Numerical Methods for Quantum Discrete Phase Space Dynamics

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Motivation

- Exact diagonalization methods are unable to access large system sizes (N>>10)
- Methods like tDMRG, which are suitable for larger systems, are mostly applicable to low energies and are inefficient for >1D systems
- MFT is limited in capturing quantum correlations

Solution: Use the Wigner picture for QM to choose probability distribution and perform Monte Carlo!

Outline

1. Review of quantum phase space dynamics
2. Construction of a discrete phase space
3. DTWA protocol + Benchmarking
4. Case Studies: a) Squeezing a) Power Law Dynamics
5. Future Directions

Wigner Picture for Quantum Phase Space

- equivalent formulation of QM in terms quasi-probability distribution

Wavefunction $\psi(x) \leftrightarrow \psi(p)$

Wigner function

$$W(x,p) = \frac{1}{\pi\hbar}\int_{-\infty}^{\infty} ds\ e^{ips/\hbar}\ \psi^*(x+s/2)\ \psi(x-s/2)$$

- easily generalized for density matrix QM

Phase point operator

$$\langle \boldsymbol{q}' | \hat{A}(\boldsymbol{q},\boldsymbol{p}) | \boldsymbol{q}'' \rangle = \frac{1}{(2\pi)^D}\,\delta\left(\boldsymbol{q} - \frac{\boldsymbol{q}'+\boldsymbol{q}''}{2}\right)\ e^{i\boldsymbol{p}\cdot(\boldsymbol{q}'-\boldsymbol{q}'')}$$

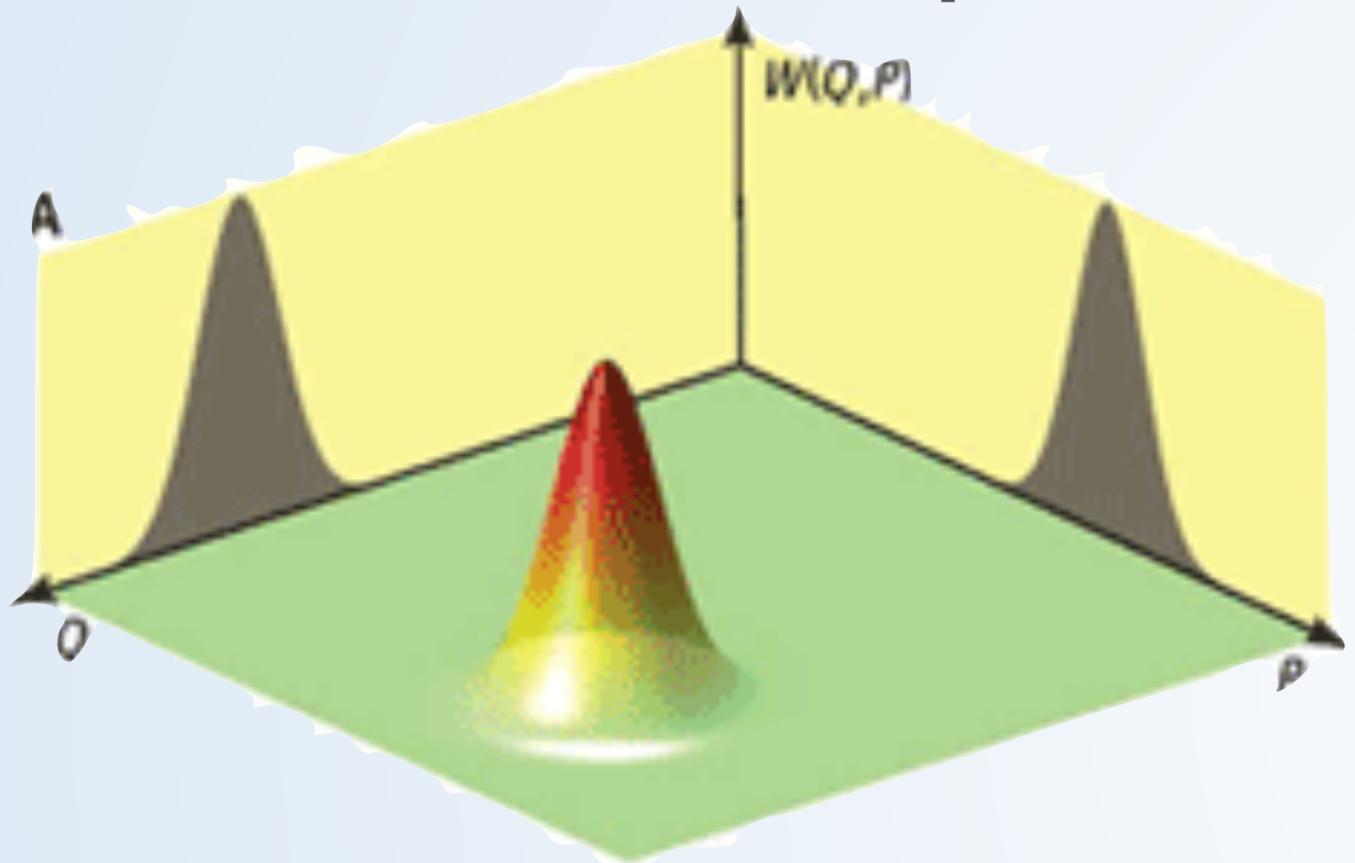
Weyl symbol

$$O_W(\boldsymbol{q},\boldsymbol{p}) = Tr(\hat{A}\hat{O})$$

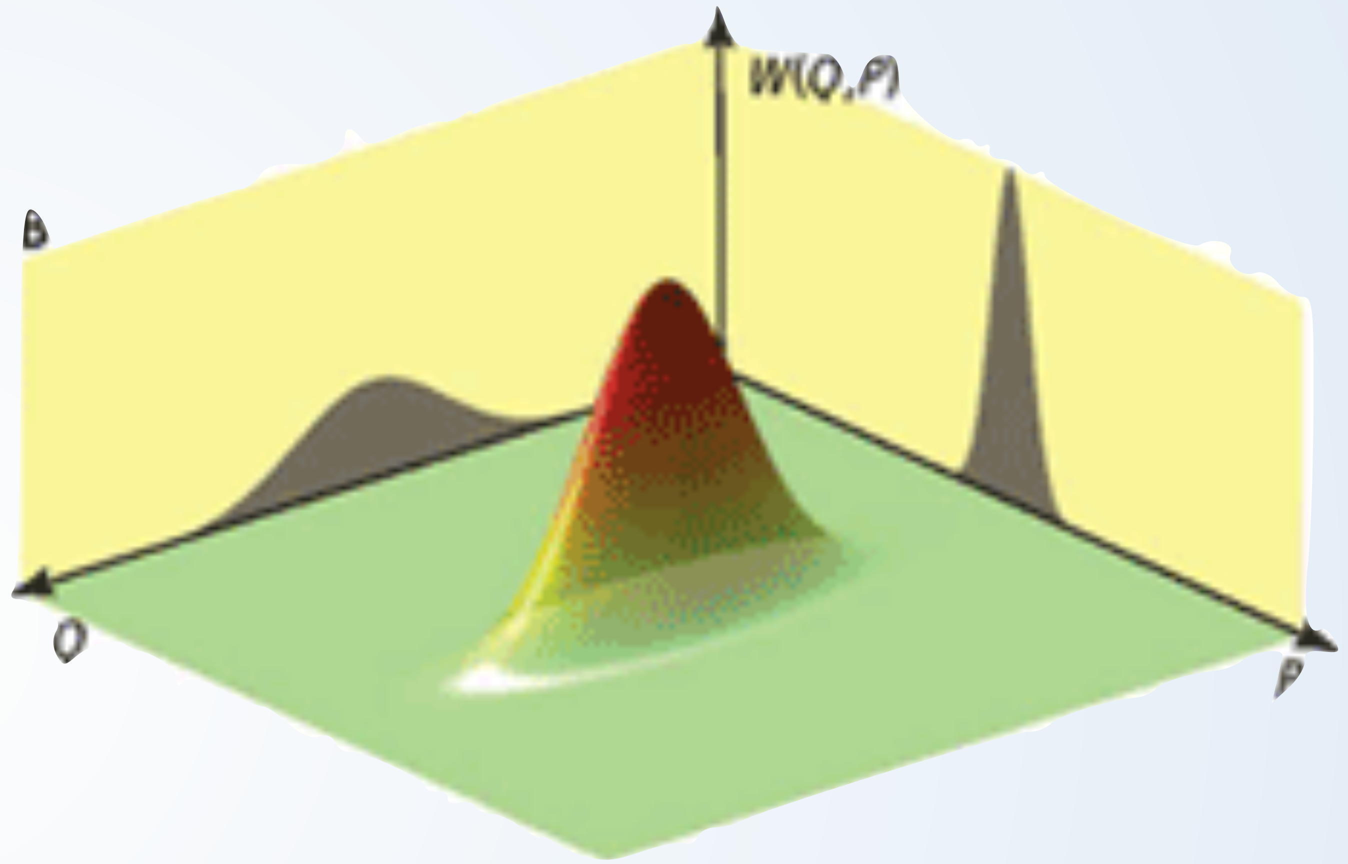
Grangier, Science 332.6027 (2011)

Wigner Function Examples

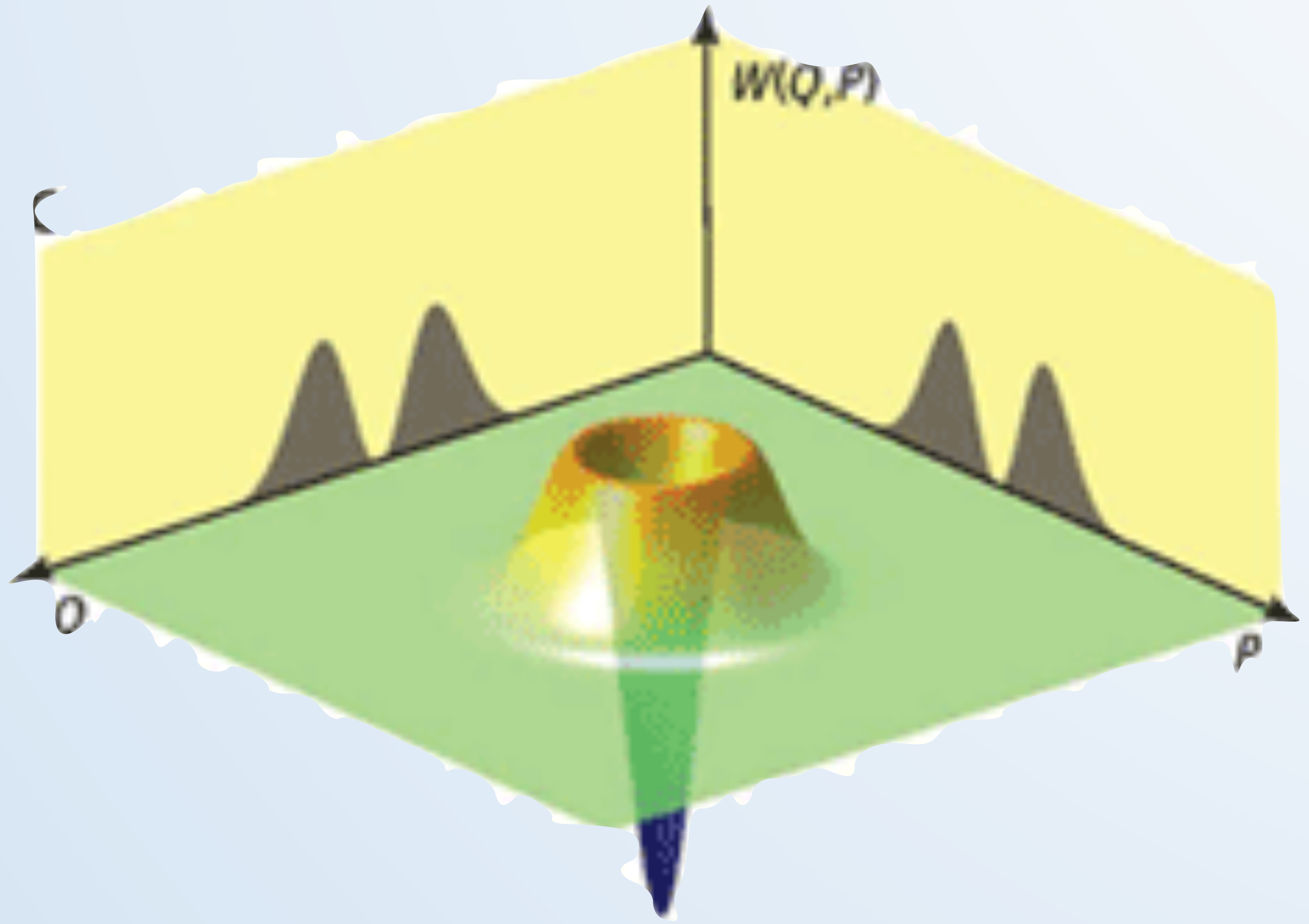
Gaussian wave packet



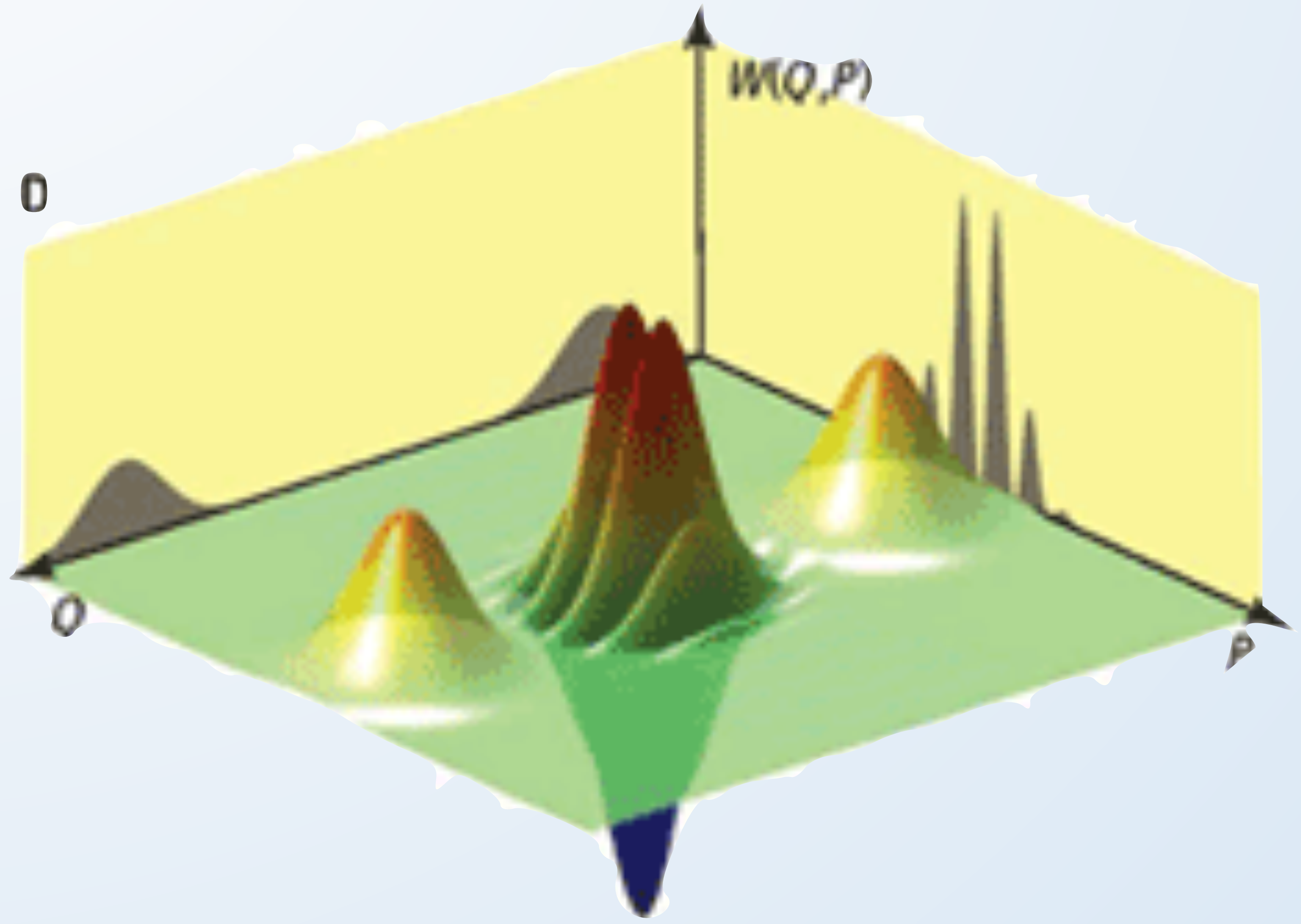
Momentum squeezed



1st excited state of QHO



Cat state



Wigner Picture

- behaves something like a joint *x*-*p* probability distribution but can be negative
  - negatives restricted to areas of ~$\hbar$ or less
  - joint (x,p) measurements associated to POVM with coherent state basis

- can show in the semiclassical limit $\hbar \to 0$ Wigner function reduces to classical probability distribution

$$\langle x \rangle = \iint dxdp\ xW(x,p)$$

$$\langle p \rangle = \iint dxdp\ pW(x,p)$$

$$H(\hat{x},\hat{p}) = T(\hat{p}) + U(\hat{x})$$

$$\langle T \rangle = \iint dxdp\ T(p)W(x,p)$$

$$\langle U \rangle = \iint dxdp\ U(x)W(x,p)$$

Wigner Phase Space Dynamics

Heisenberg

$$\frac{d}{dt}\hat{O}(t) = \frac{1}{i\hbar}[\hat{H}, \hat{O}(t)]$$

$\longleftrightarrow$

Wigner

$$\frac{\partial}{\partial t}O_W = \{\{H, O_W\}\}$$

Moyal bracket

$\xrightarrow{\hbar \to 0}$

Wigner approximation

$$\frac{\partial}{\partial t}O_W = \{H, O_W\} + \mathcal{O}(\hbar^2)$$

Poisson bracket

- Time evolution of expectation values

$$\langle \hat{O}(\hat{\boldsymbol{x}}, \hat{\boldsymbol{p}}, t)\rangle = \int d\boldsymbol{x}d\boldsymbol{p}\ O_W\left(\boldsymbol{x}(t), \boldsymbol{p}(t), t\right)\ W(\boldsymbol{x}_0, \boldsymbol{p}_0) \xrightarrow{\hbar \to 0} \int d\boldsymbol{x}d\boldsymbol{p}\ O_W\left(\boldsymbol{x}_{cl}(t), \boldsymbol{x}_{cl}\ (t), t\right)\ W(\boldsymbol{x}_0, \boldsymbol{x}_0)$$

$\Longrightarrow$ **Can perform Monte Carlo numerics!**

- can perform $\hbar^2$ quantum corrections —> makes contact with Feynman path integral

Truncated Wigner Approximation (TWA)

- Takes first order quantum fluctuations into account
- continuous dof
- In Heisenberg picture:

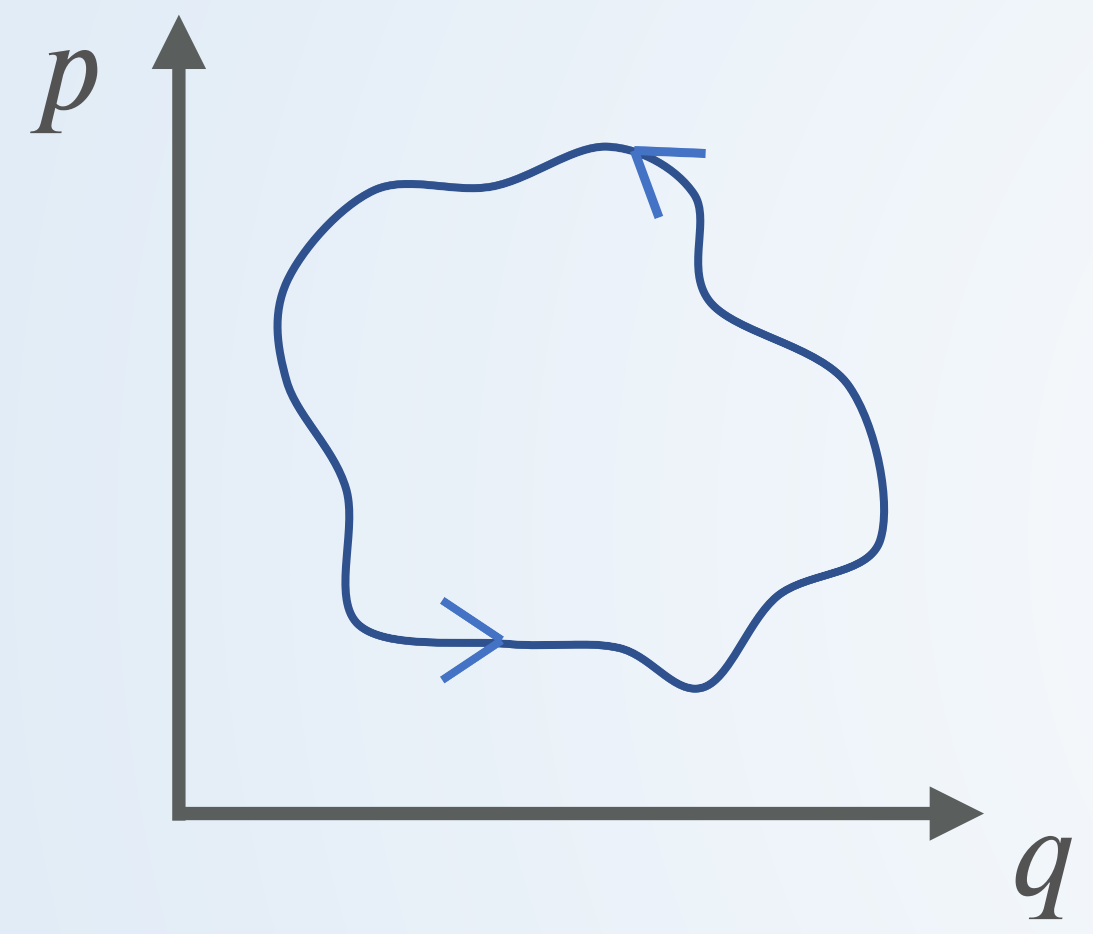
$$\langle O \rangle(t) = \int d\boldsymbol{x} d\boldsymbol{p}\ O_W(\boldsymbol{x}_{cl}(t), \boldsymbol{p}_{cl}(t), t)\ W_0(\boldsymbol{x}_0, \boldsymbol{p}_0)$$

1. Calculate initial Wigner function
2. Calculate classical EOM for x_{cl} and p_{cl}
3. Plug expressions into Weyl symbol for operator
4. Integrate over phase space

Phase Space

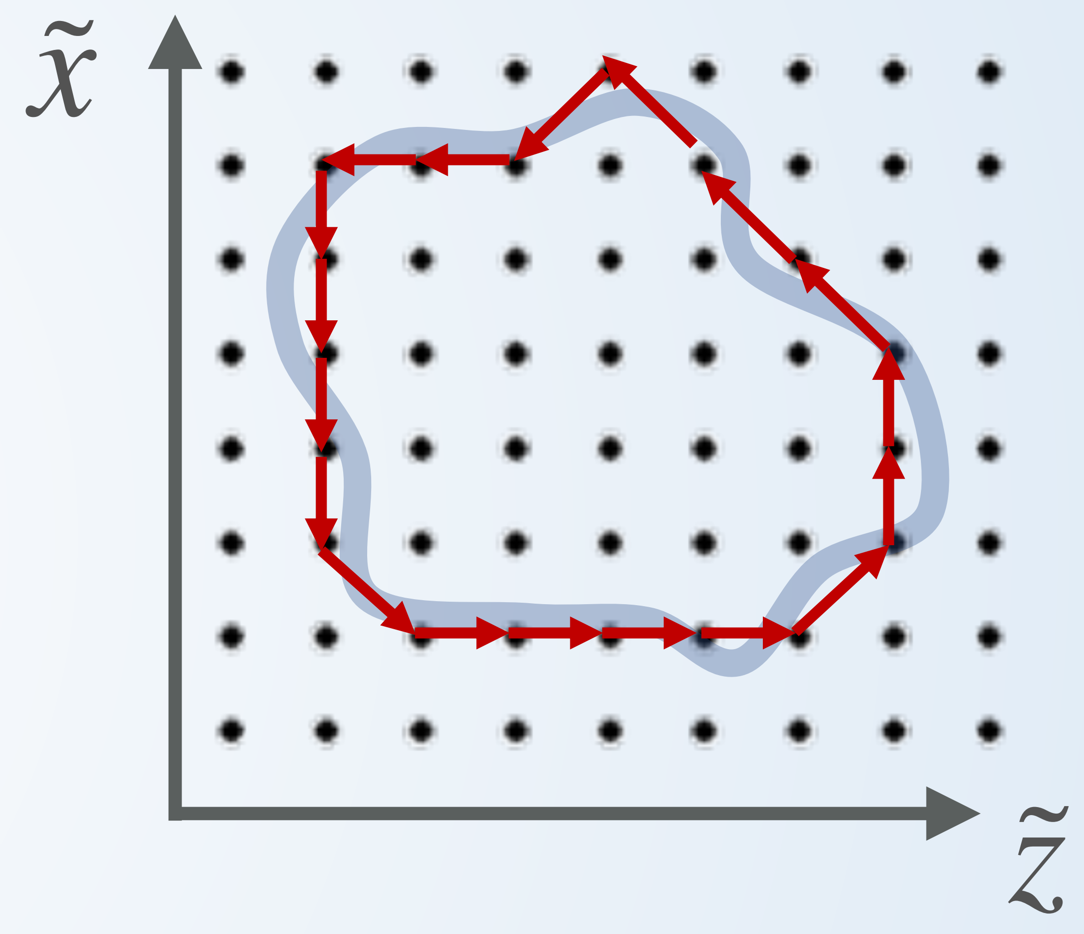
*More details in Wootters

Continuous phase space



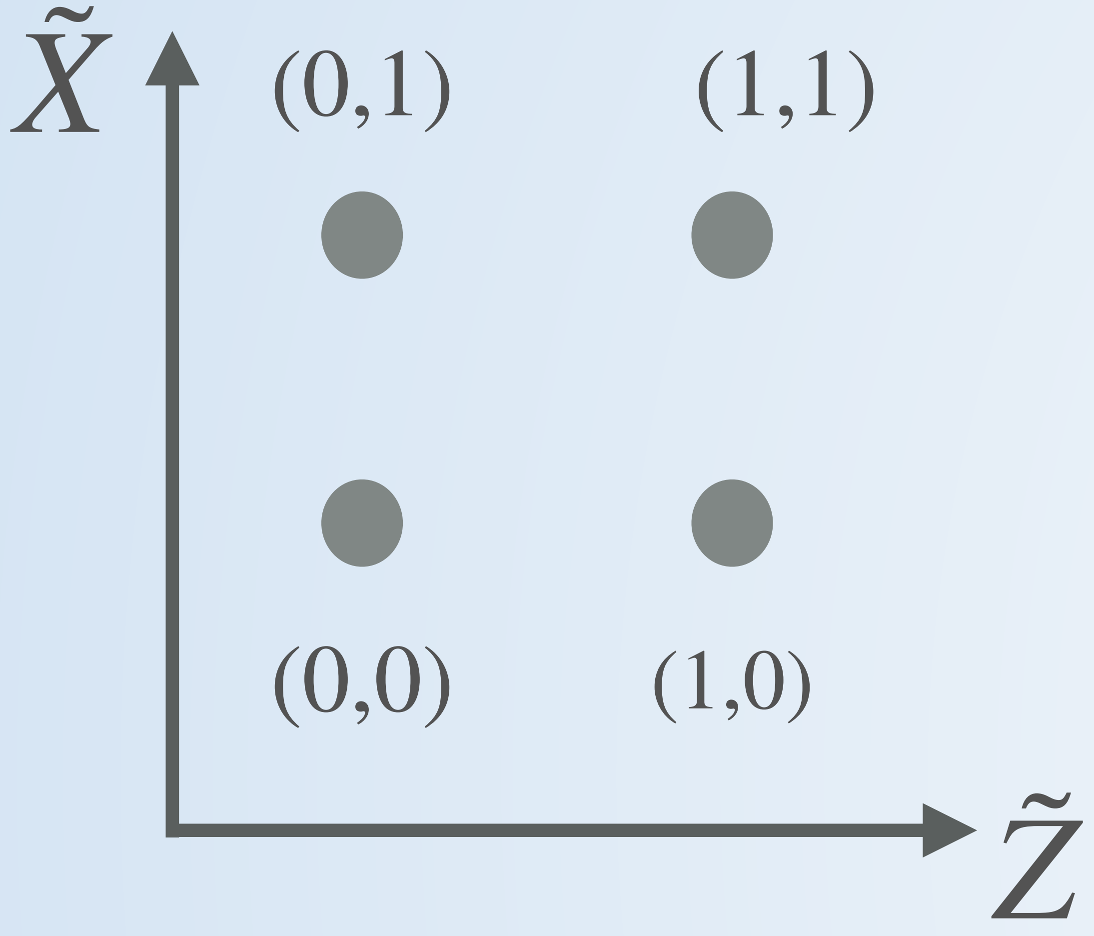
- conjugate variables with canonical commutation relation assigned to axes
- lines associated to variables of the form aq + bp

Discrete phase space



- non-commuting observables assigned to coordinate axes
- lines associated to variables of the form ax + bz

Discrete Phase space



$$\tilde{Z} \equiv \left(\mathbb{I} - \frac{1}{2}\hat{Z}\right) \qquad \tilde{X} \equiv \left(\mathbb{I} - \frac{1}{2}\hat{X}\right)$$

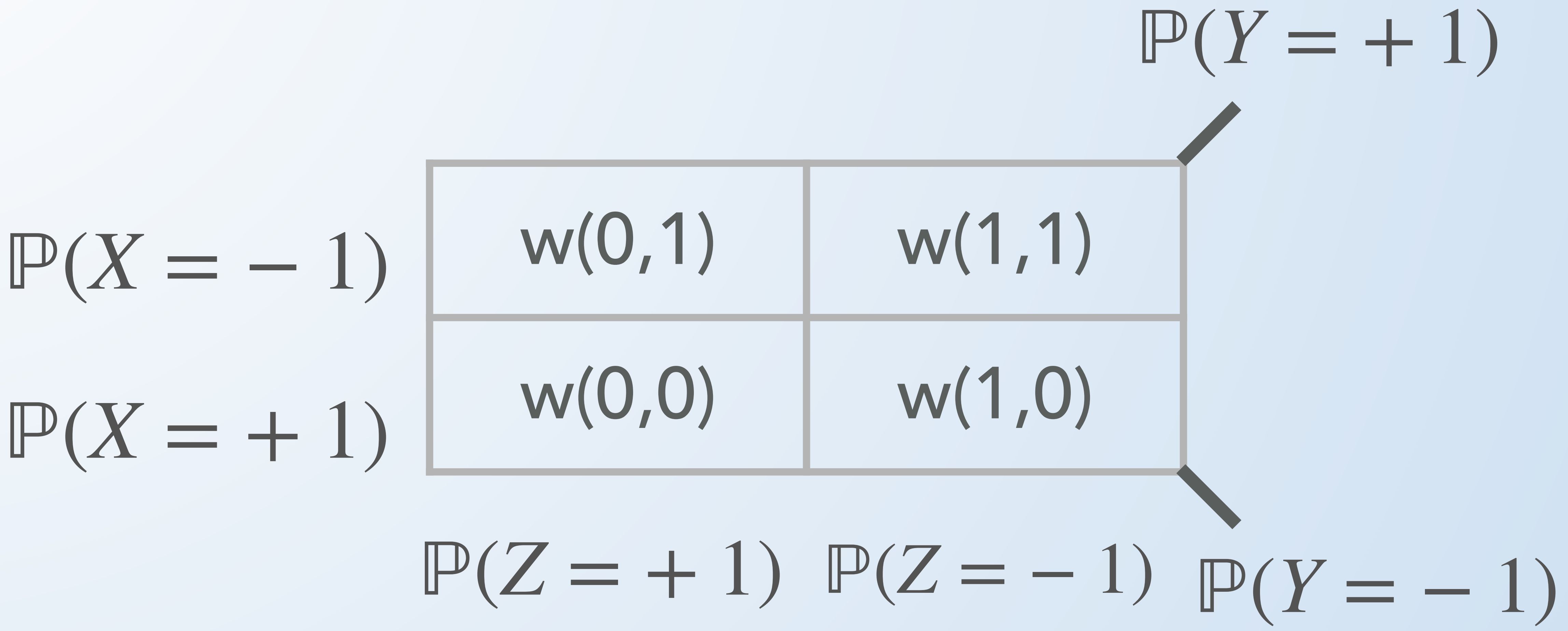
- Expectation values of $\tilde{Z}$, $\tilde{X}$ obtained by summing quasi probabilities over vertical, horizontal slices
- Expectation value of $\tilde{Y}$ obtained by summing over diagonal

Phase point operator

$$\hat{A}(\alpha) = \mathbb{I} \ + \boldsymbol{r}_\alpha \cdot \boldsymbol{\sigma}$$

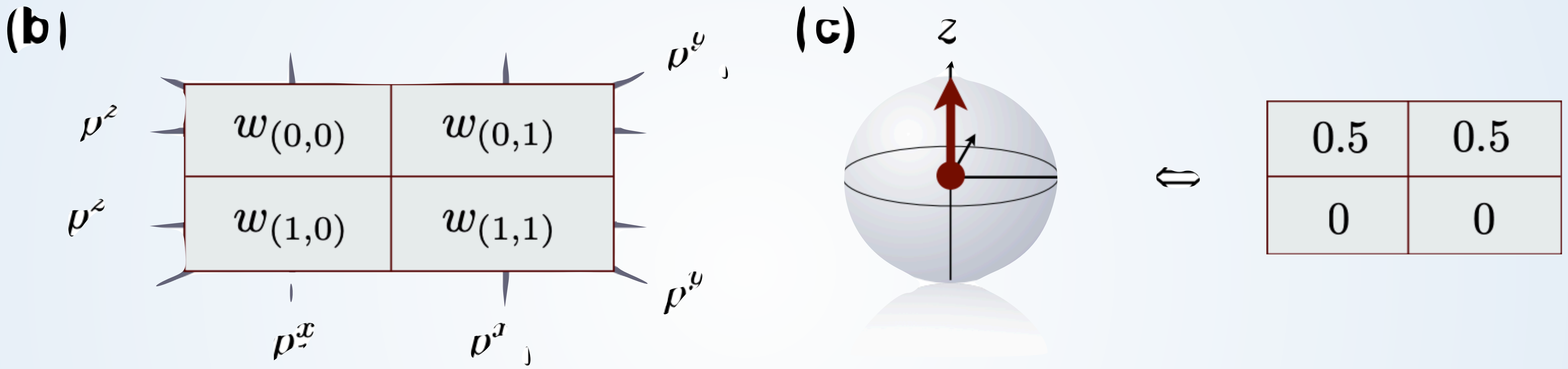
$$O_W(\alpha) = Tr(\hat{O}\hat{A}_\alpha)$$

$$(0,0) \leftrightarrow \mathbb{I} + \hat{X} + \hat{Y} + \hat{Z}$$
$$(1,0) \leftrightarrow \mathbb{I} + \hat{X} - \hat{Y} - \hat{Z}$$
$$(0,1) \leftrightarrow \mathbb{I} - \hat{X} + \hat{Y} - \hat{Z}$$
$$(1,1) \leftrightarrow \mathbb{I} - \hat{X} - \hat{Y} + \hat{Z}$$



Discrete Wigner Picture

- degrees of freedoms match: 2 $\mathbb{C}$ numbers = 4 $\mathbb{R}$ per qubit
- Examples:



$+1$ eigenstate of Y

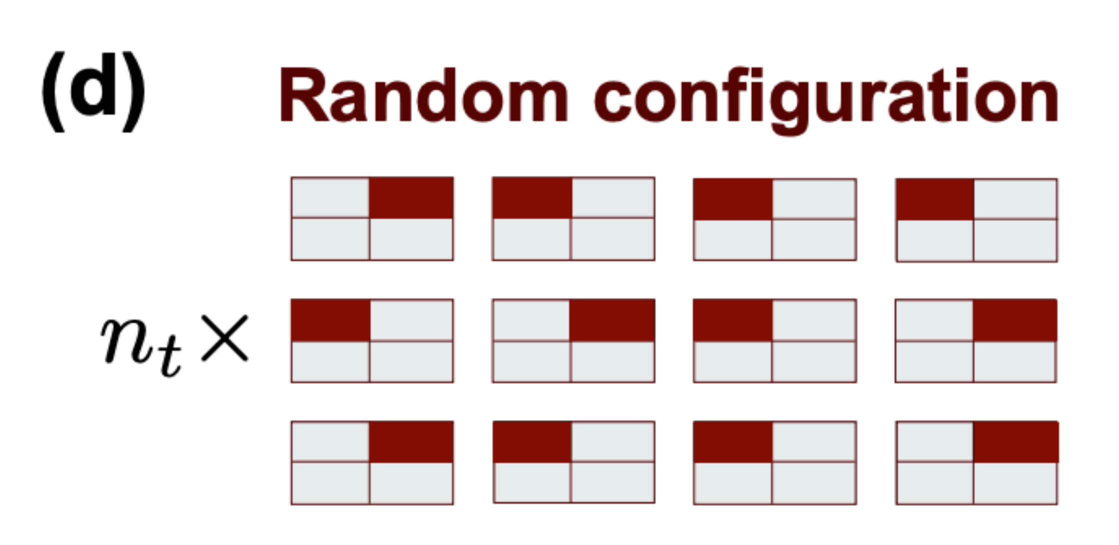
	+z	-z
-x	0	1/2
+x	1/2	0

mixed state $\rho = \mathbb{I}/2$

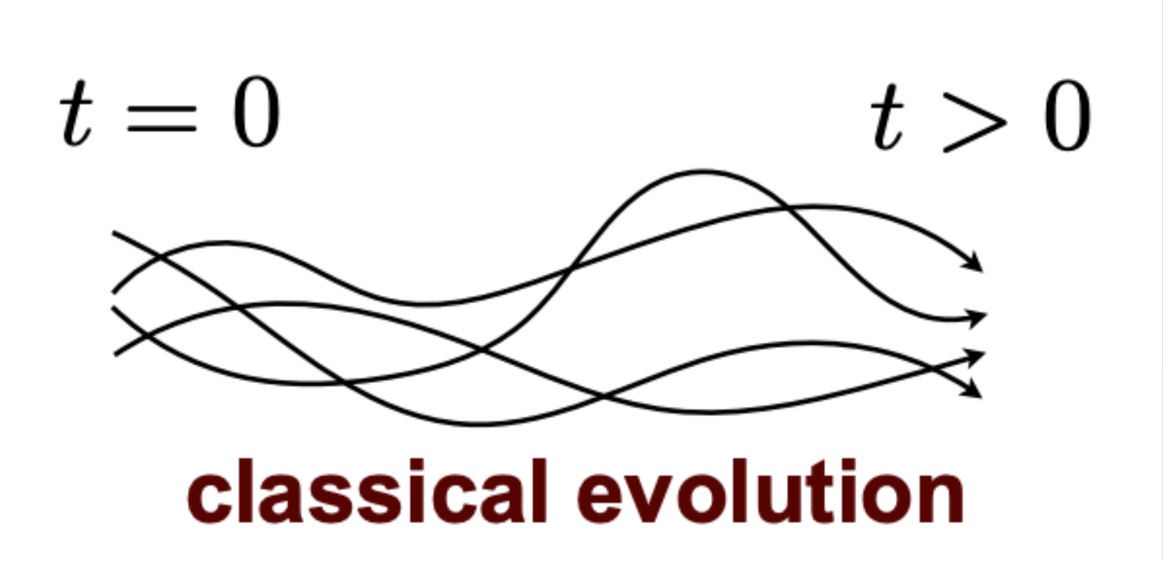
	+z	-z
-x	1/4	1/4
+x	1/4	1/4

DTWA Protocol

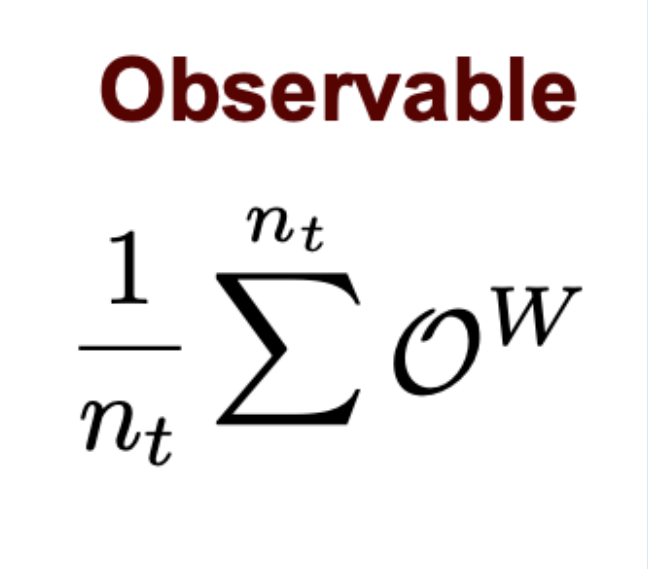
1. **Initialize configurations** using chosen discrete weyl probability distribution
   a) probabilities must be strictly positive



2. **Simulate classical evolution** of each configuration within probability distribution

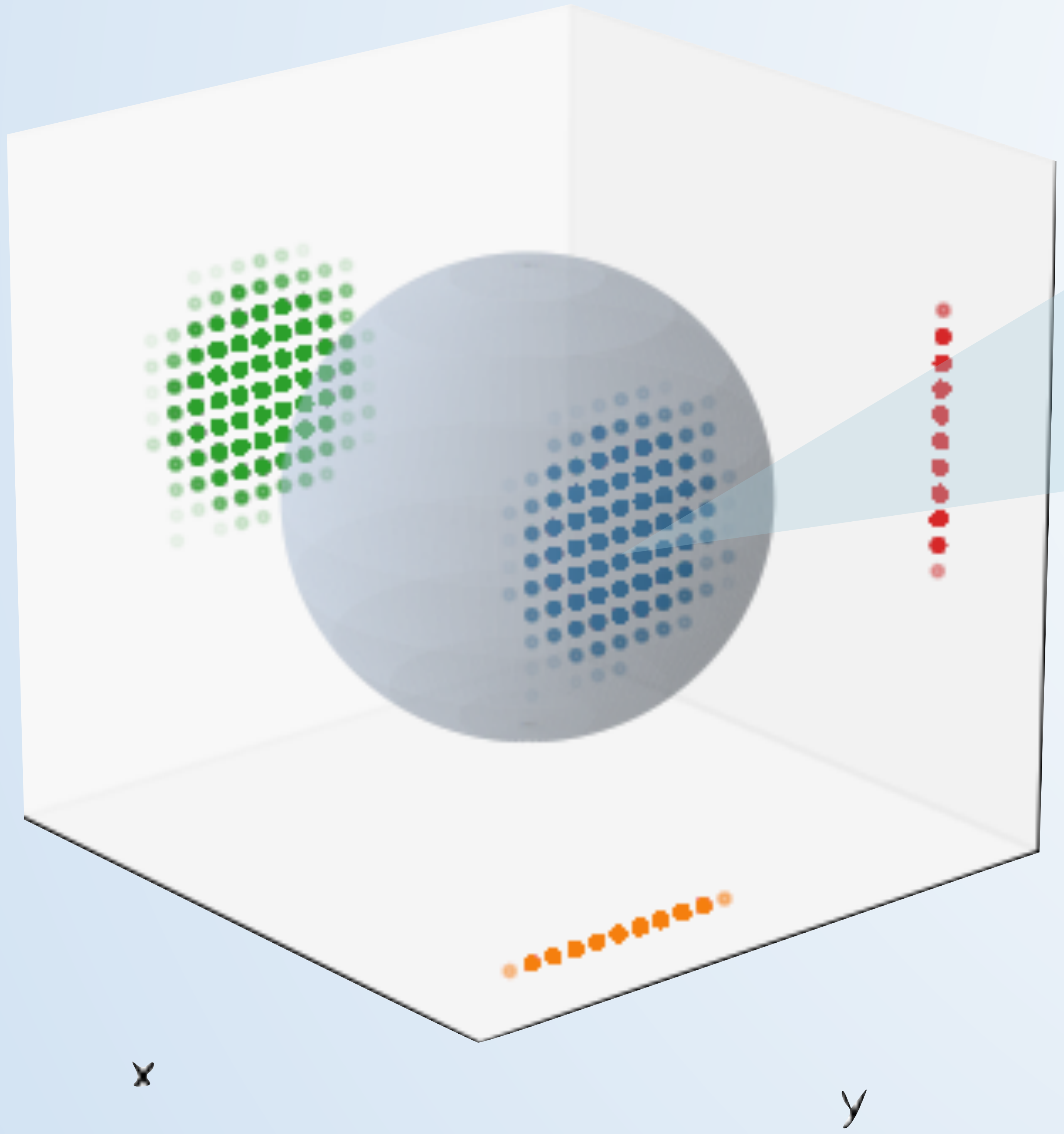


3. **Compute expectation** values classically



DTWA Protocol

1. Initialize configurations



$\vec{s}_1$

x	y	z
+	+	-
+	-	+
+	-	-
+	...	

$+$

$\vec{s}_2$

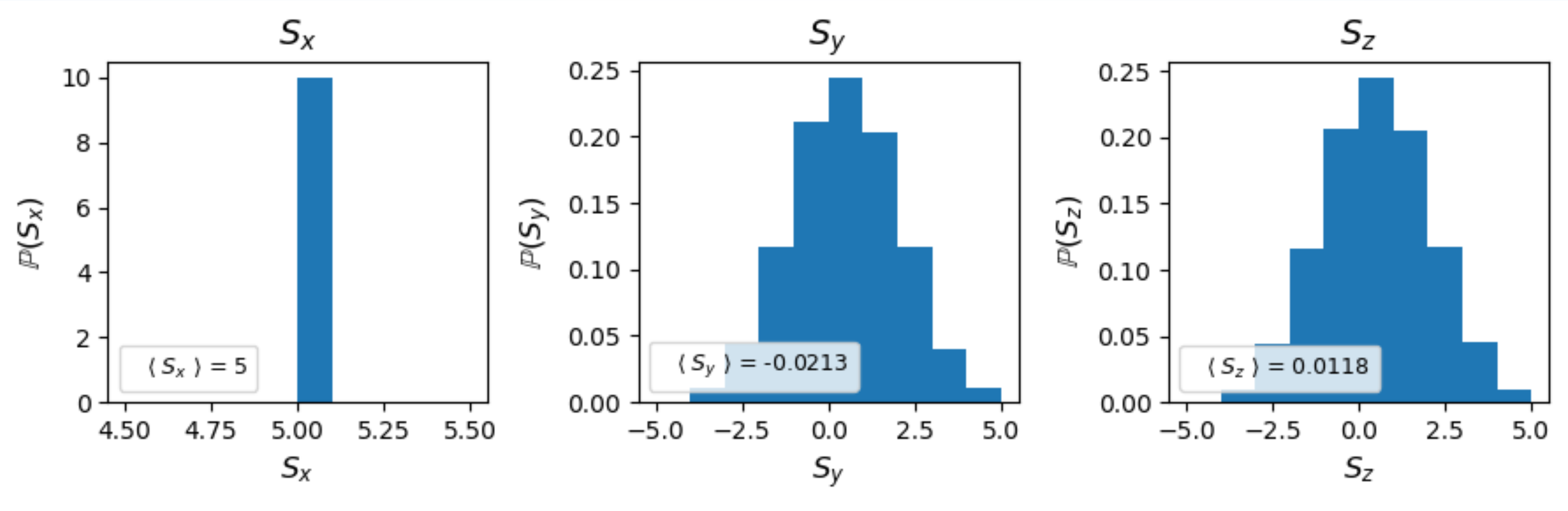
x	y	z
+	-	+
+	-	+
+	+	-
+	...	

$+ \dots$

DTWA Protocol

1. Initialize configurations

$$N = 10,\ n_t = 10^4$$



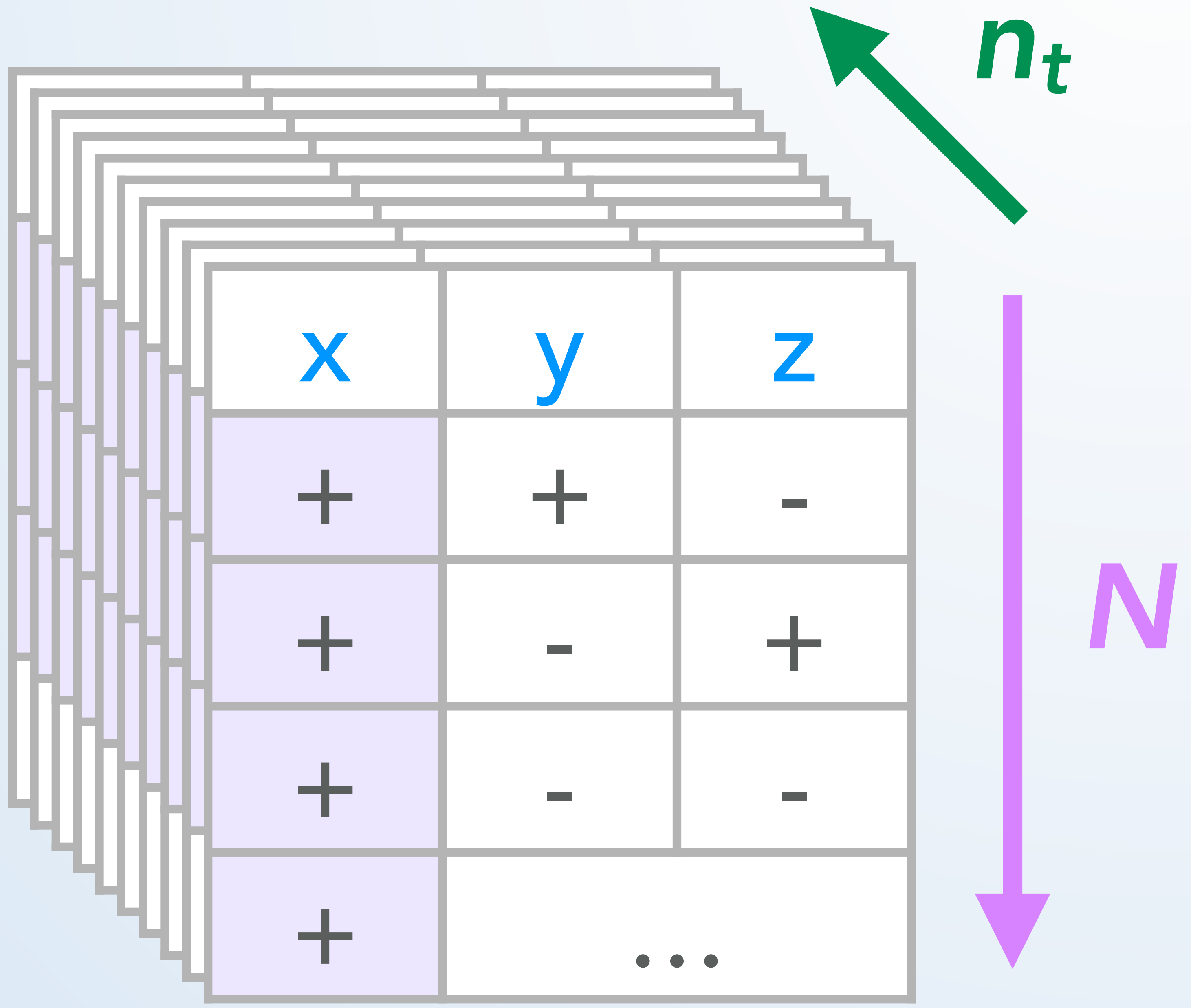
DTWA Protocol

2. **Simulate classical evolution**

$$\dot{s}_i^\alpha = \{s_i^\alpha, H_{cl}\} = 2\sum_\beta \epsilon_{\alpha\beta\gamma} s_i^\gamma \frac{\partial H}{\partial s_i^\beta}$$

generically gives a set of coupled differential equations!

3. **Compute expectation values**



Ex: $S_y = \frac{1}{n_t}\sum_{n_t}\left(\sum_i s_i^y\right)$

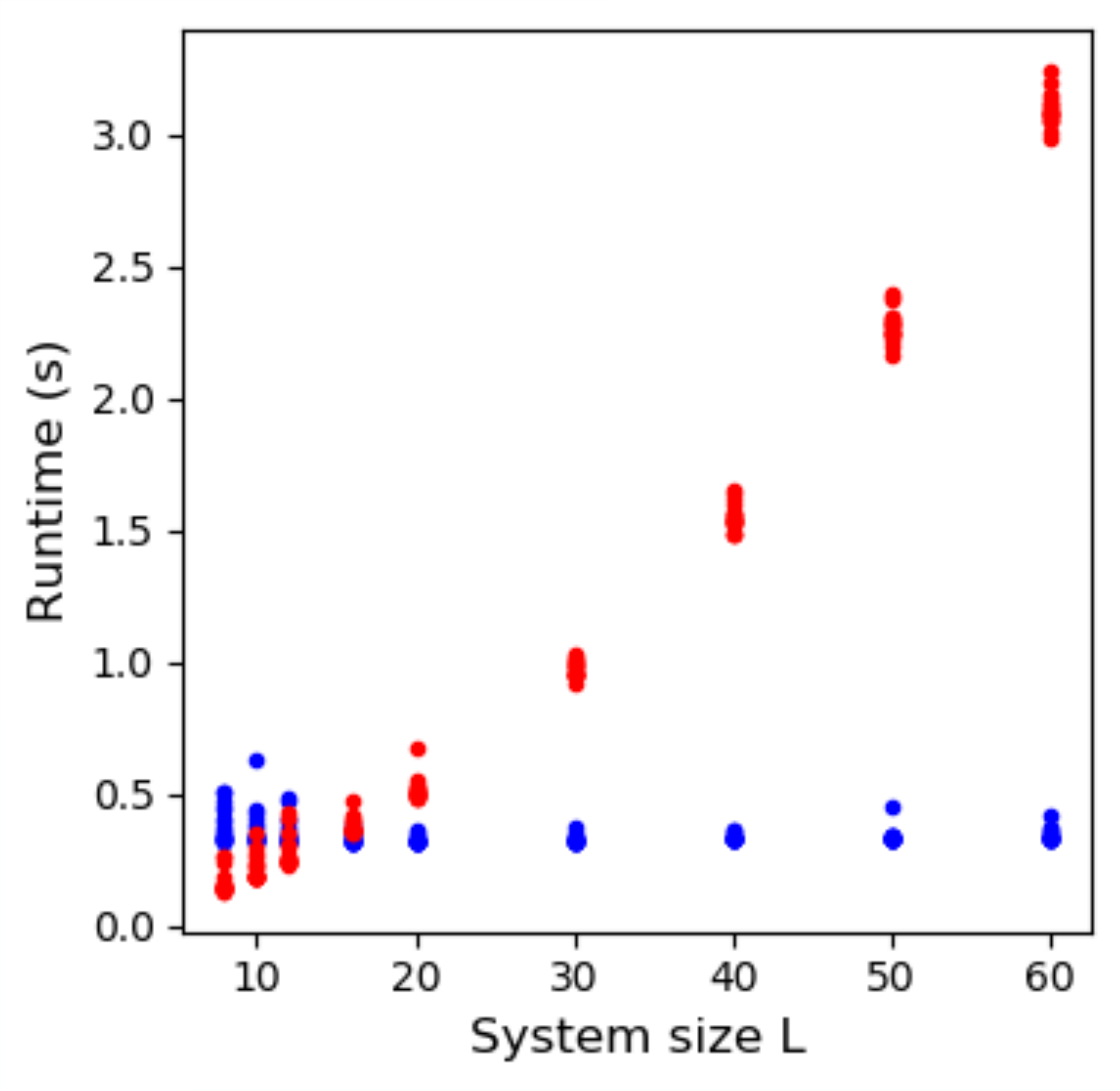
Scalability

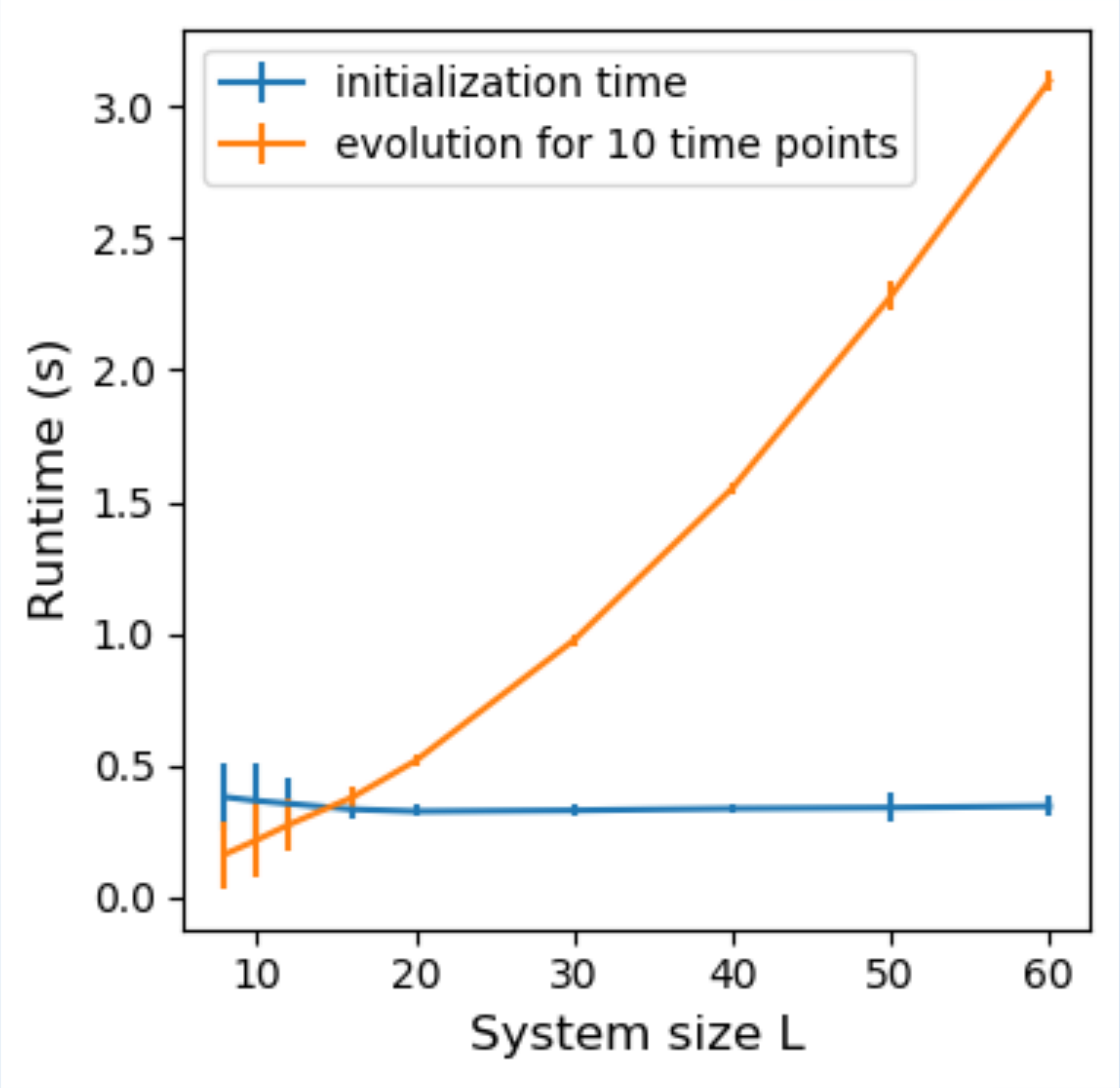
- Most challenging aspect is finding classical EOM. For simple Hamiltonians like the Ising Hamiltonian, exact evolution can be computed.
- can simulate ~100 spins on a laptop
- *not* strongly computationally limited by system size, but rather by number of trajectories and resolution of time dynamics

Benchmarking

- Examining runtime dependence on system size

$$N = 10,\ n_t = 10^4, \text{trials} = 20$$





Range of Validity

- **Require**: strictly positive initial probability distribution
- Semiclassical limit: large system size and large energies
- Becomes “exact" for quadratic potentials - error for certain observables is computable
- Error in expectation values is operator-dependent

What we've won

- traded exponential complexity in space for smaller time complexity with vanishingly small error
  - diagonalizing large matrices ~$\mathcal{O}\left(2^{N^3}\right)$ vs. weak ~$\mathcal{O}\left(N^2\right)$ dependence
- can easily accommodate various interactions, spin geometries, etc
- can accommodate $\frac{1}{\hbar^2}$ corrections via quantum jumps
- **The unique content of DTWA is the sampling scheme. Using an initial configuration that echoes initial probability distribution instead of mean-field approximation + Gaussian initial conditions wins us the ability to capture late time quantum dynamics.**

Performance compared to other methods

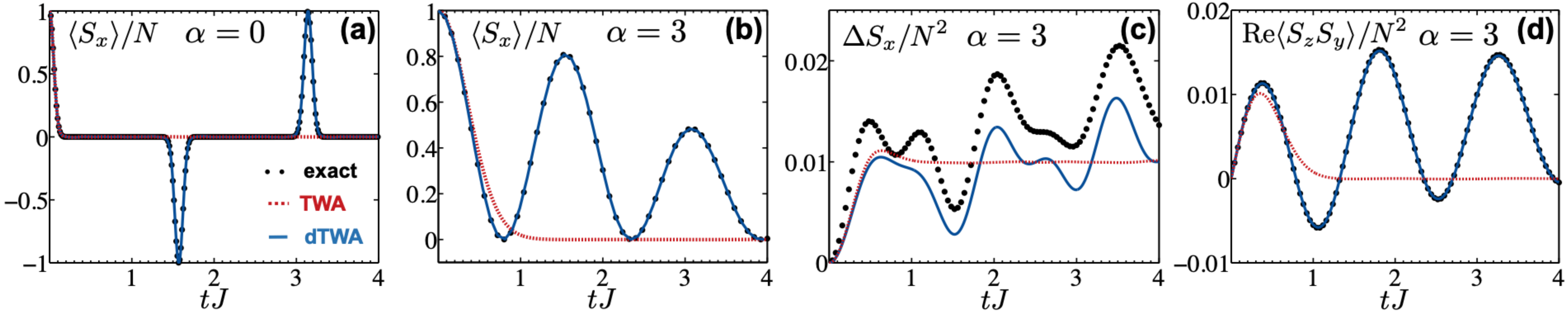


Figure 2. *Dynamics for Ising interactions.* Circles denote the exact solution, dashed lines are traditional TWA results, solid lines denote DTWA results, for 1D, $N = 100$ spins. (a-b) Evolution of $\langle S_x \rangle$, for all-to-all (decay exponent $\alpha = 0$) and dipolar ($\alpha = 3$) interactions, respectively. Traditional TWA captures only the initial decay and no oscillations or revivals. In contrast, DTWA becomes exact (on top of the black symbols). (c/d) The evolution of the correlation functions $\Delta S_x = \langle S_x^2 \rangle - \langle S_x \rangle^2$ and $\mathrm{Re}\langle S_y S_z \rangle$ for dipolar interactions. While the latter one is exactly captured in DTWA, ΔS_x shows deviations. DTWA improves traditional TWA predictions in all panels.

Schachenmayer, J., Pikovski, A., & Rey, A. M. (2015). *PRX* 5(1), 011022.

Case Study: Squeezing

- Good way to diagnose if method captures quantum correlations
- Examined evolution squeezing parameter as a function of time under Ising interactions and compared results to known analytics/ED
- Squeezing useful for applications in high-precision metrology + interferometry, quantum sources of light, etc

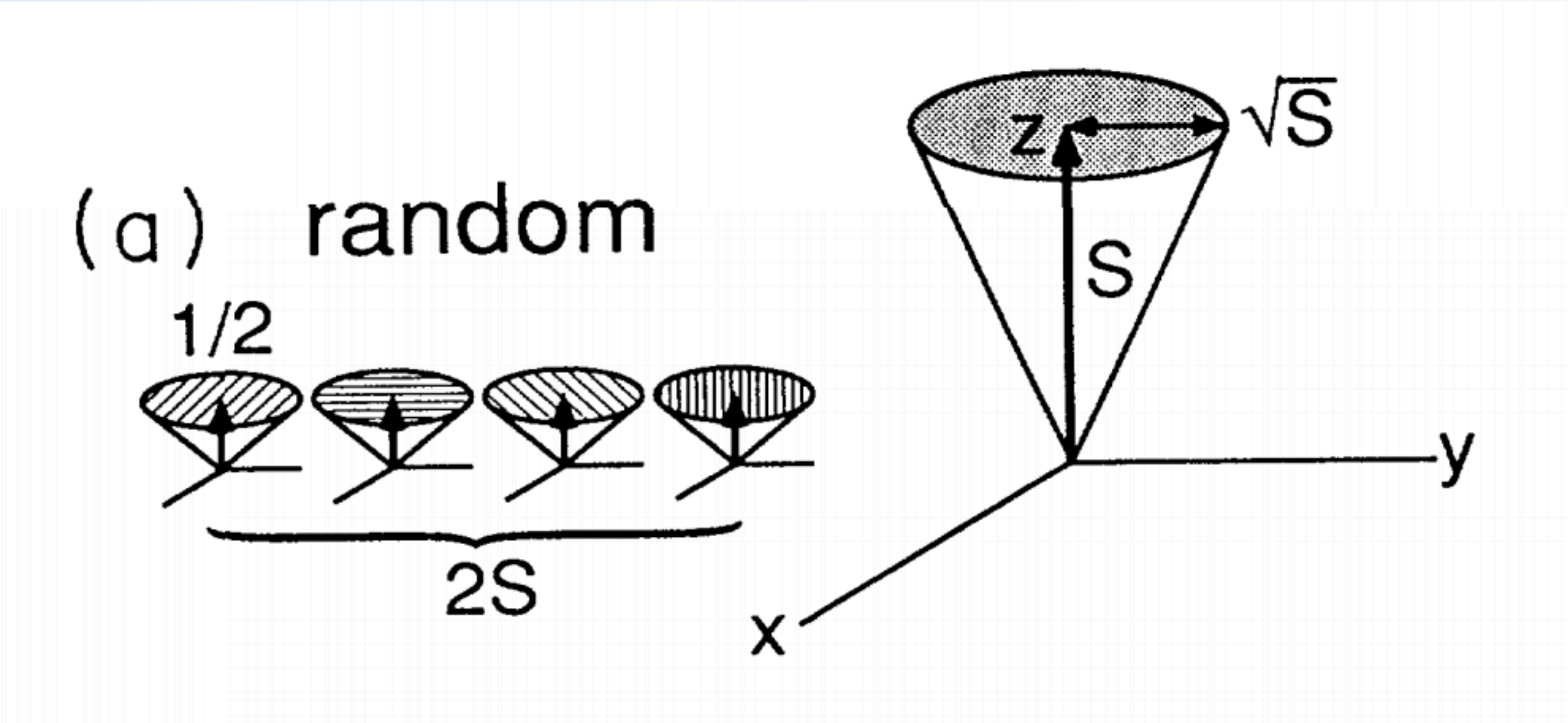
Kitagawa, et al. *Physical Review* A 47.6 (1993): 5138.

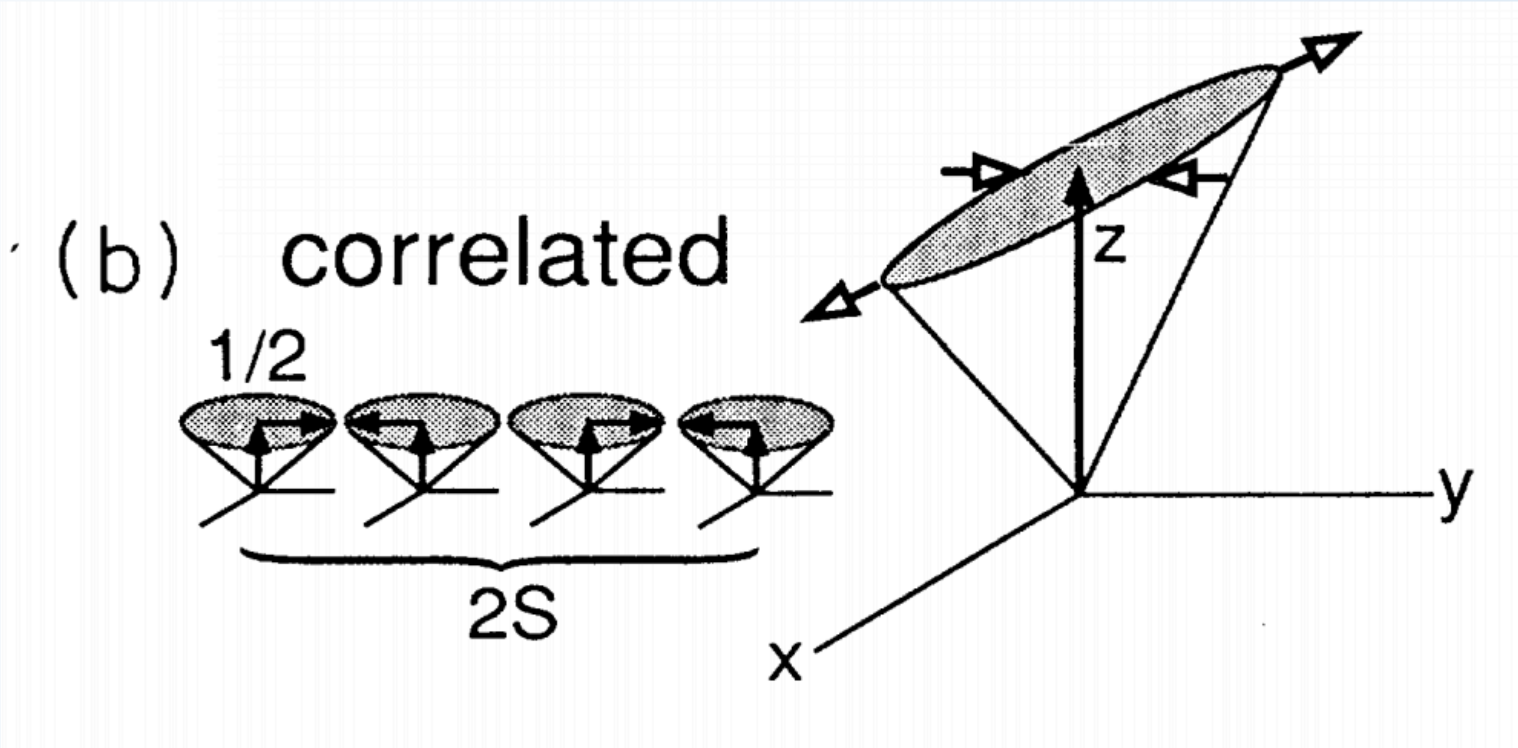
Squeezing Basics

- Uncertainty relation: lower bound on product of uncertainties of operators set by their anticommutator

$$\Delta A \Delta B \geq \frac{1}{2} \left| \langle [A, B] \rangle \right|$$

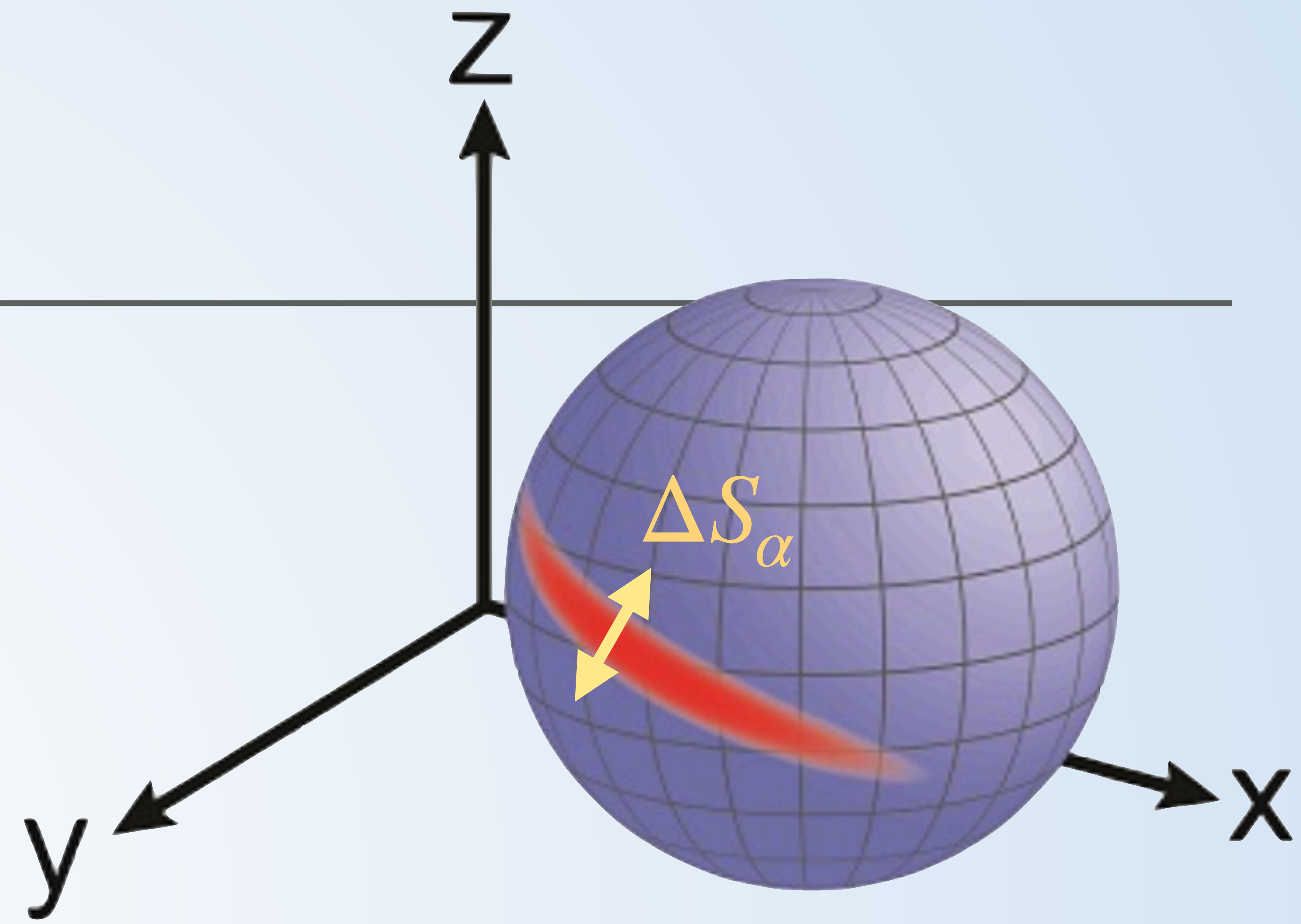
- A system of 2S spins has a representation as a spin-S particle
  - If spins are uncorrelated, variances will add to give $(\Delta S)^2 = S/2$
  - If correlations develop, the covariances can conspire to reduce variance in one quadrature at the expense of the other





Squeezing Basics

- Squeezing parameter $$\xi = \frac{\sqrt{N}\Delta S_\alpha}{|\boldsymbol{S}|}$$



https://nicholsonlabs.quantumlah.org/research/squeezed-clock-spectroscopy/

- Examined squeezing under Ising Hamiltonian with uniform and power law interactions

$$H = \sum_{ij} J_{ij}(\boldsymbol{r}_i - \boldsymbol{r}_j) s_i^z s_j^z = \sum_{i \neq j} 2J_{ij}(\boldsymbol{r}_i - \boldsymbol{r}_j) s_i^z s_j^z$$

Case Study: Squeezing

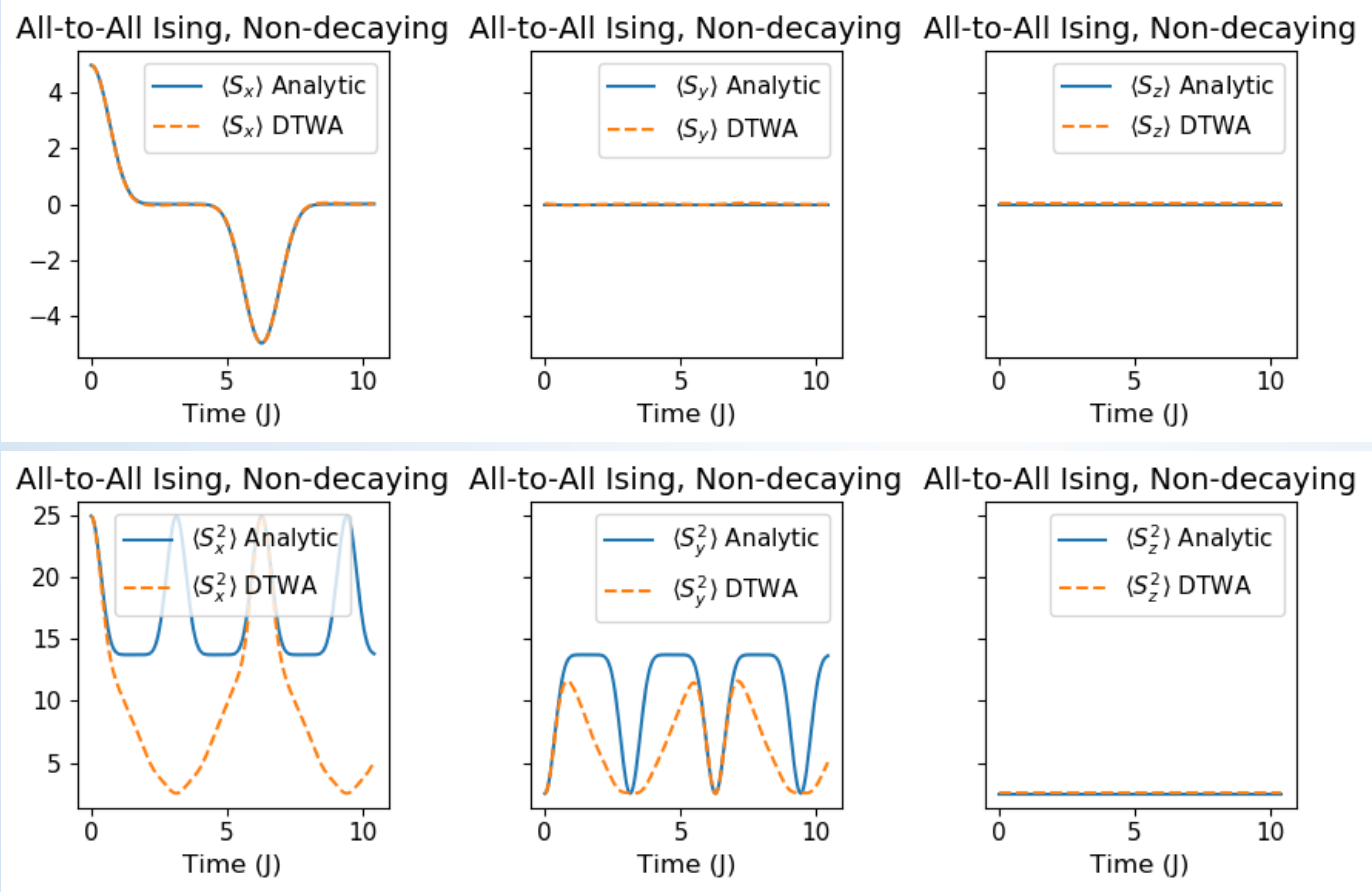
1. **Initialize configurations** with all spins with x = +1/2 and with y, z chosen randomly

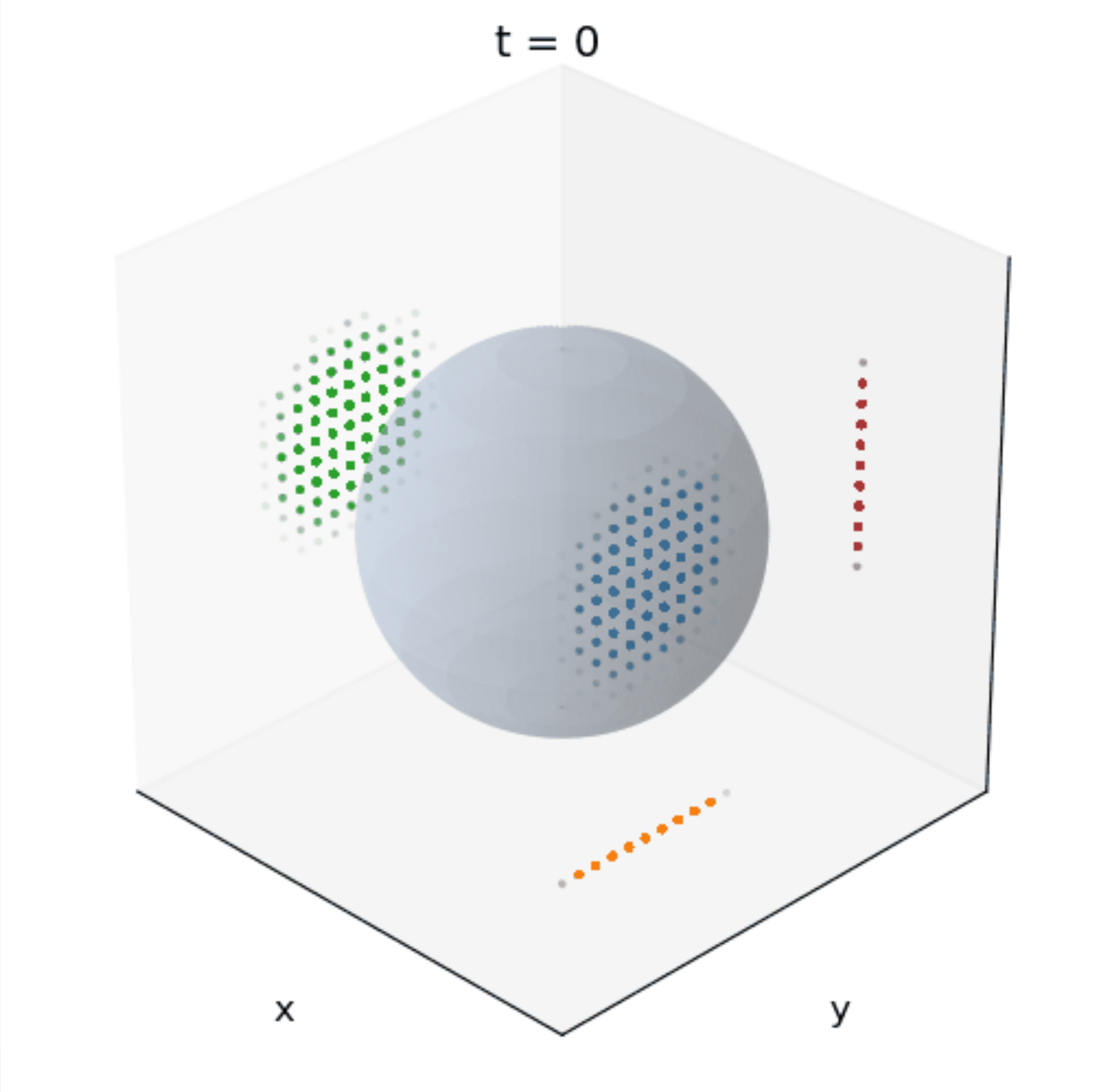
2. **Simulate classical evolution** by switching to ladder basis +/-/z and using the solution to the EOM:

$$s_n^{\pm}(t) = s_n^{\pm}(0)\ \exp\left(\pm 2it \sum_{j\neq n} J_{jn} s_j^z\right)$$

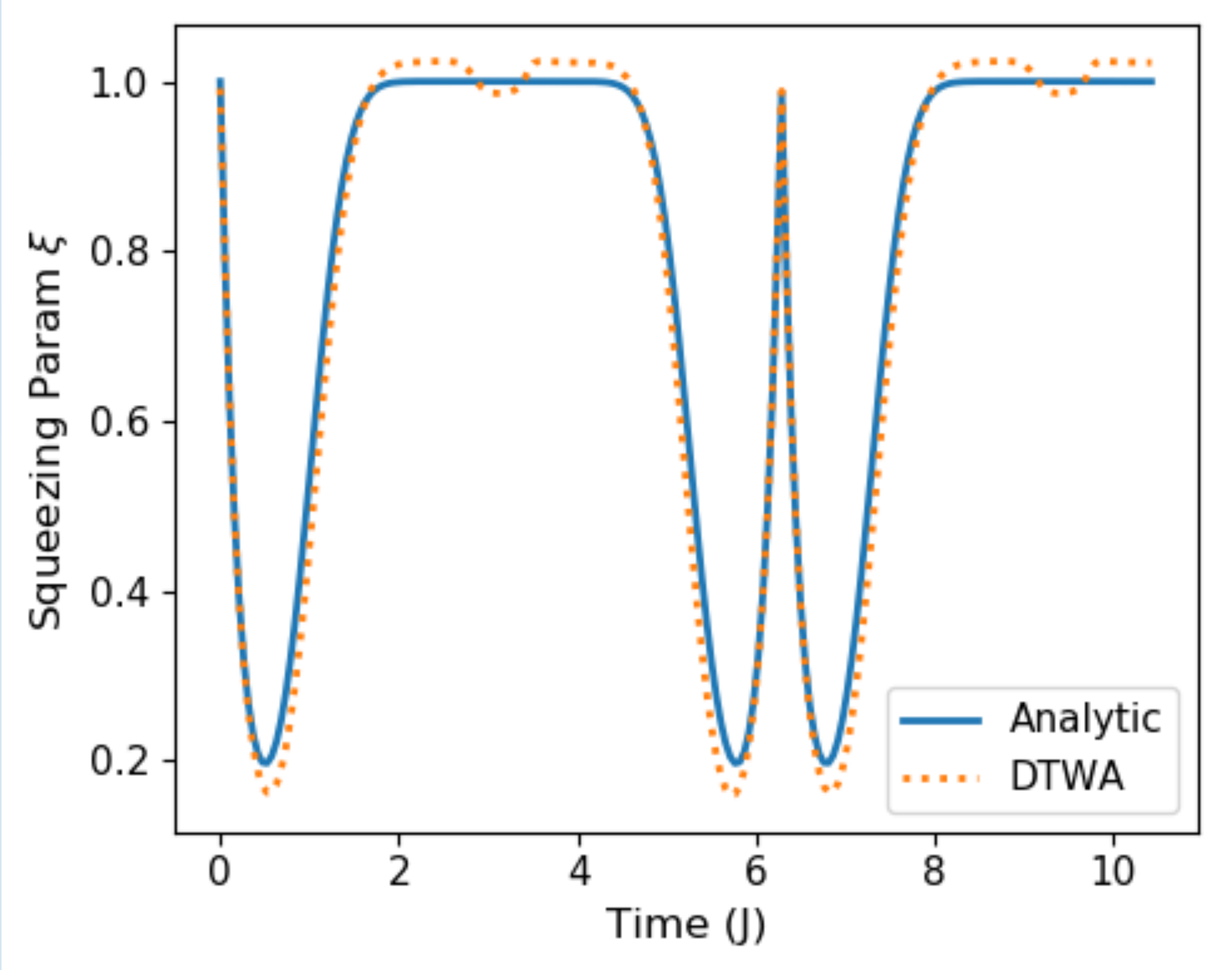
3. Reconvert back to x/y/z basis to **compute expectation** values classically

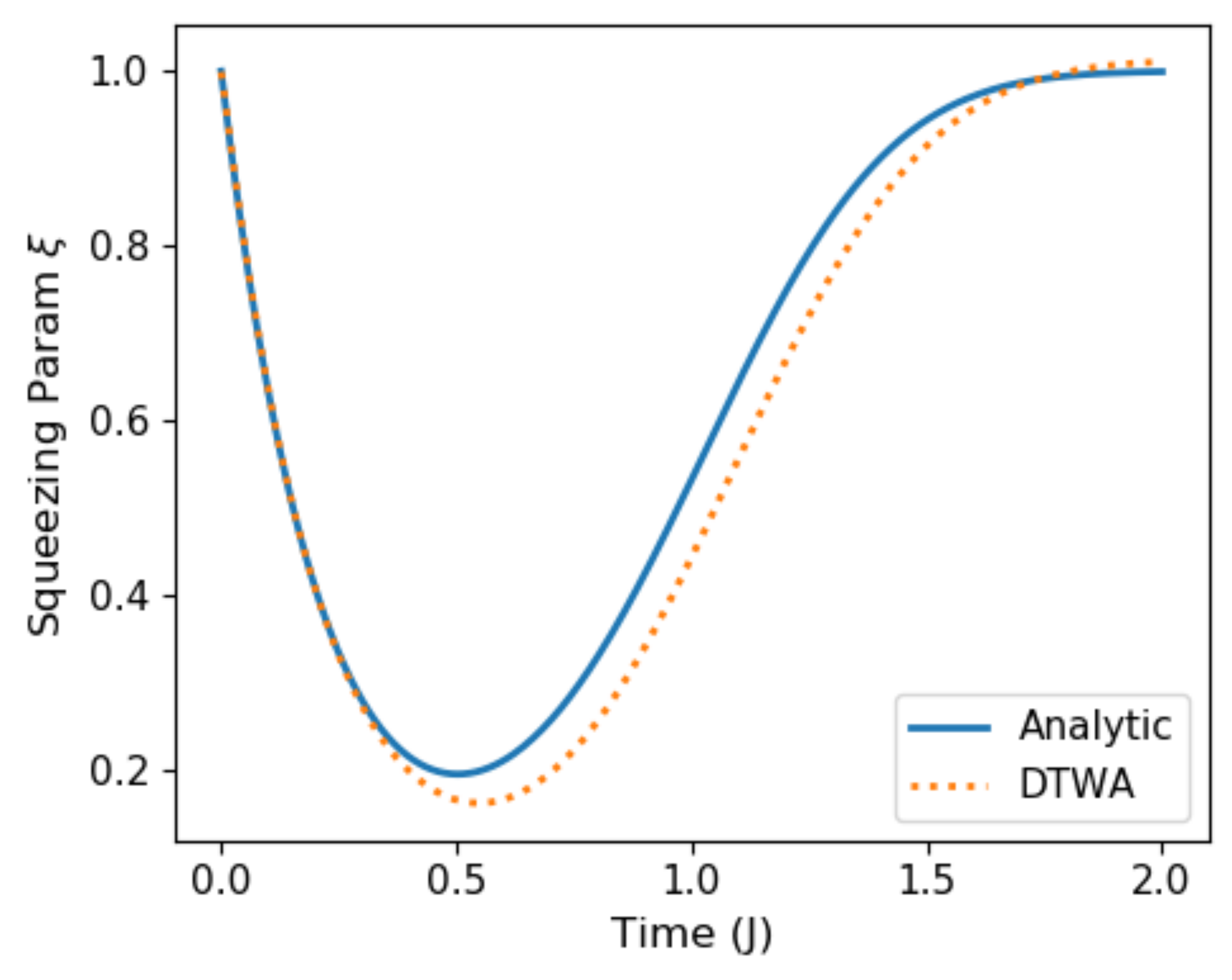
Case Study: Squeezing

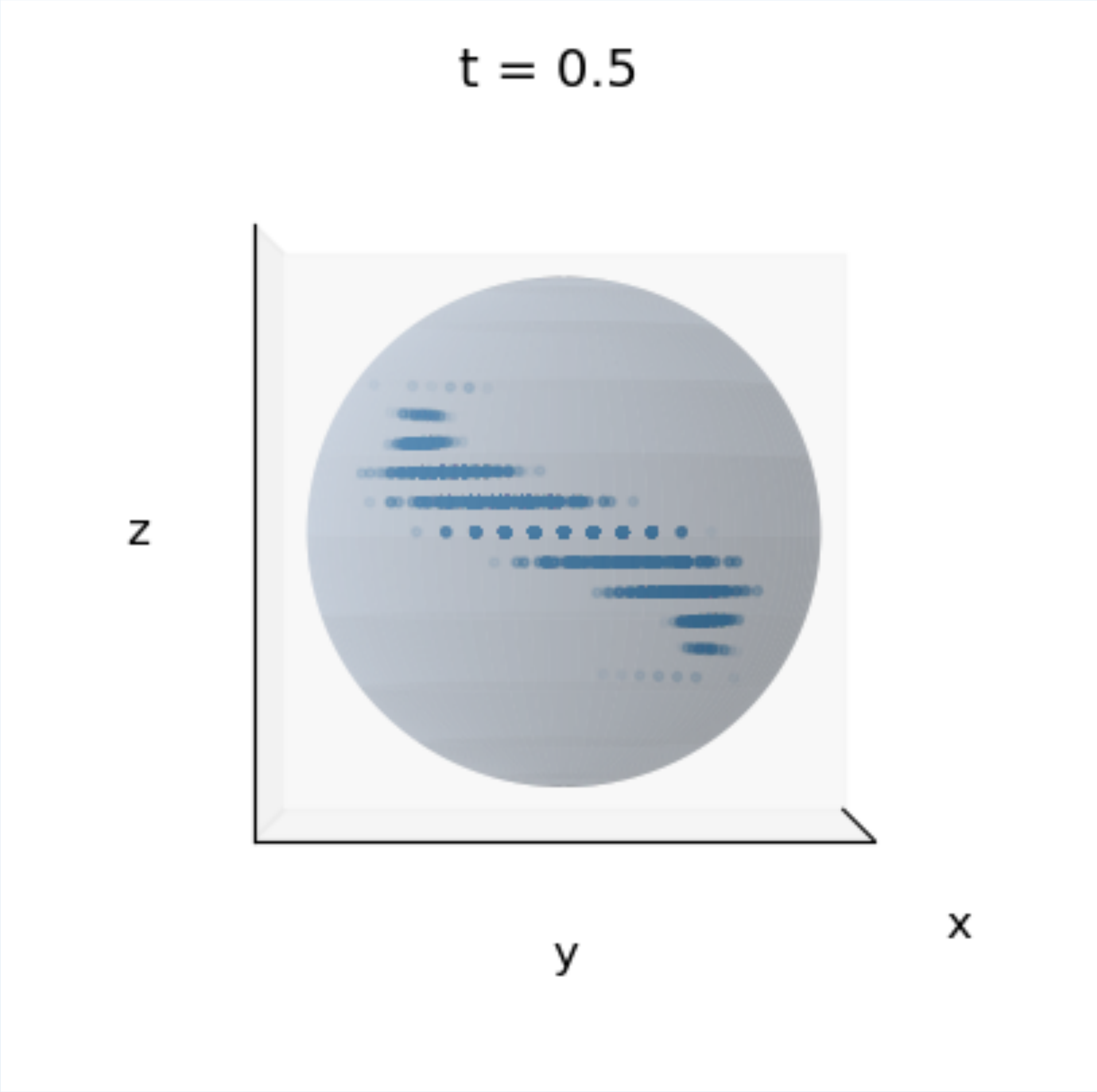




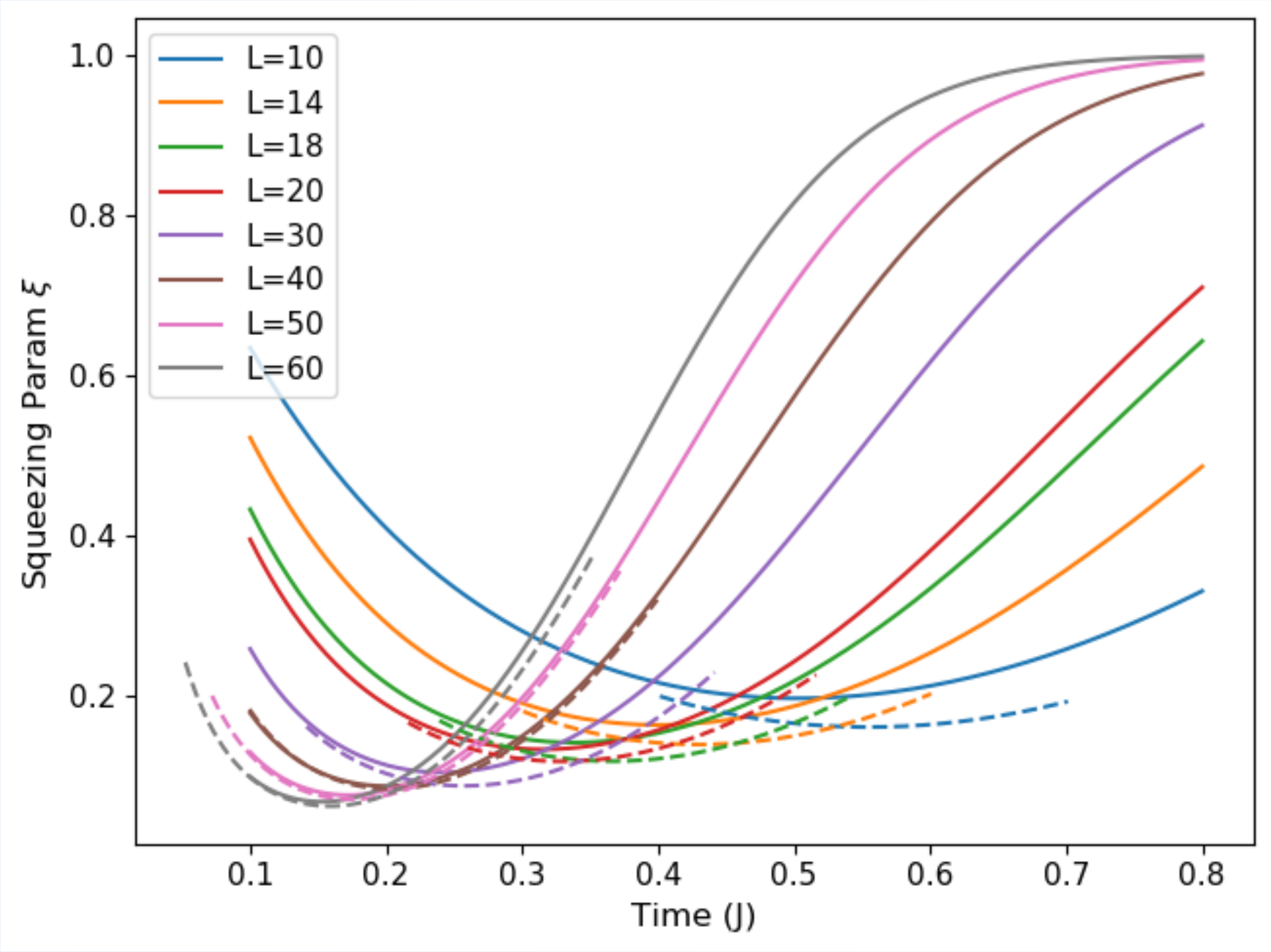
Case Study: Squeezing

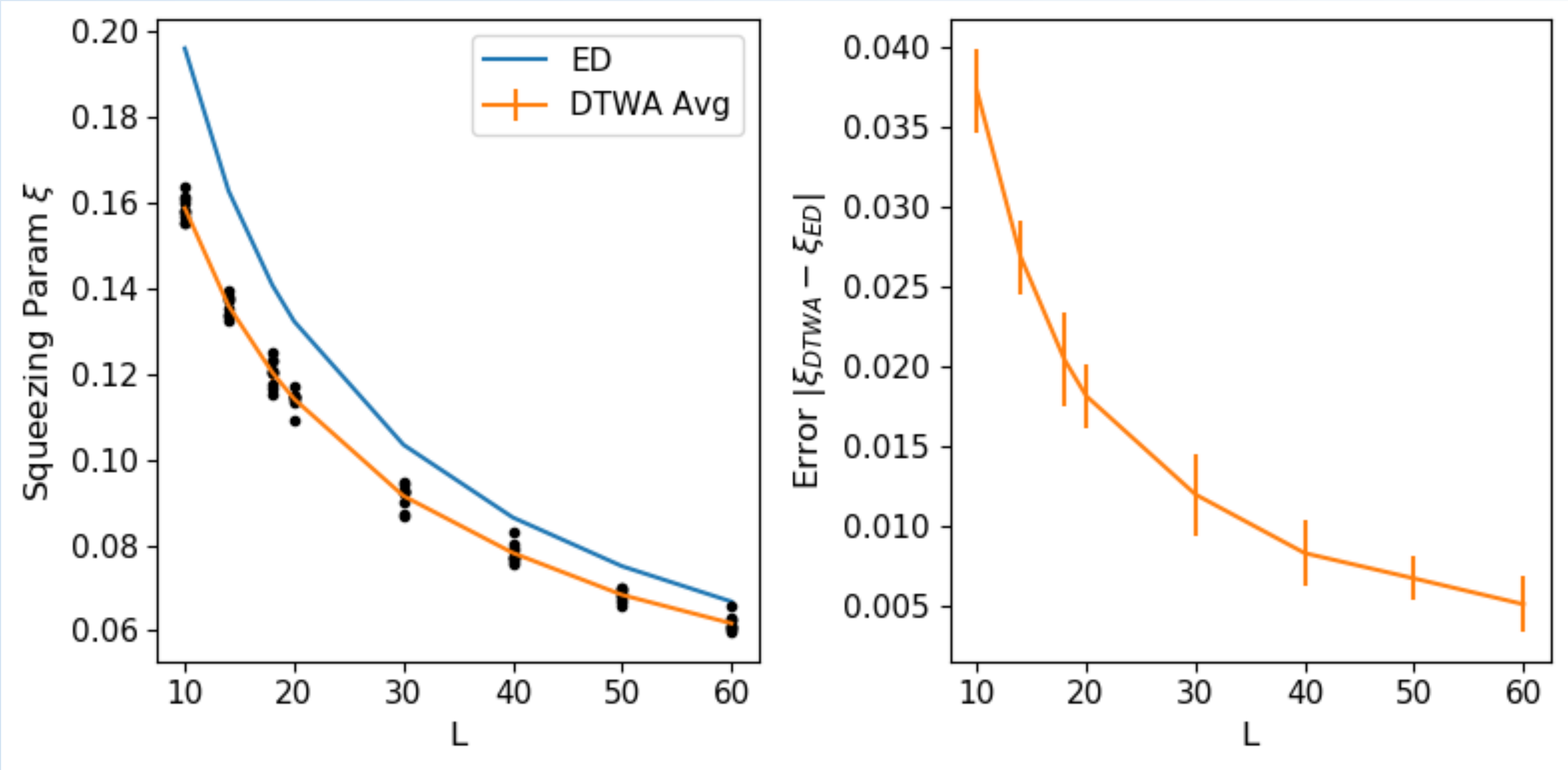




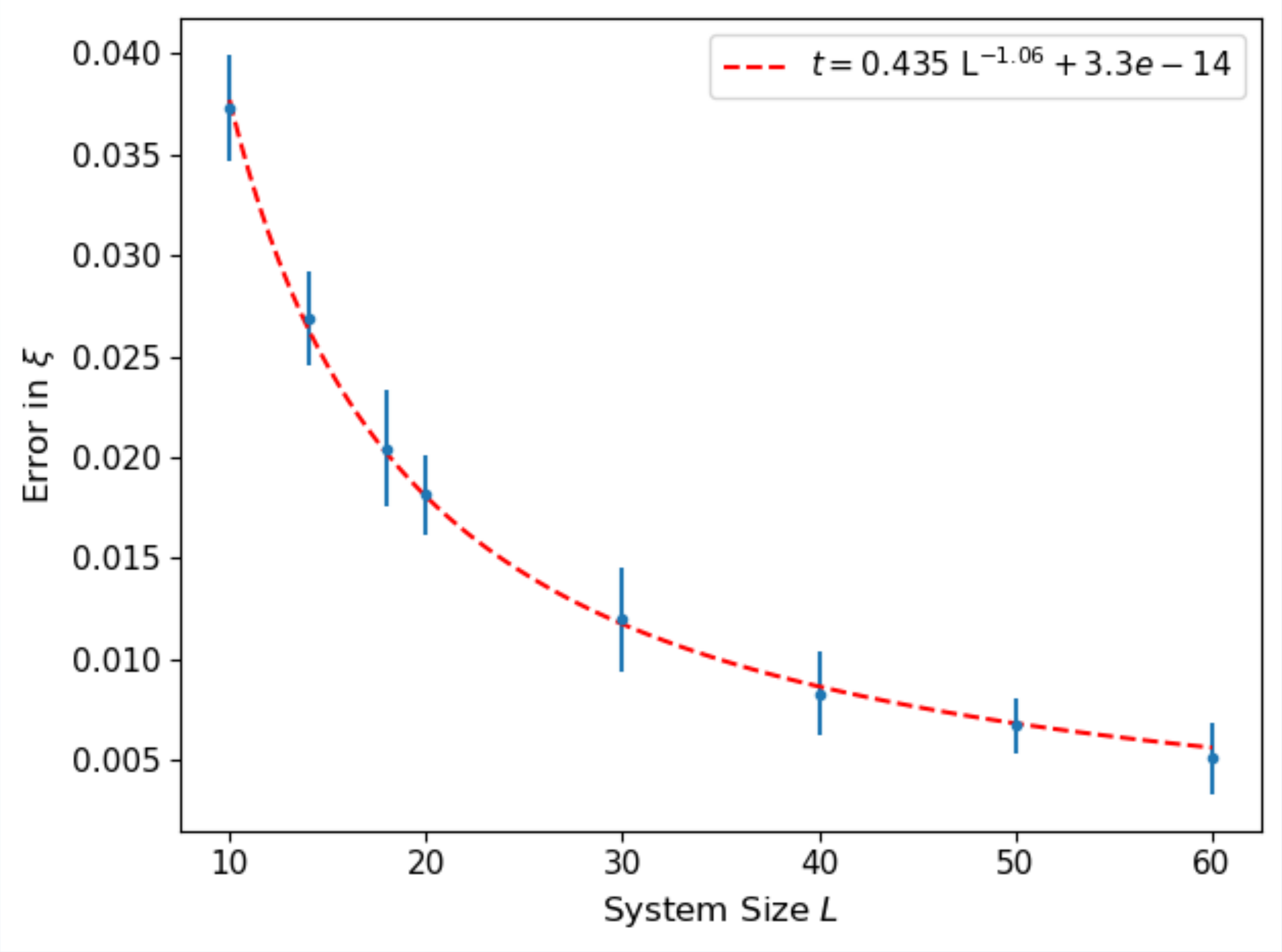


Dependence on System Size



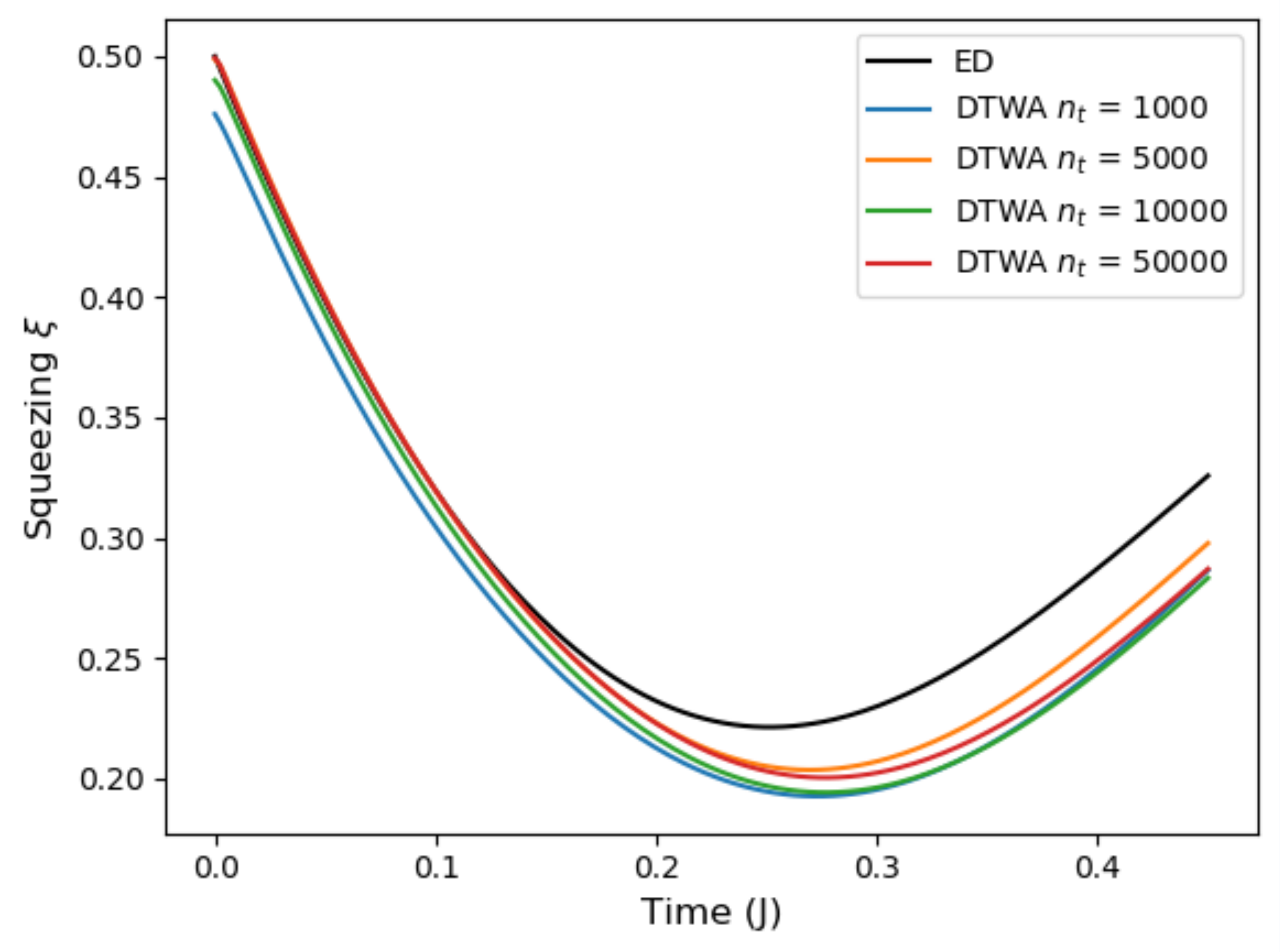


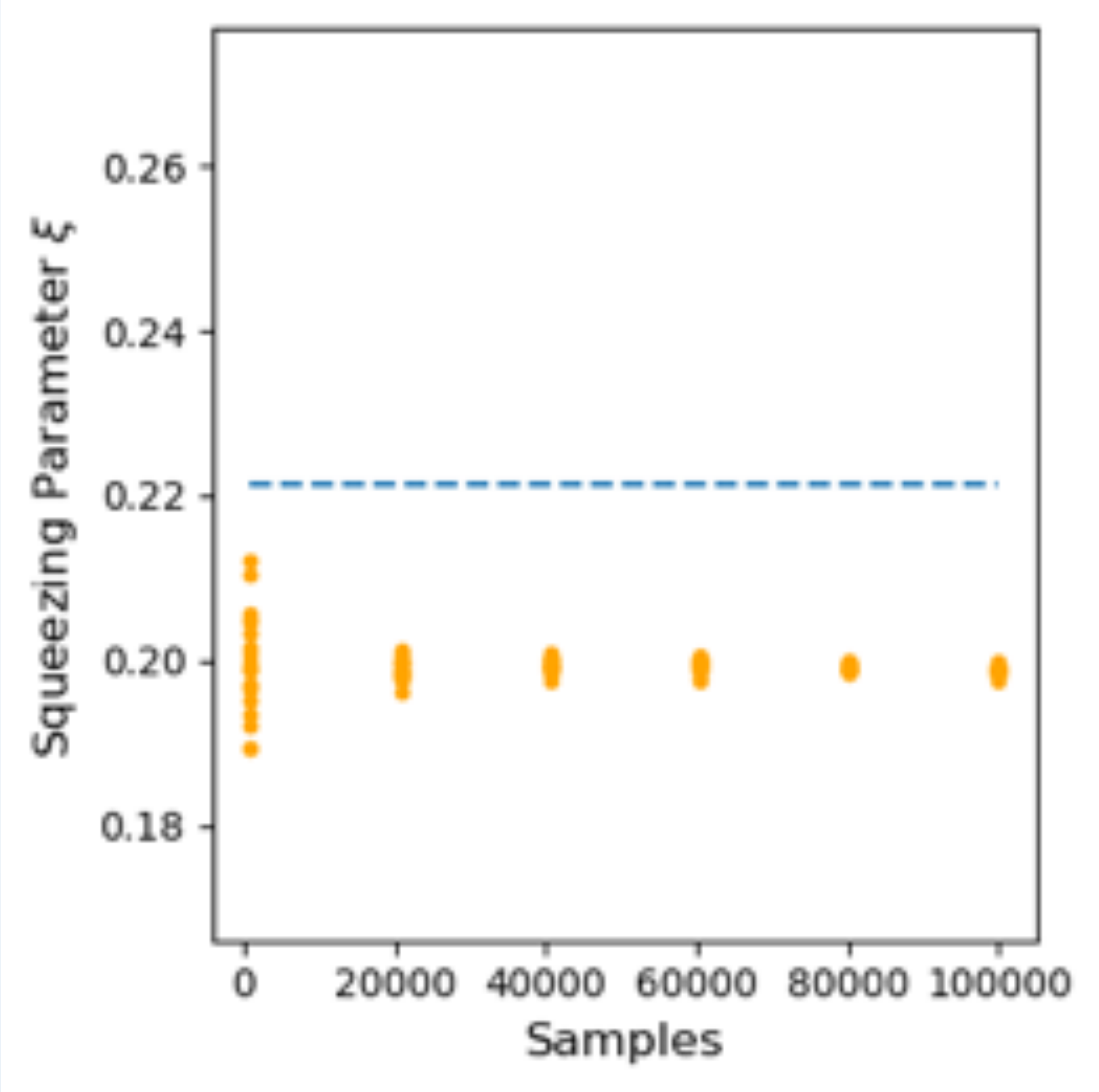
1/L scaling of error, as expected

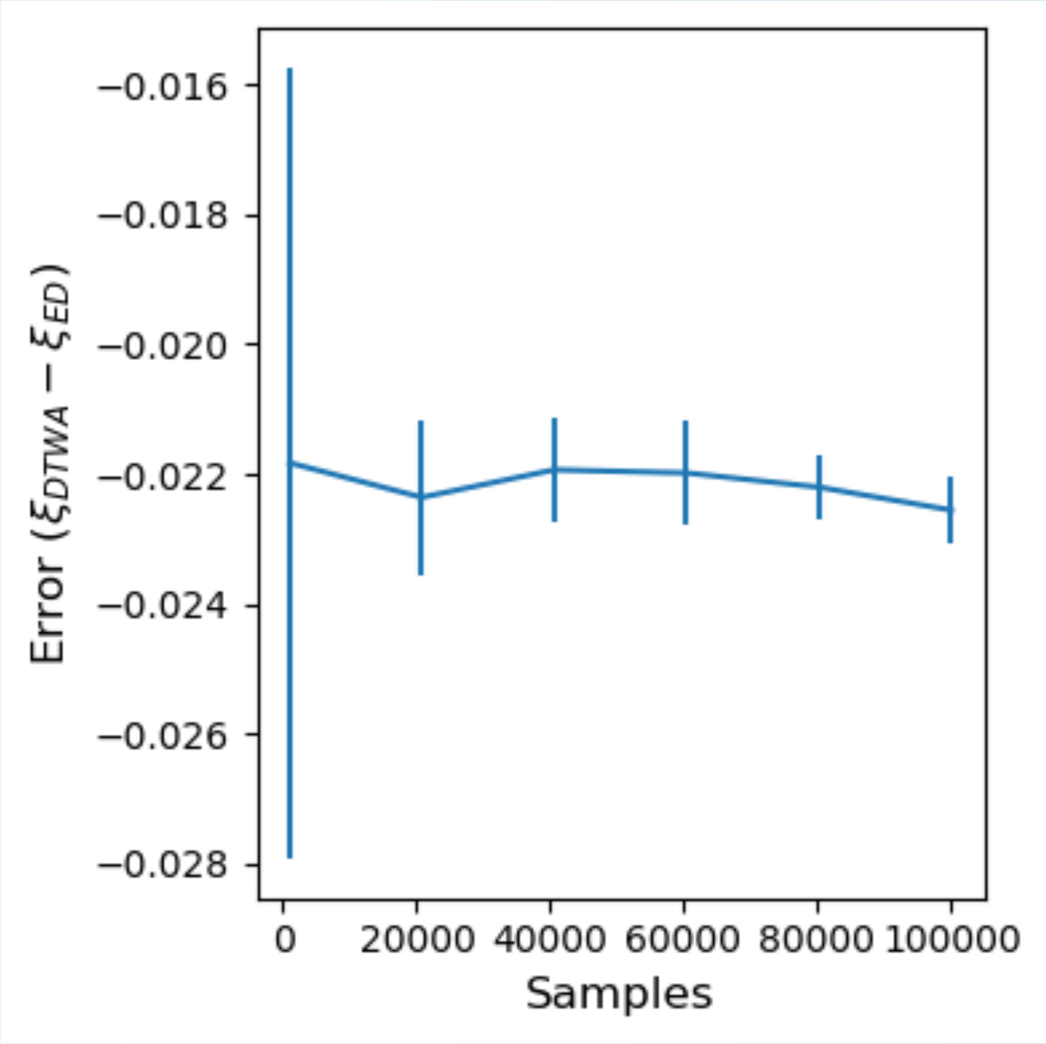


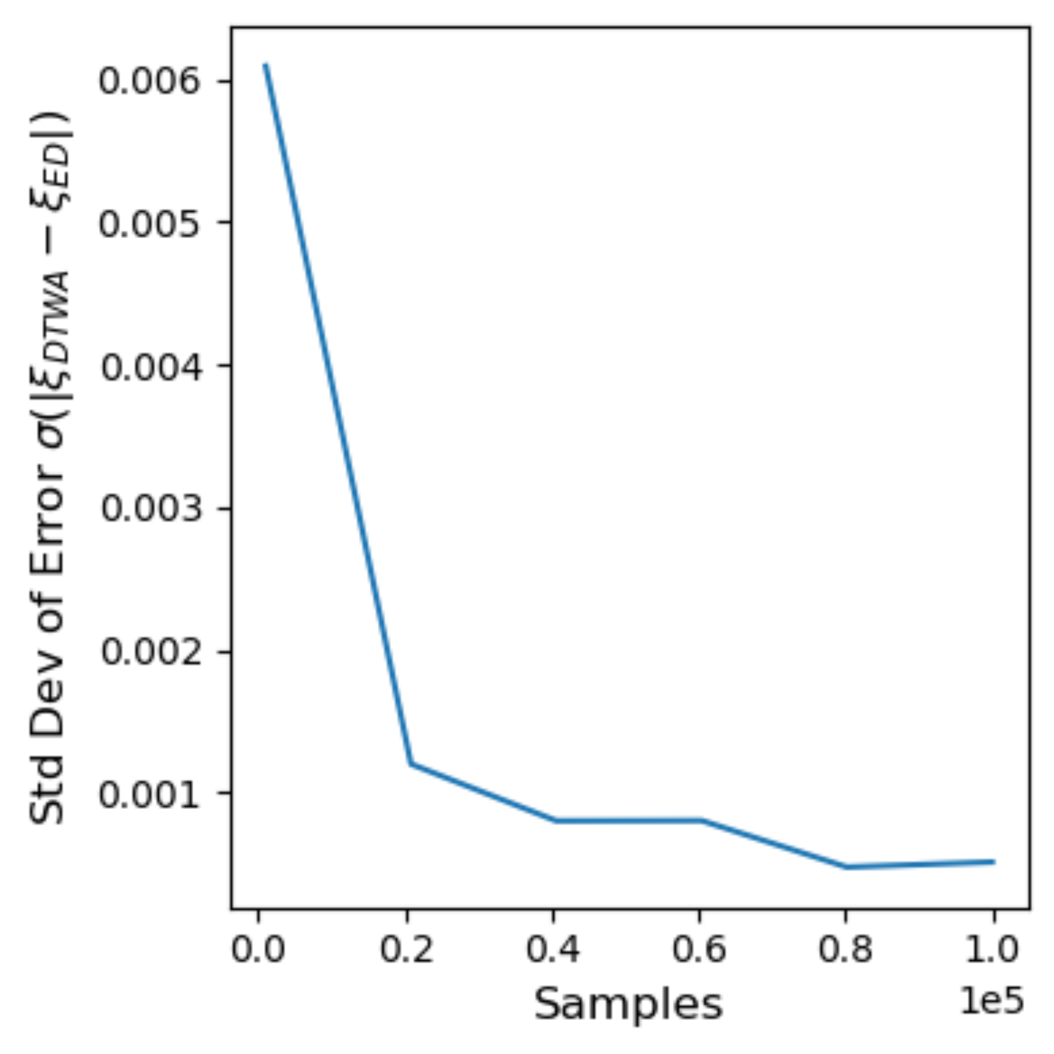
Numerical Convergence

Average squeezing parameter is constant with fluctuations decreasing as a function of number of trajectories





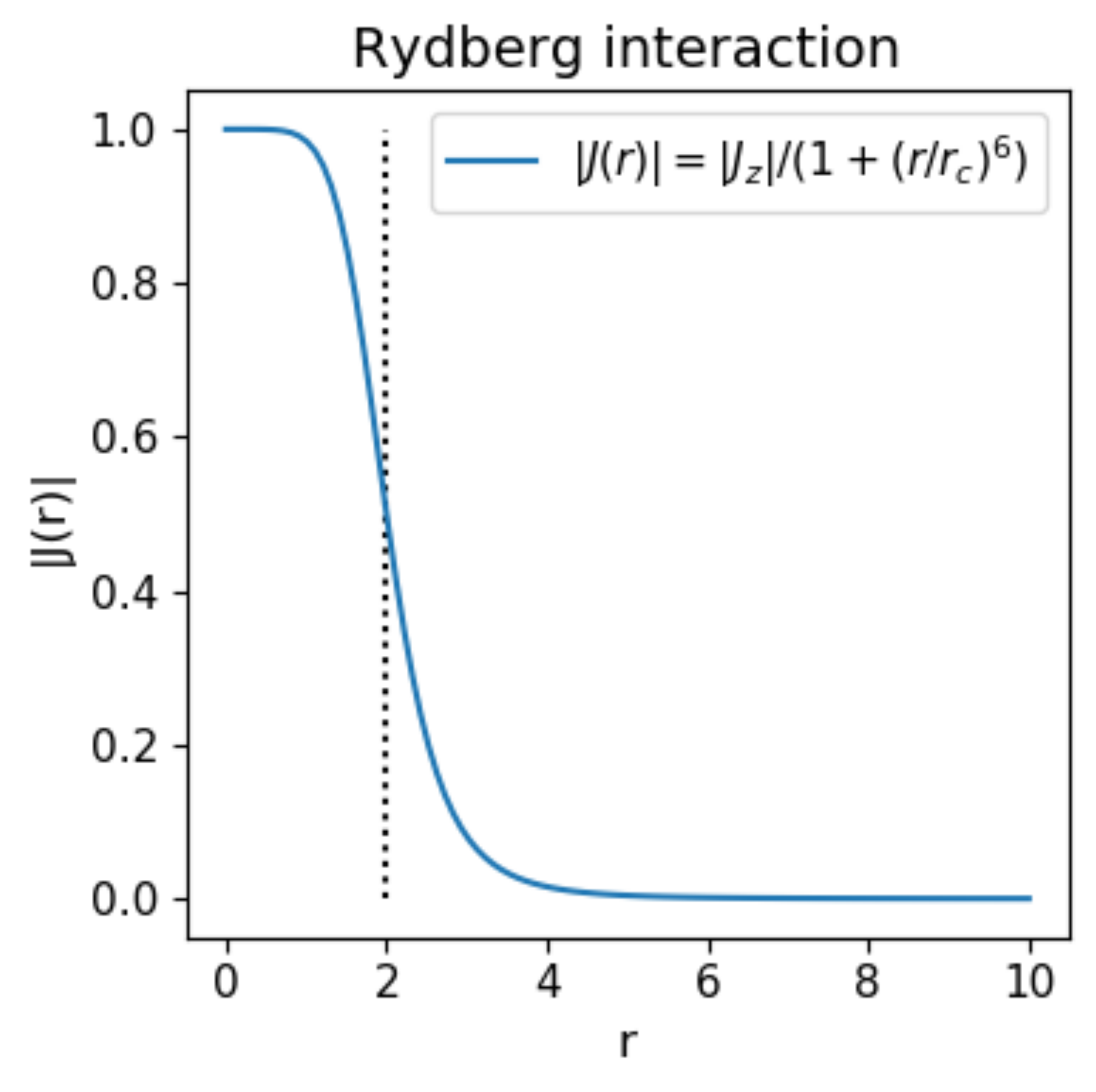


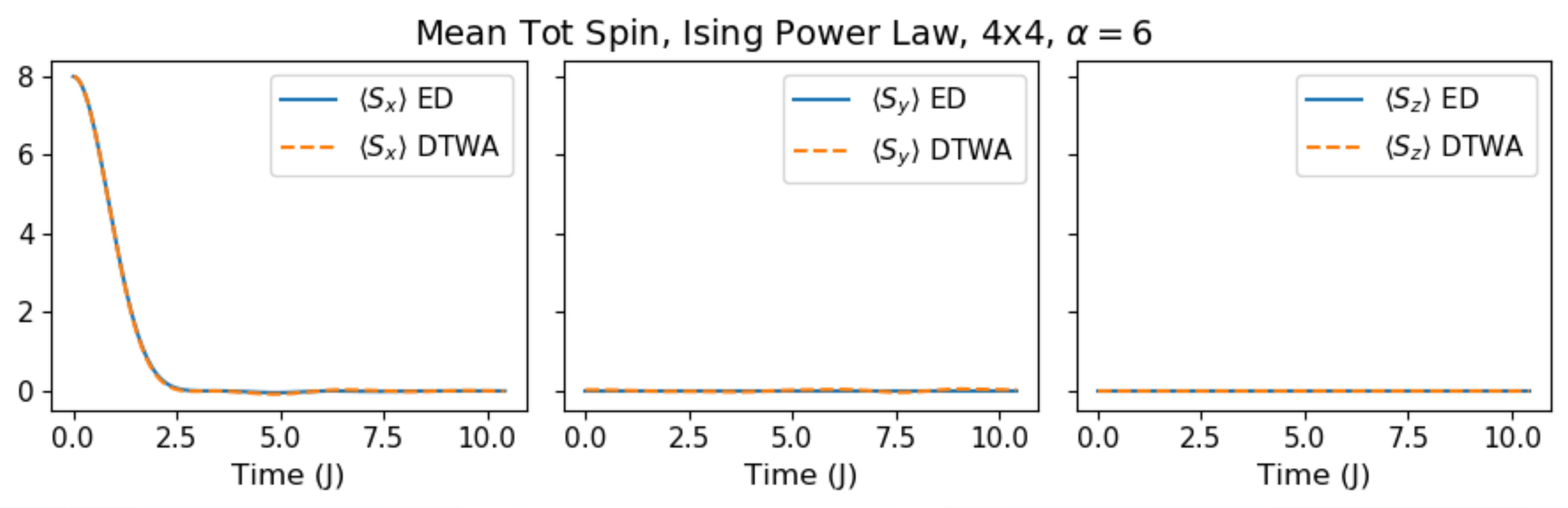


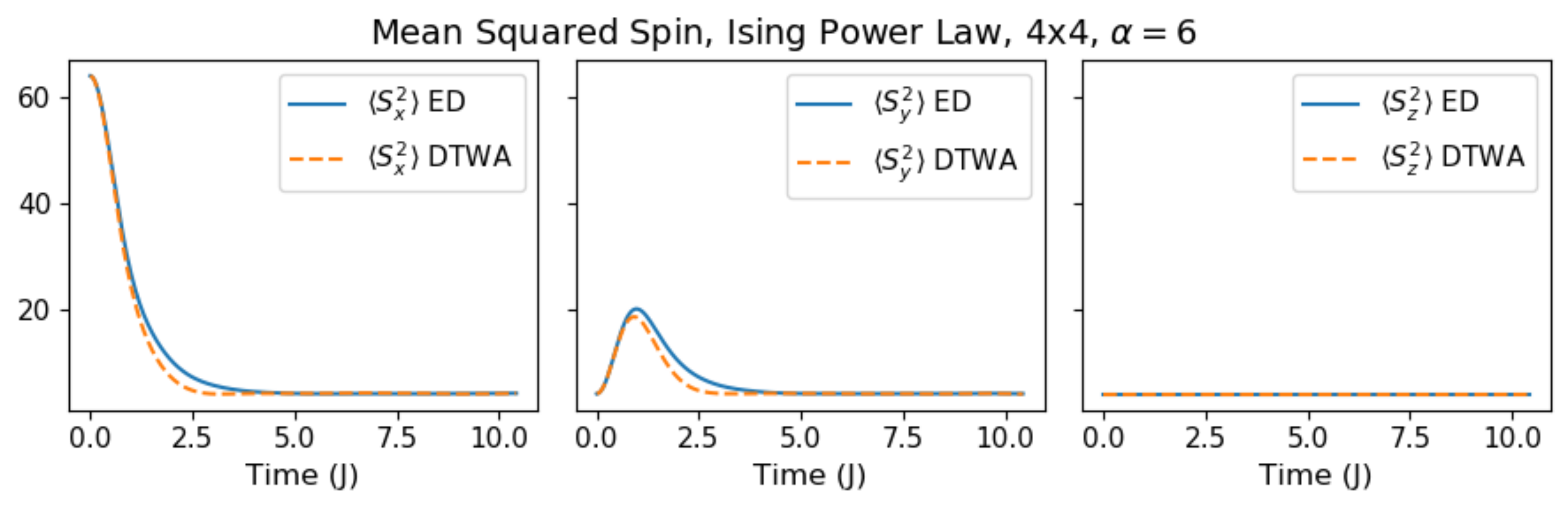
Case Study: Power Law Interactions in 2D

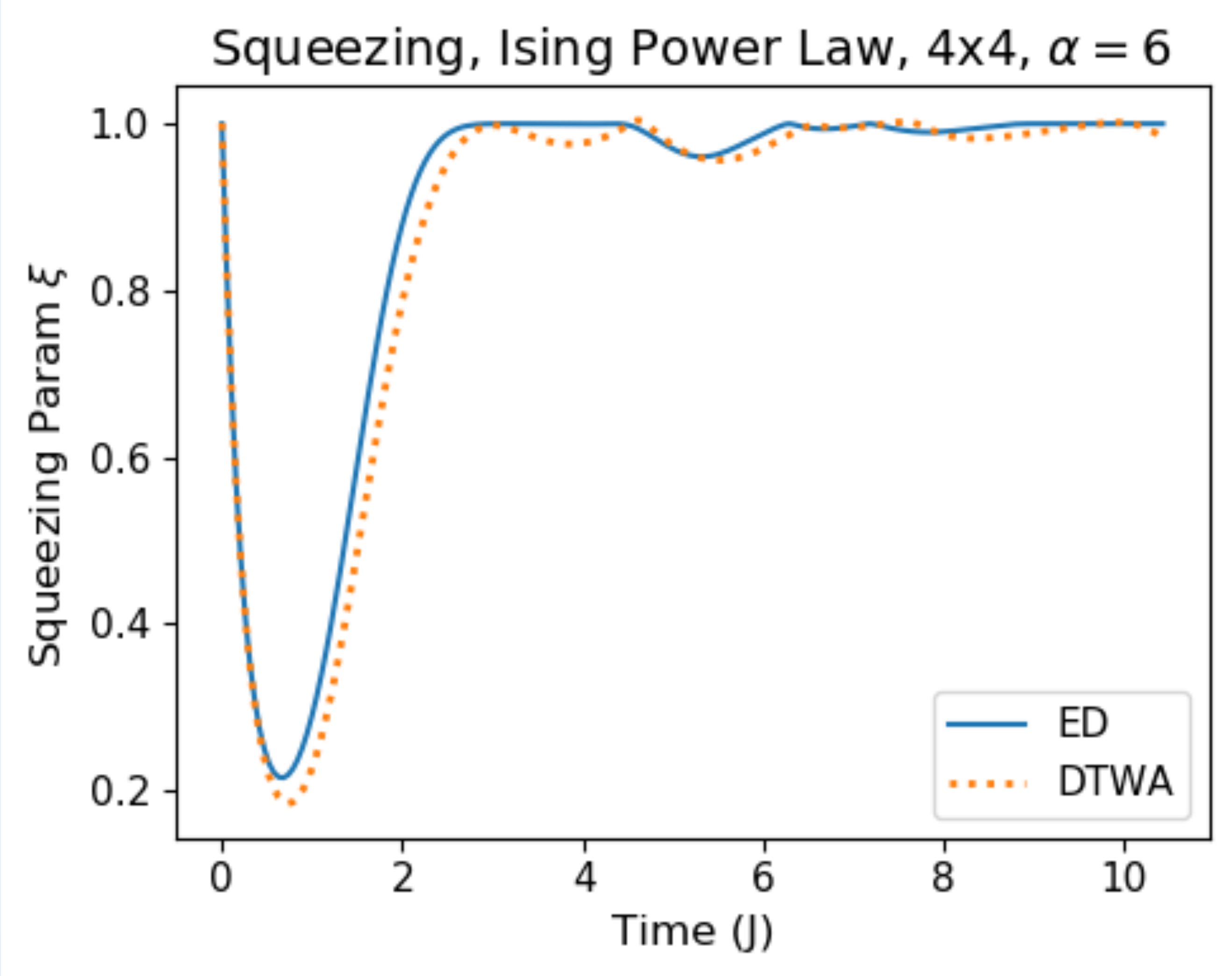
$$J_{ij}(r) \sim J_z \frac{1}{1 + (r/r_c)^6}$$

DTWA is still able to track ED results well

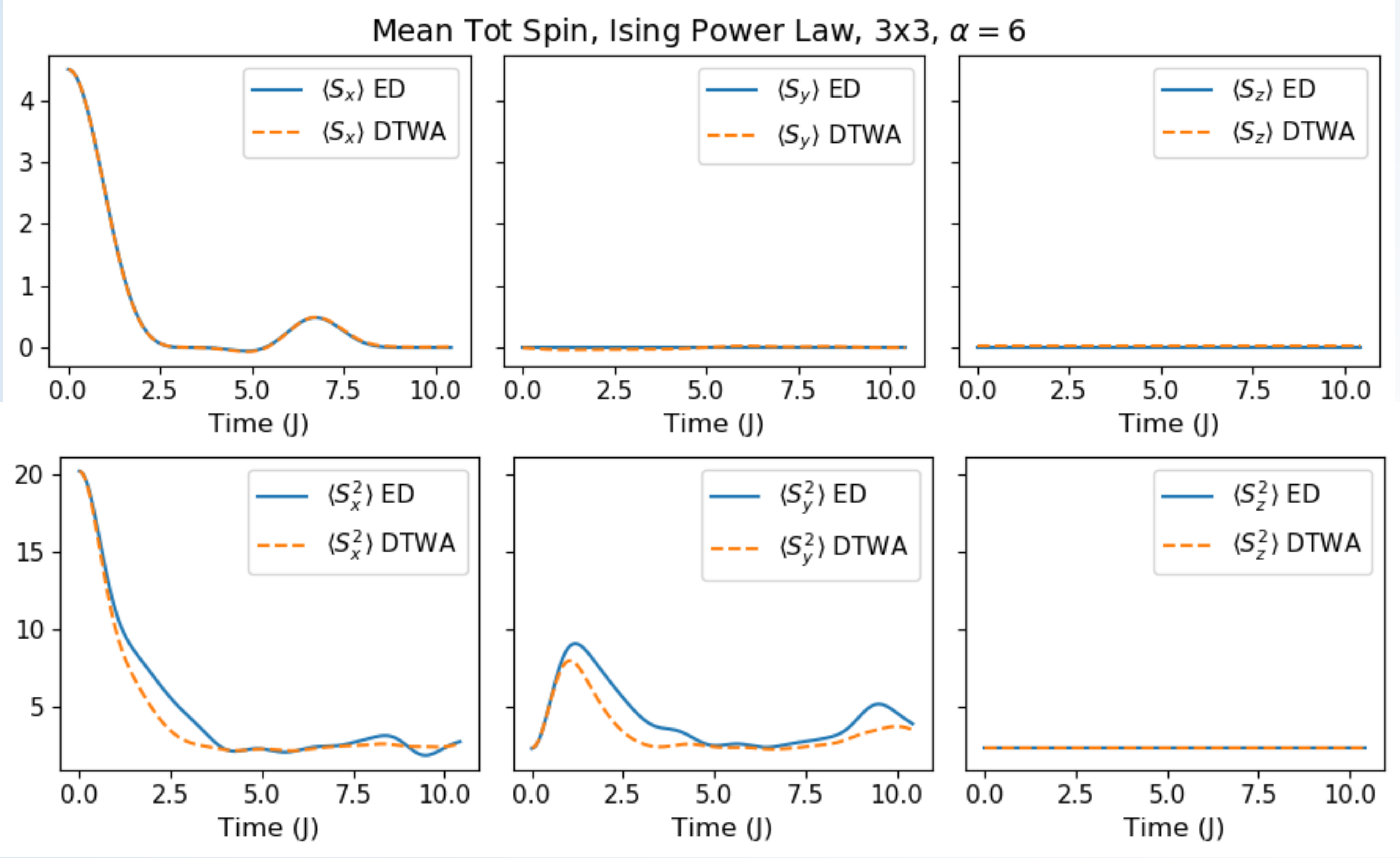


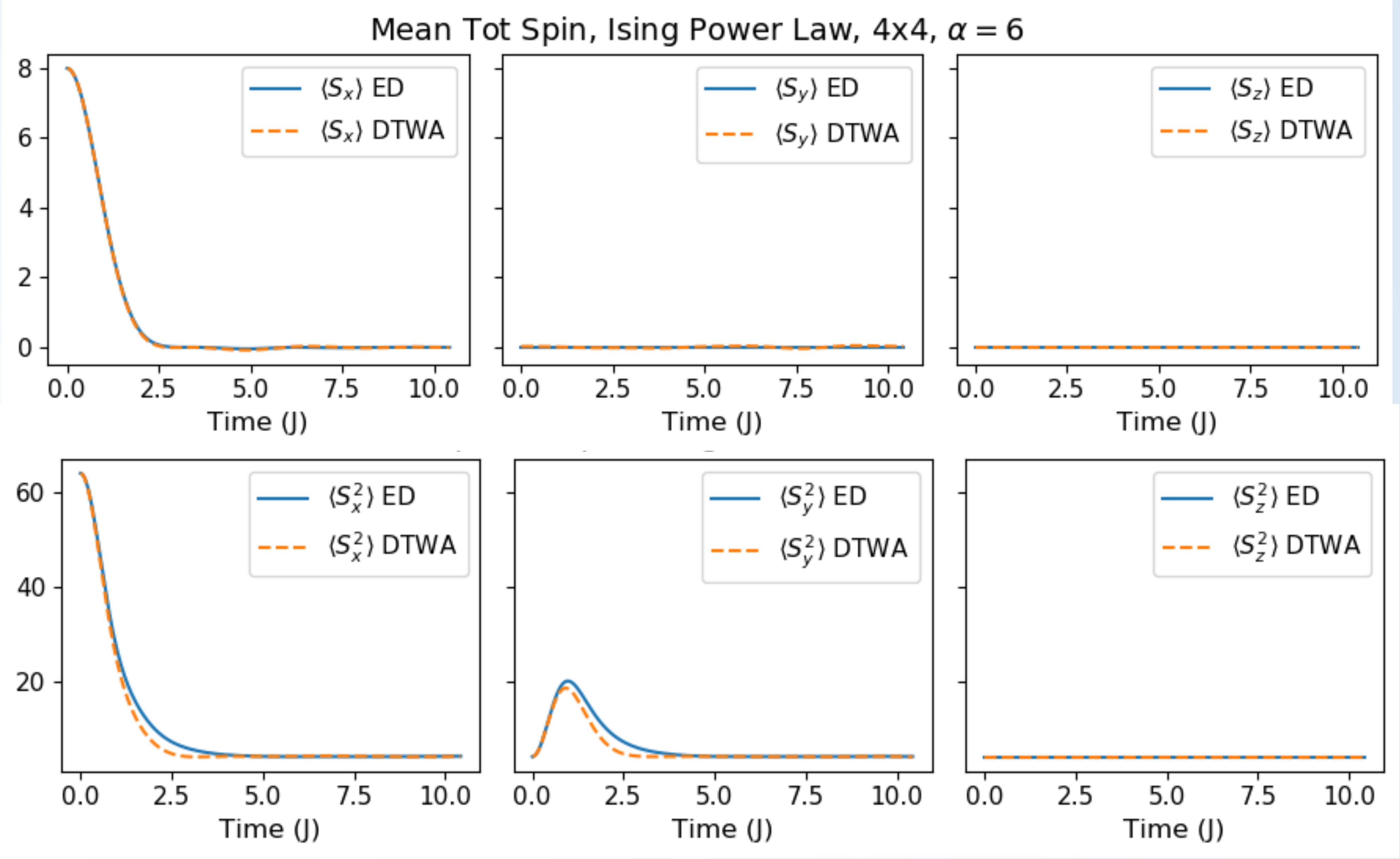


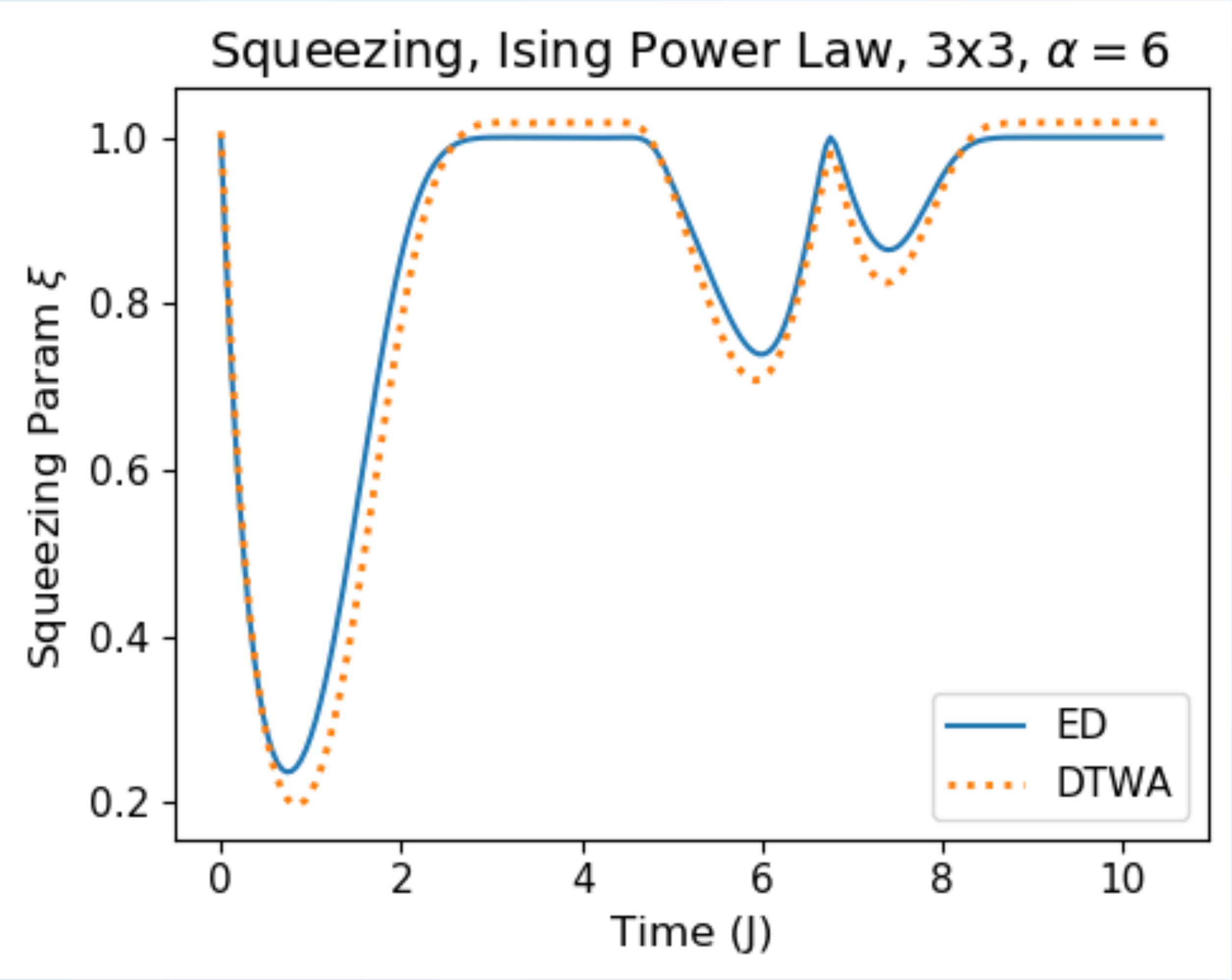


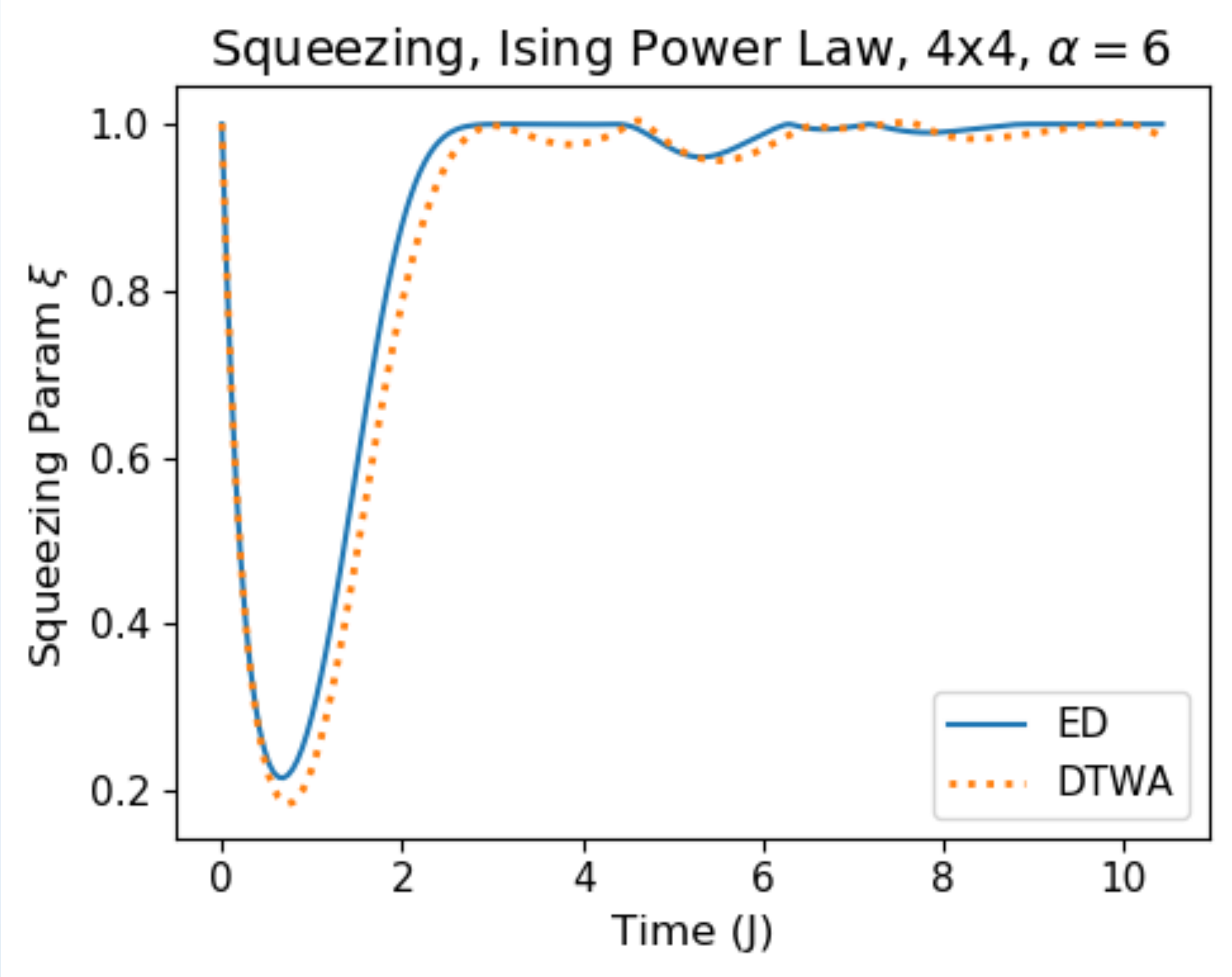


Case Study: Power Law Interactions in 2D









Conclusions

- Explored theoretical backing for the DTWA
- Examined scaling behavior of runtime, dependency on trajectories, and system size
- Demonstrated proof-of-principle numerics with uniform and power-law interactions

Future Directions

- Designing optimal pulse sequences for
  - extreme squeezing
  - QAOA
- Time-evolving spatial maps of correlations

Coding Suite

- Will be available soon on GitHub with:
  - Python library
  - IPython Tutorial
  - presentation + notes

```
]: # IMPORT LIBRARIES
   from fractions import Fraction

   from DTWA_Lib import *

   %matplotlib notebook
```

```
#### Generates general all-to-all Heisenberg model
# Hamilt: sum_ij[ (Jx_ij(X_i X_j) + Jy_ij(Y_i Y_j)) +  Jz_ij(Z_i Z_j)] + hx * sum_i[X_i] + hz * sum_i[Z_i]
# if Jperp = (Jx, Jy), then have XYZ. ow have XXZ w/ Jx = Jy = Jperp/2
# L = vector containing number of spins along each dimension
# PauliBool = (optional) True to switch to Pauli operators; False to use Spin Operators
# opList = (optional) to provide list
# Jfunc = (optional) list of functions for Jx, Jy, Jz to compute interaction between every pair of spins; may be distance-dependent
# coord = (optional) Nxd numpy arrays representing the d coordinates of each spin; default gives regular lattice with spacing a=1
# alpha = (optional) exponent of decay for interaction strength  J_ij ~ 1/|r_ij|^α
def Heisenberg_A2A(L, Jperp, Jz, hx, hz, PauliBool = False, opList=[], Jfunc=[], coord = [], alpha=[]):
    if not coord==[] and np.prod(L)!=coord.shape[0]:
        raise Exception("Number of coordinates doesn't match number of spins!")
        print(np.prod(L))
    N = np.prod(L)  # total number of spins = product of number of spins along each direction
    # print("N: %d" %N)

    if opList==[]:
        if PauliBool:
            opList = genPauliList(N)
        else:
            opList = genSpinOpList(N)
    sx, sy, sz, sp, sm = opList
    # print("number of spin ops: %d" %len(sx))
    # print("dimension of spin op: %s" %(sx[0].shape,))

    # Generate coupling strengths
    if isinstance(Jperp,(float, int)):   # XXZ CHAIN
        Jx = Jperp/2
        Jy = Jperp/2

    elif isinstance(Jperp,(list,tuple,np.ndarray)) and len(Jperp)==2:
        Jx = Jperp[0]
        Jy = Jperp[1]
    else:
        raise Exception("Wrong number of elements in Jperp!")
    # print("Jx: %g \t Jy: %g \t Jz: %g" % (Jx,Jy,Jz))

    H_int = []
```

Thanks for listening!

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