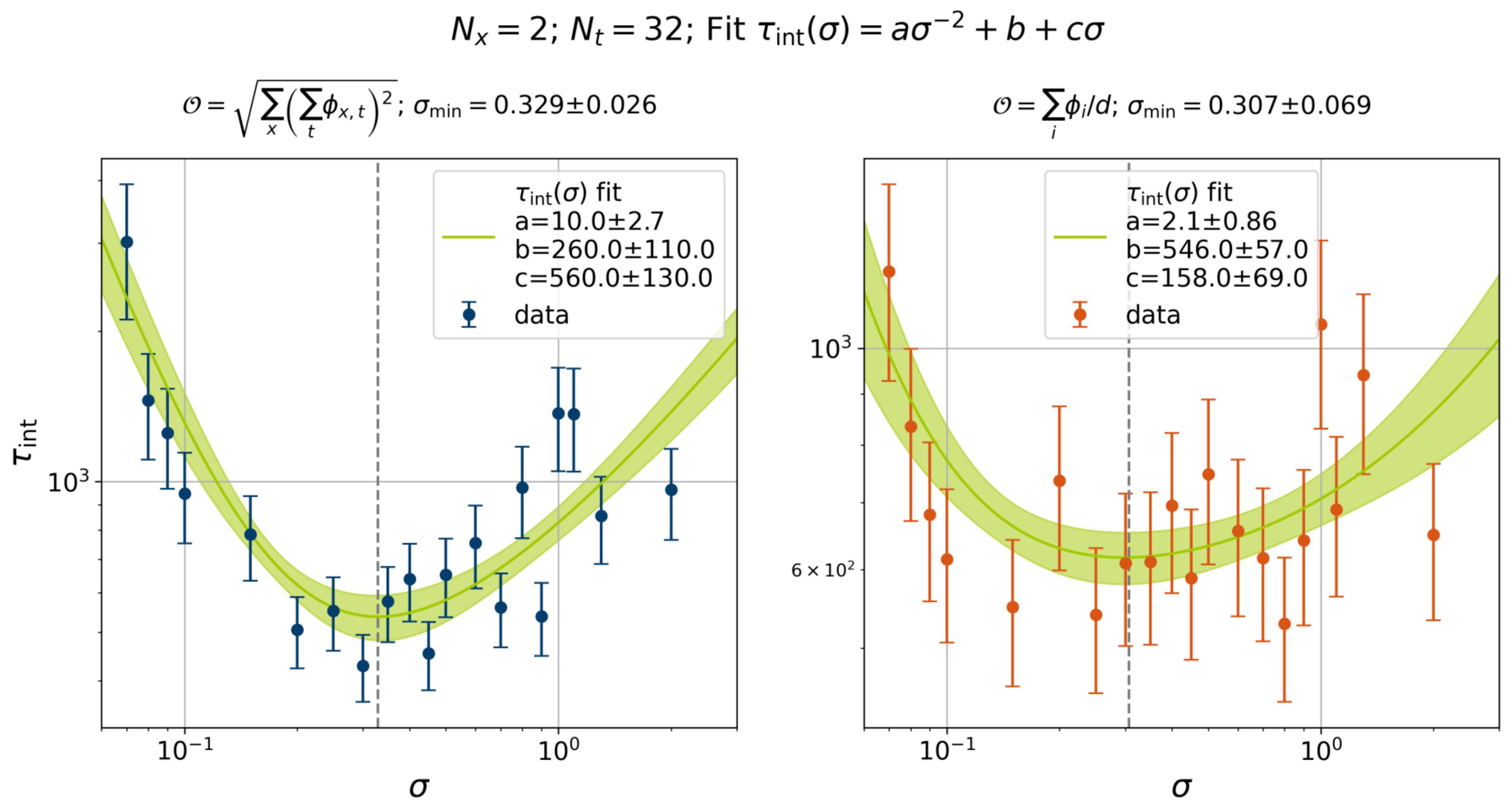

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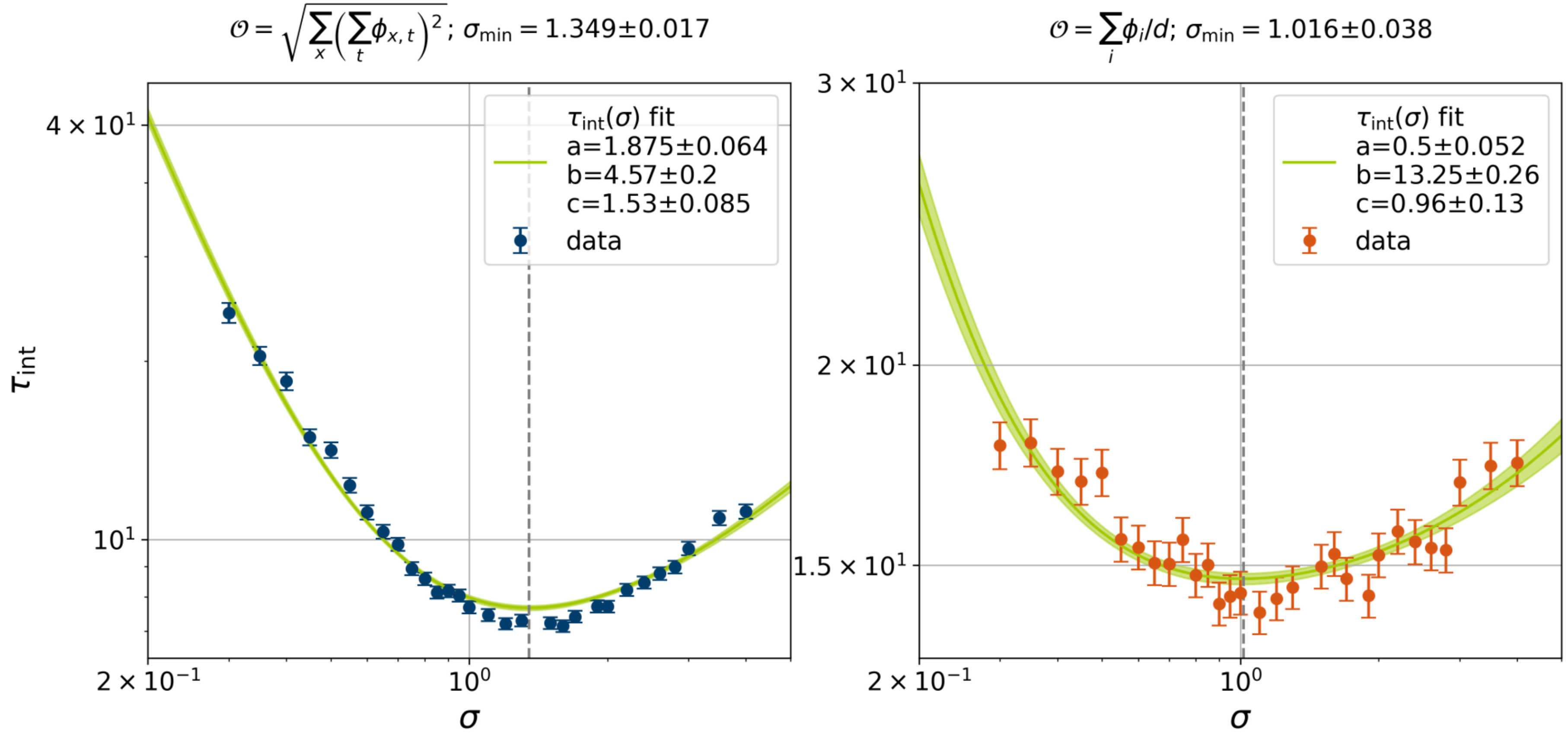
PRELIMINARY RESULTS
4-SITE MODEL

RESULTS – 4-SITE MODEL

Autocorrelations, Scaling and Parameter Tuning

$N_x = 4;\ N_t = 1;$ Fit $\tau_{\text{int}}(\sigma) = a\sigma^{-2} + b + c\sigma$



- Fit function

$$\tau_{\text{int}}(\sigma) = a\sigma^{-2} + b + c\sigma$$

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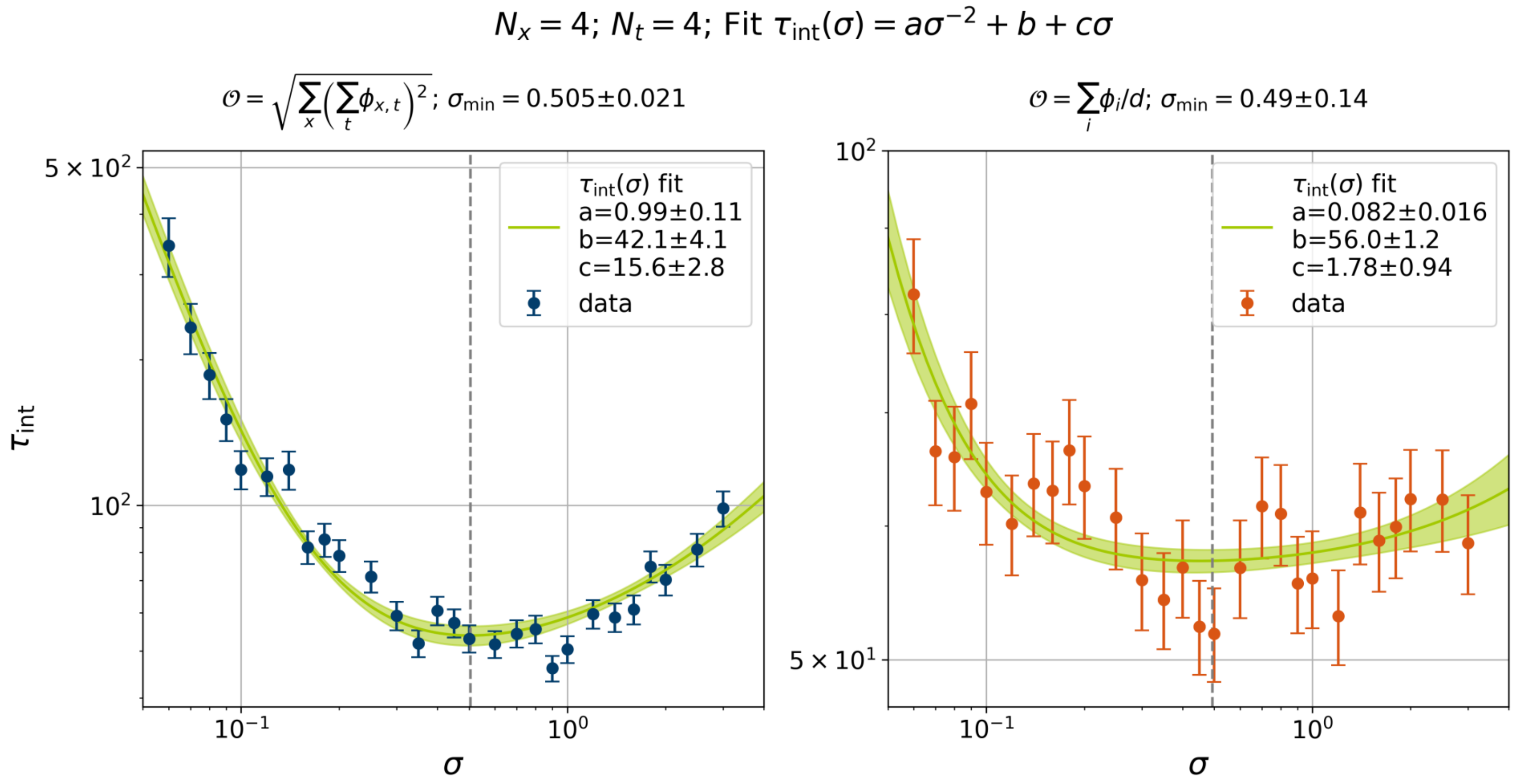
RESULTS – 4-SITE MODEL

Autocorrelations, Scaling and Parameter Tuning



- Fit function

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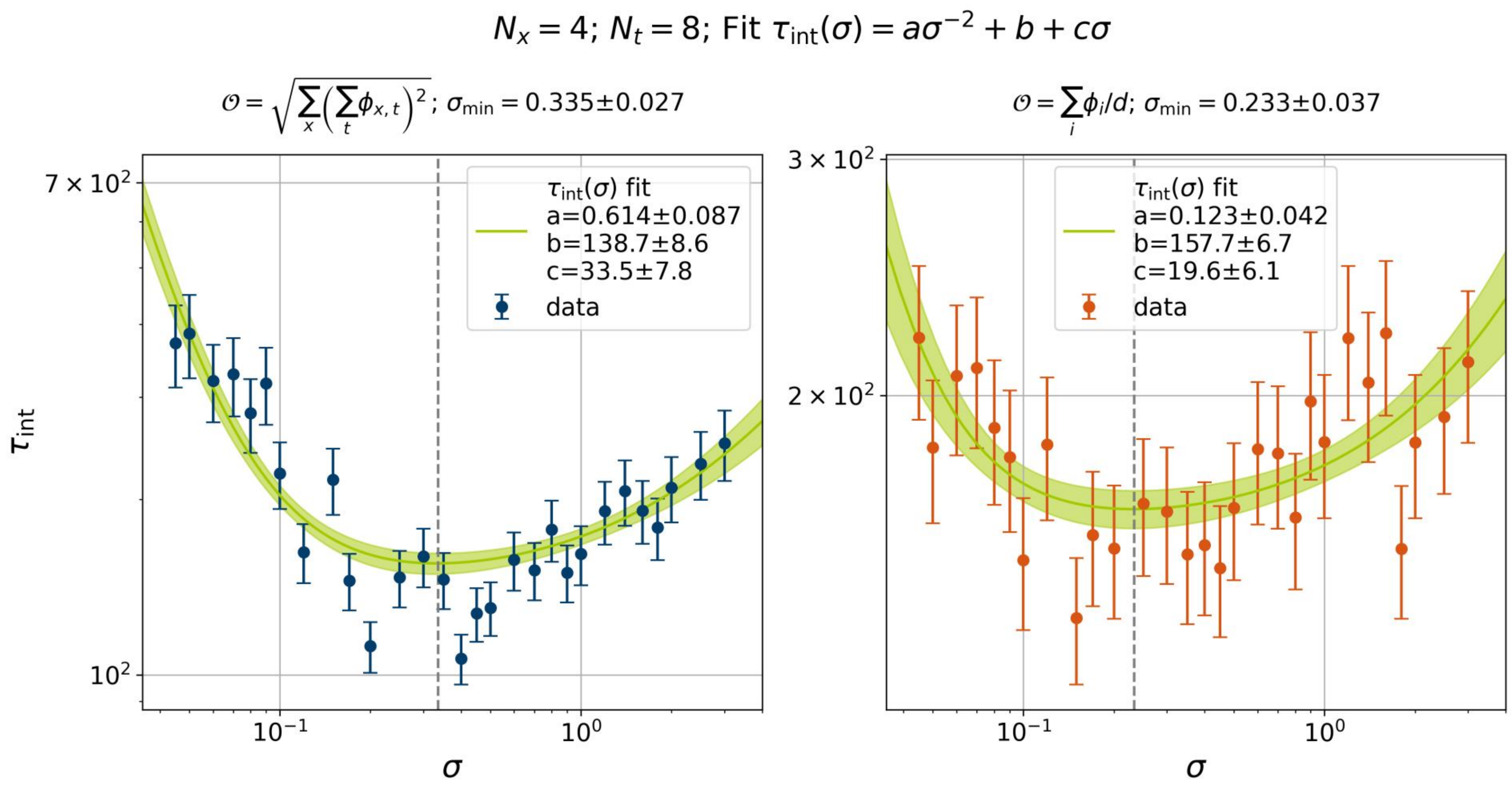
RESULTS – 4-SITE MODEL

Autocorrelations, Scaling and Parameter Tuning



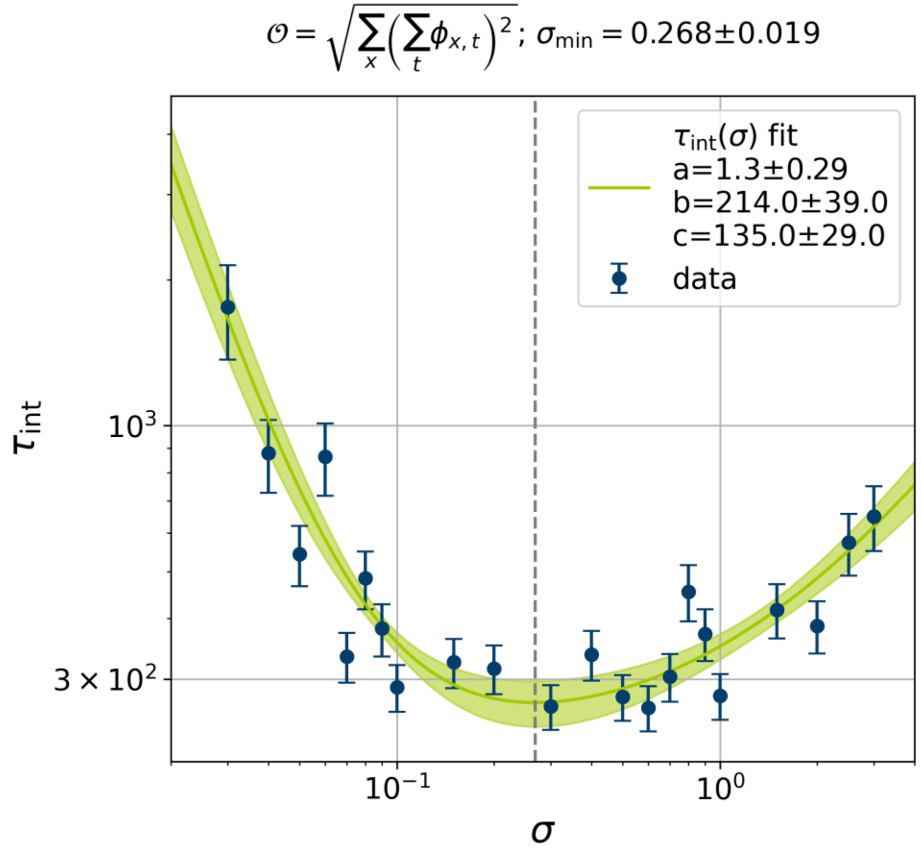
- Fit function

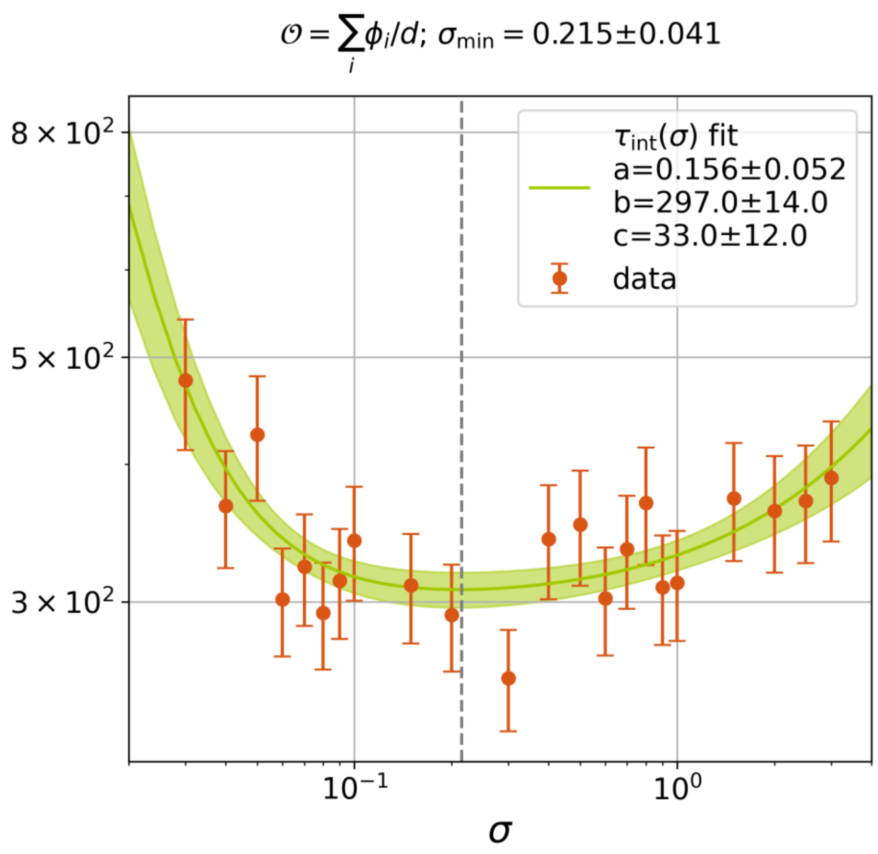
$$\tau_{\text{int}}(\sigma) = a\sigma^{-2} + b + c\sigma$$

RESULTS – 4-SITE MODEL

Autocorrelations, Scaling and Parameter Tuning

$N_x = 4$; $N_t = 16$; Fit $\tau_{\text{int}}(\sigma) = a\sigma^{-2} + b + c\sigma$





- Fit function

$$\tau_{\text{int}}(\sigma) = a\sigma^{-2} + b + c\sigma$$

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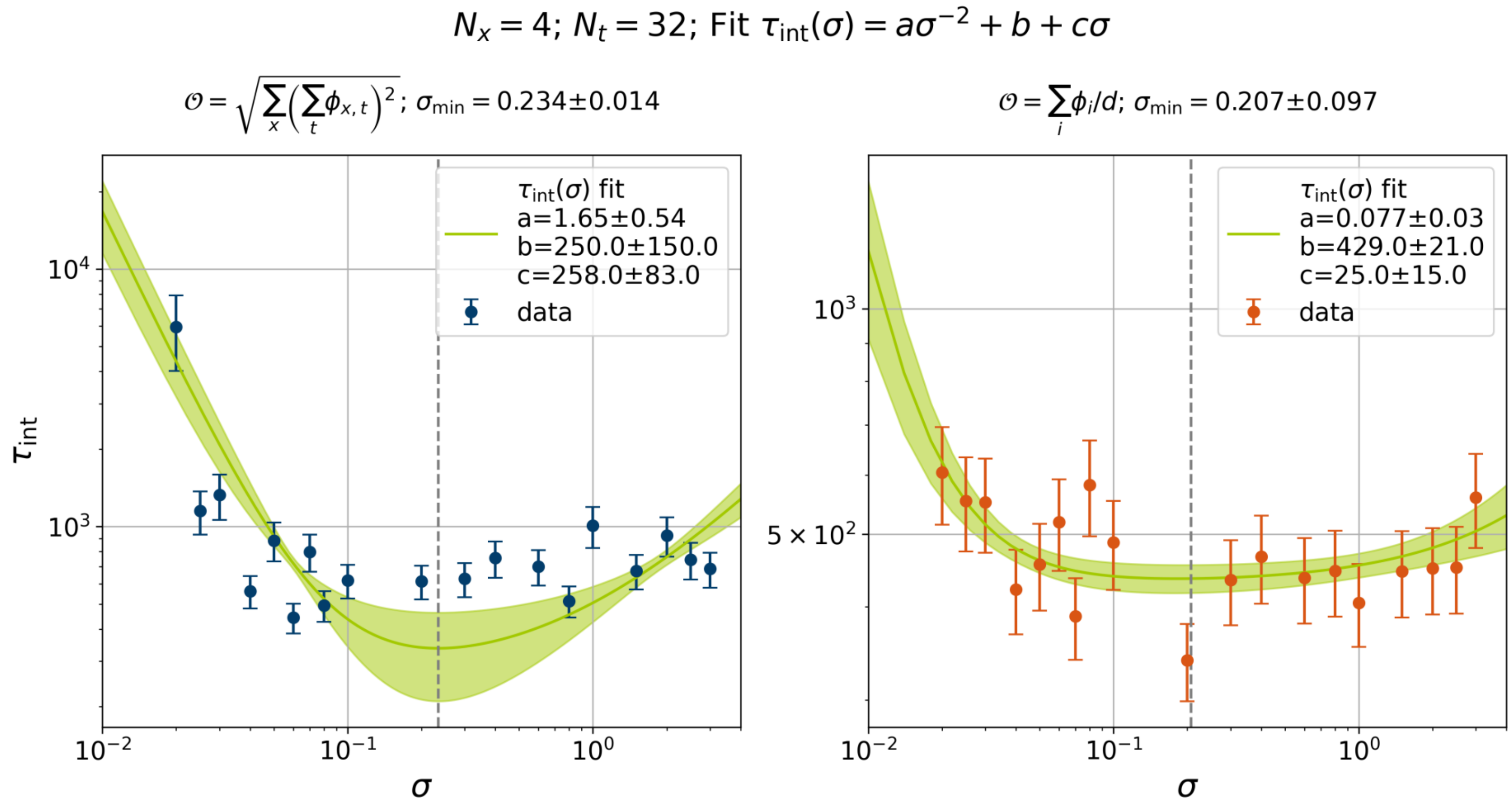
RESULTS – 4-SITE MODEL

Autocorrelations, Scaling and Parameter Tuning

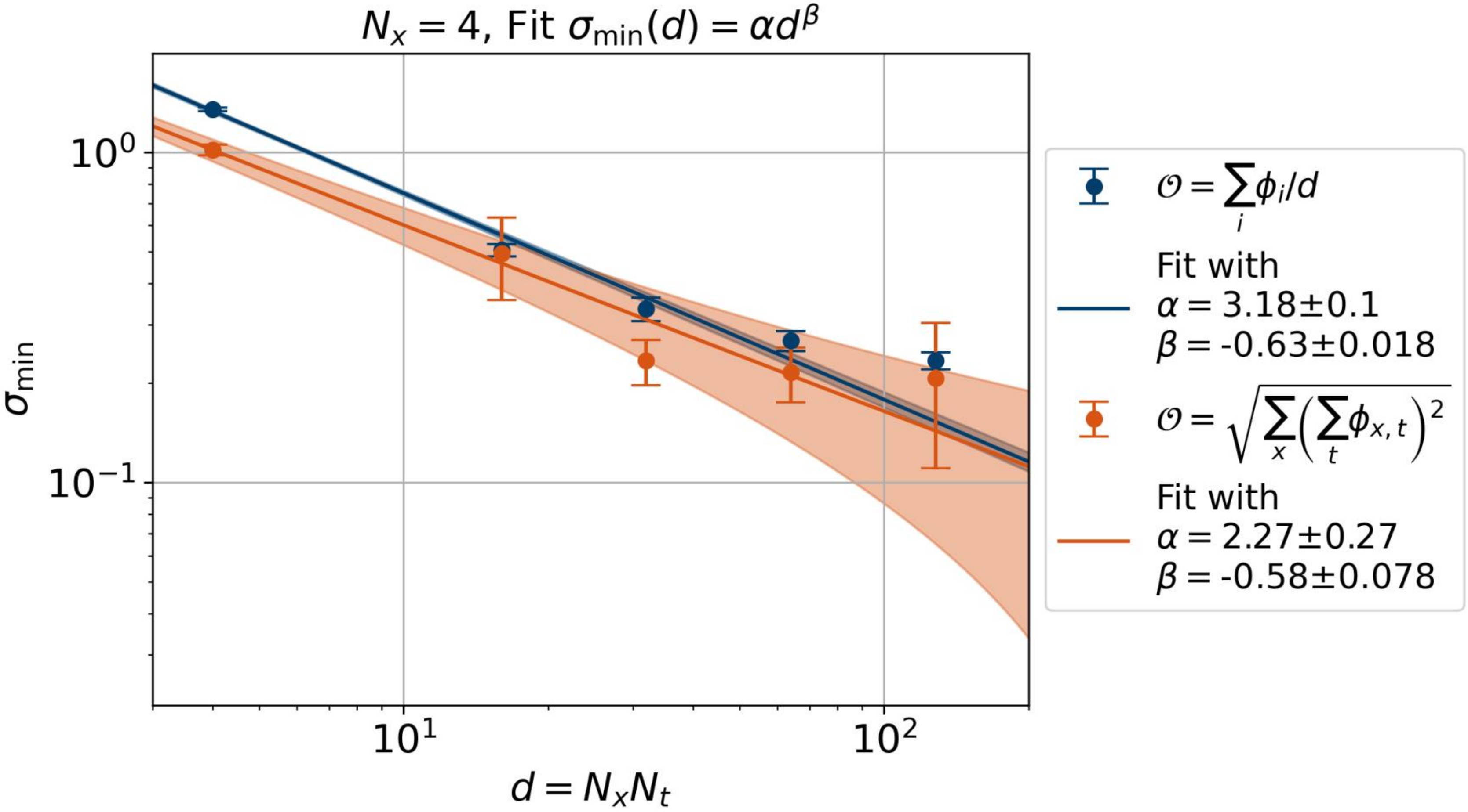


- Fit function

$$\tau_{\mathrm{int}}(\sigma) = a\sigma^{-2} + b + c\sigma$$

RESULTS – 4-SITE MODEL

Autocorrelations, Scaling and Parameter Tuning



- From theoretical considerations

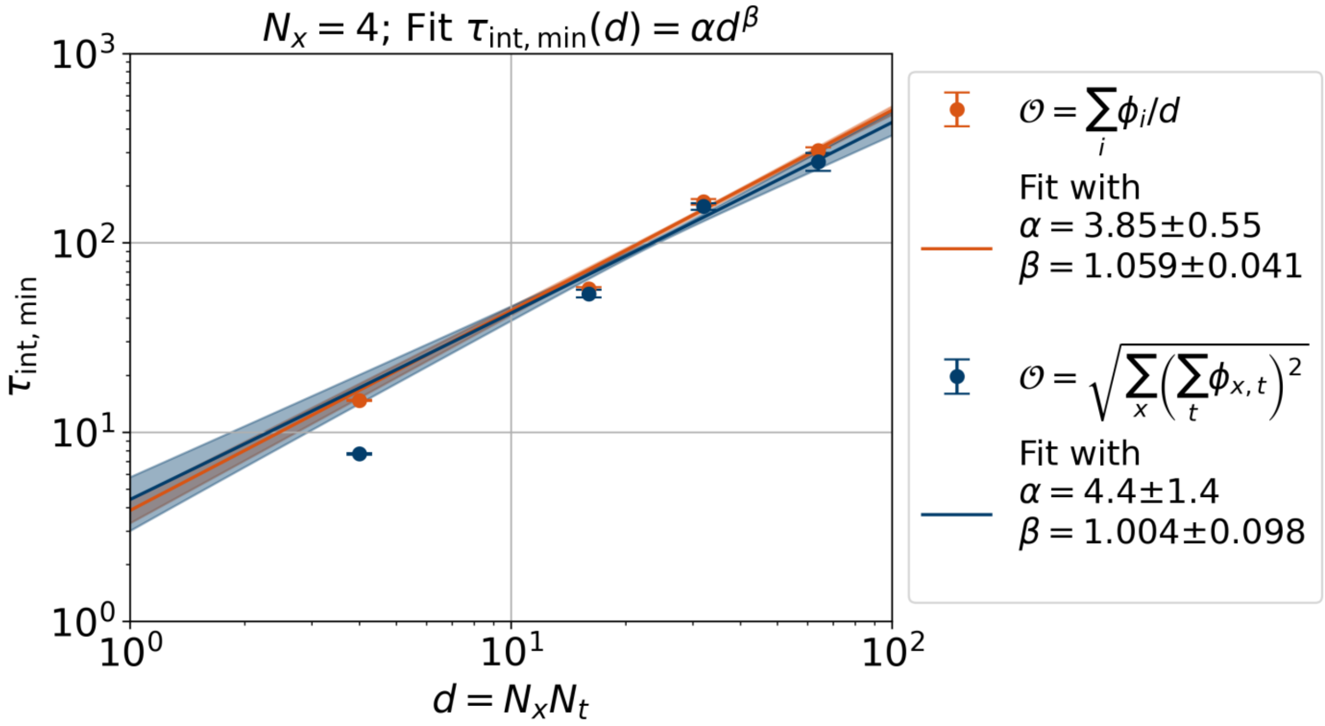
$$\sigma_{\min}(d) \propto d^{-0.5} + \mathcal{O}(d^{-1})$$

- Fit function

$$\sigma_{\min}(d) = \alpha d^{\beta}$$

RESULTS – 4-SITE MODEL

Autocorrelations, Scaling and Parameter Tuning



- $\tau_{\text{int}}(\sigma_{\text{min}})$ scales almost linearly with d

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