The quantum many-body non-equilibrium problem in phase space

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The quantum many-body non-equilibrium problem in phase space

Goal:

A tour through numerical methods for simulating large quantum many-body dynamics (in general and) with a focus on phase space concepts

Lecture 1: Exact numerical methods and their limitations. How to to go beyond?

Lecture 2: Introduction to quantum physics on phase space. The truncated Wigner approximation (TWA).

Lecture 3: Simulating quantum many-body dynamics with the discrete TWA (DTWA)

- Some text recommendations:
  - *For phase-space methods: Online lecture notes: A. Polkovnikov, Boulder summer school 2013: https://boulderschool.yale.edu/2013/boulder-school-2013-lecture-notes*
- Language recommendation (used for examples): Julia, **https://julialang.org/** (open source, easy, fast linear algebra)
- What these lectures are **not:**
  - *Complete: Many techniques are not discussed, many proofs are skipped: The big picture instead*
  - *Computer science class*
- Two types of lectures: Theory intro and "tutorial style" (sometimes mixed)
  Will provide code snippets, but no copy and paste!
- Philosophy: Use toolboxes only for basics (linear algebra, statistics)… let's understand things from scratch

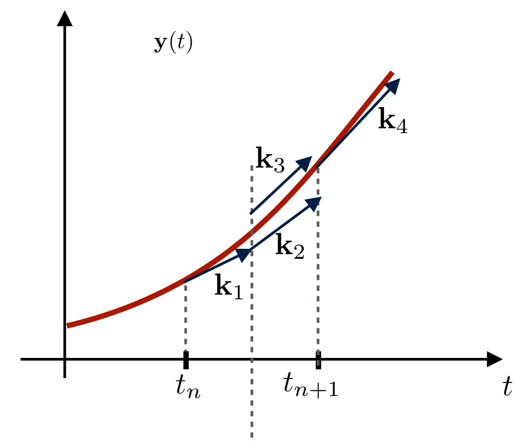
Lecture 3 - Plan for today

Today 50/50: Tutorial style | Theory lecture style

- **Part 3.1:** Introduce Runge-Kutta methods

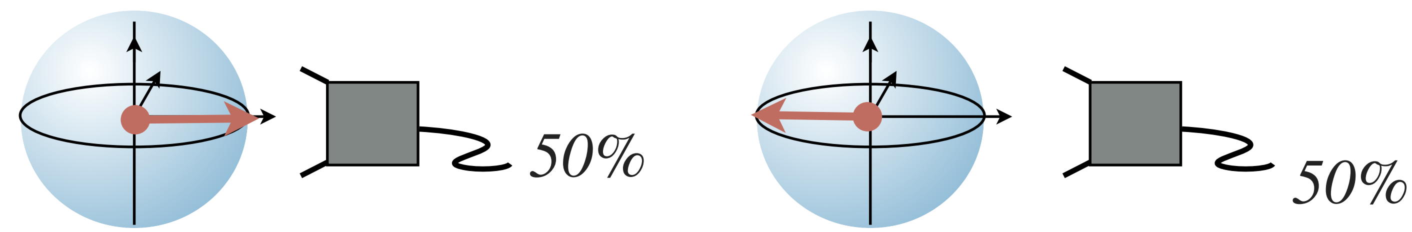
Swiss army knife for solving ODE dynamics

$$\mathbf{k}_1 = f(t_n, \mathbf{y}_n)$$
$$\mathbf{k}_2 = f\left(t_n + \frac{h}{2}, \mathbf{y}_n + \frac{h}{2}\mathbf{k}_1\right)$$
$$\mathbf{k}_3 = f\left(t_n + \frac{h}{2}, \mathbf{y}_n + \frac{h}{2}\mathbf{k}_2\right)$$
$$\mathbf{k}_4 = f\left(t_n + h, \mathbf{y}_n + h\mathbf{k}_3\right)$$
$$\mathbf{y}_{n+1} \approx \mathbf{y}_n + \frac{h}{6}(\mathbf{k}_1 + 2\mathbf{k}_2 + 2\mathbf{k}_3 + \mathbf{k}_4)$$



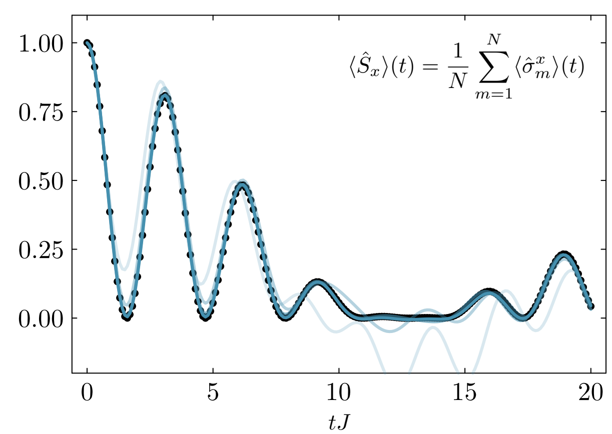
- **Part 3.2:** Back to phase space: The discrete TWA (DTWA) for generic spin-1/2 model dynamics

$$W(+1,+1,-1) = 1/4$$
$$W(-1,+1,-1) = 1/4$$
$$W(+1,-1,-1) = 1/4$$
$$W(-1,-1,-1) = 1/4$$

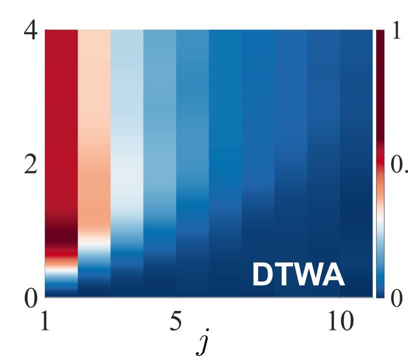


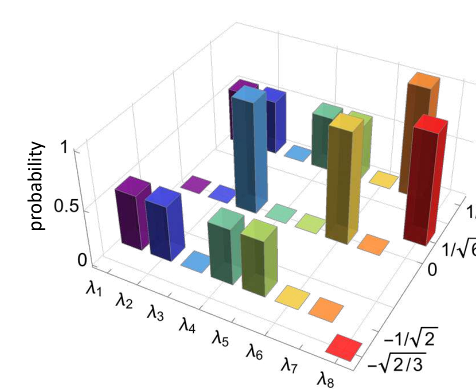
- **Part 3.3:** Set up a DTWA code for Ising model simulations. Understand the approximation better

$$\mathbf{Y} \equiv (\mathbf{Y}_1 \quad \mathbf{Y}_2 \quad \dots \quad \mathbf{Y}_{n_T}) = \begin{pmatrix} x_{1,1} & x_{1,2} & & x_{1,n_T} \\ \vdots & \vdots & & \\ x_{N,1} & x_{N,2} & & x_{N,n_T} \\ y_{1,1} & y_{1,2} & & y_{1,n_T} \\ \vdots & \vdots & \dots & \\ y_{N,1} & y_{N,2} & & y_{N,n_T} \\ z_{1,1} & z_{1,2} & & z_{1,n_T} \\ \vdots & \vdots & & \\ z_{N,1} & z_{N,2} & & z_{N,n_T} \end{pmatrix}$$



- **Part 3.4:** Generalizations to spin > 1/2 models and use case examples





Lecture 3.1 - Runge-Kutta Methods

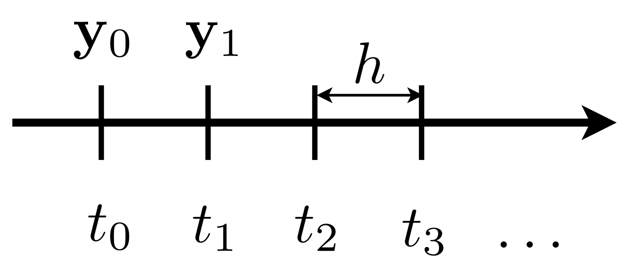
- A general class of standard methods for initial value problems ("Swiss army knife")

$$\dot{\mathbf{y}}(t) = f(t, \mathbf{y}(t)) \qquad \mathbf{y}(t_n) = \mathbf{y}_n \qquad \textit{Find:} \quad \mathbf{y}_{n+1} \approx \mathbf{y}(t_n + h)$$

$\mathbf{y}(\dots)$ *"exact"*

$\mathbf{y}_n$ *"numerical approximation"*

- Time-discretization:



- Note: This includes linear Schrödinger equation, but also non-linear (e.g. mean-field/Gross-Pitaevskii) problems

Schrödinger equation

$$\frac{d}{dt}|\psi\rangle = -\mathrm{i}\hat{H}|\psi\rangle$$

$$f(t, \mathbf{y}(t)) = \mathbf{A} \cdot \mathbf{y}(\mathbf{t})$$

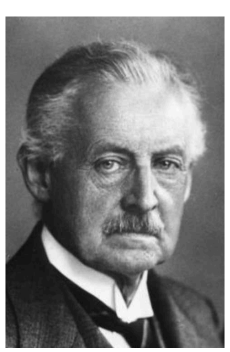
GP equation

$$\frac{d}{dt}\psi(x,t) = -\mathrm{i}\left(\frac{\hat{p}^2}{2m} + V(x) + g|\psi(x,t)|^2\right)\psi(x,t)$$

discretized $\quad \psi(x,t) = \psi_i(t)$

$$f(t, \mathbf{y}(t)) = \mathbf{A}(\mathbf{y}(t)) \cdot \mathbf{y}(\mathbf{t})$$

$$\mathbf{y} = \begin{pmatrix} \psi_1 \\ \psi_2 \\ \vdots \\ \psi_{M-1} \\ \psi_M \end{pmatrix}$$



Carl David Tolmé Runge (1856-1927)

Martin Kutta (1867–1944)

Lecture 3.1 - Runge-Kutta Methods: 1st order - explicit Euler

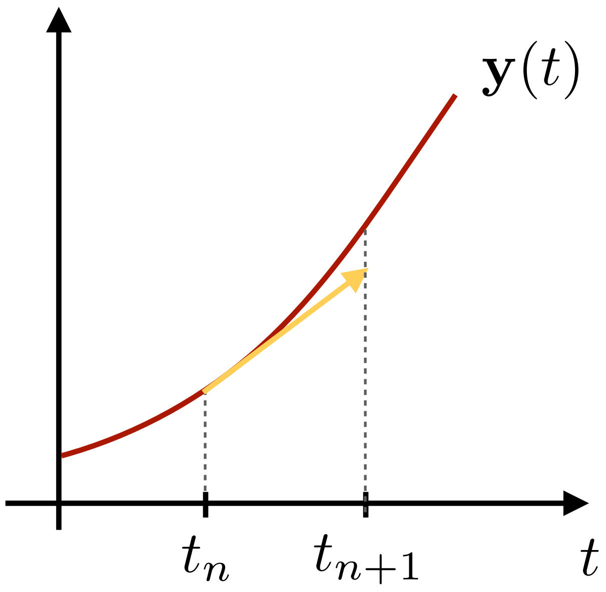
$$\dot{\mathbf{y}}(t) = f(t, \mathbf{y}(t)) \qquad \mathbf{y}(t_n) = \mathbf{y}_n \qquad \textit{Find:} \quad \mathbf{y}_{n+1} \approx \mathbf{y}(t_n + h)$$

- Let's find a method from Taylor expansion of $\mathbf{y}(t)$

$$\mathbf{y}(t_n + h) = \mathbf{y}(t_n) + h\dot{\mathbf{y}}(t_n) + \frac{h^2}{2}\ddot{\mathbf{y}}(t_n) + \cdots = \boxed{\mathbf{y}(t_n) + hf(t_n, \mathbf{y}_n)} + \mathcal{O}(h^2)$$

$$\boxed{\mathbf{y}_{n+1} \approx \mathbf{y}_n + hf(t_n, \mathbf{y}_n)}$$

"explicit Euler method"

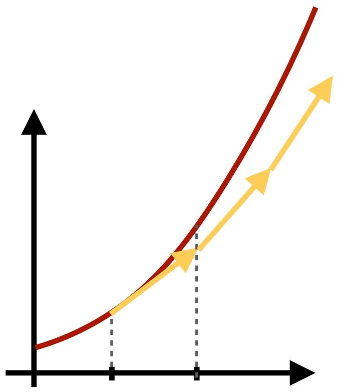


- Not a good method for several reasons

Error is large $\mathcal{O}(h^2)$

... need tiny h

Solution is often not stable!



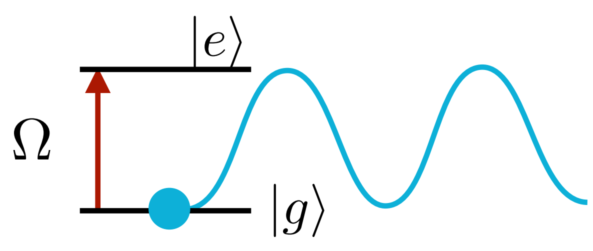
"error grows in same direction"

Lecture 3.1 - Runge-Kutta Methods: 1st order

$$\dot{\mathbf{y}}(t) = f(t, \mathbf{y}(t)) \qquad \mathbf{y}(t_n) = \mathbf{y}_n \qquad \textit{Find:} \quad \mathbf{y}_{n+1} \approx \mathbf{y}(t_n + h)$$

- … very simple example (Rabi oscillations)

$$\hat{H} = \begin{pmatrix} 0 & \Omega \\ \Omega & 0 \end{pmatrix} \qquad \frac{d}{dt}|\psi\rangle = -\mathrm{i}\hat{H}|\psi\rangle \qquad |\psi_0\rangle = \begin{array}{cc} \begin{pmatrix} 1 \\ 0 \end{pmatrix} & \begin{array}{c} |g\rangle \\ |e\rangle \end{array} \end{array}$$



Compute:

$$n_e(t) = |\,\langle\psi(t)|e\rangle\,|^2$$

Exact:

$$n_e(t) = \sin^2(t\Omega)$$

$\Omega \equiv 1$

```
h = 0.05
steps = 200

psi = [1;0]
ne = zeros(steps+1)
ne[1] = abs(psi[2])^2
for tt = 1:steps
    psi = rk1(H, psi, h)
    ne[tt+1] = abs(psi[2])^2
end
```

- Explicit Euler method: $\mathbf{y}_{n+1} \approx \mathbf{y}_n + hf(t_n, \mathbf{y}_n)$

"explicit Euler method"

```
function rk1(H, y, h)
    y += h .* (-1im .* H * y)
    return y
end
```

Lecture 3.1 - Runge-Kutta Methods: 1st order

$$\dot{\mathbf{y}}(t) = f(t, \mathbf{y}(t)) \qquad \mathbf{y}(t_n) = \mathbf{y}_n \qquad \textit{Find:} \quad \mathbf{y}_{n+1} \approx \mathbf{y}(t_n + h)$$

- Explicit Euler method:

$$\mathbf{y}_{n+1} \approx \mathbf{y}_n + hf(t_n, \mathbf{y}_n)$$

"explicit Euler method"

```
function rk1(H, y, h)
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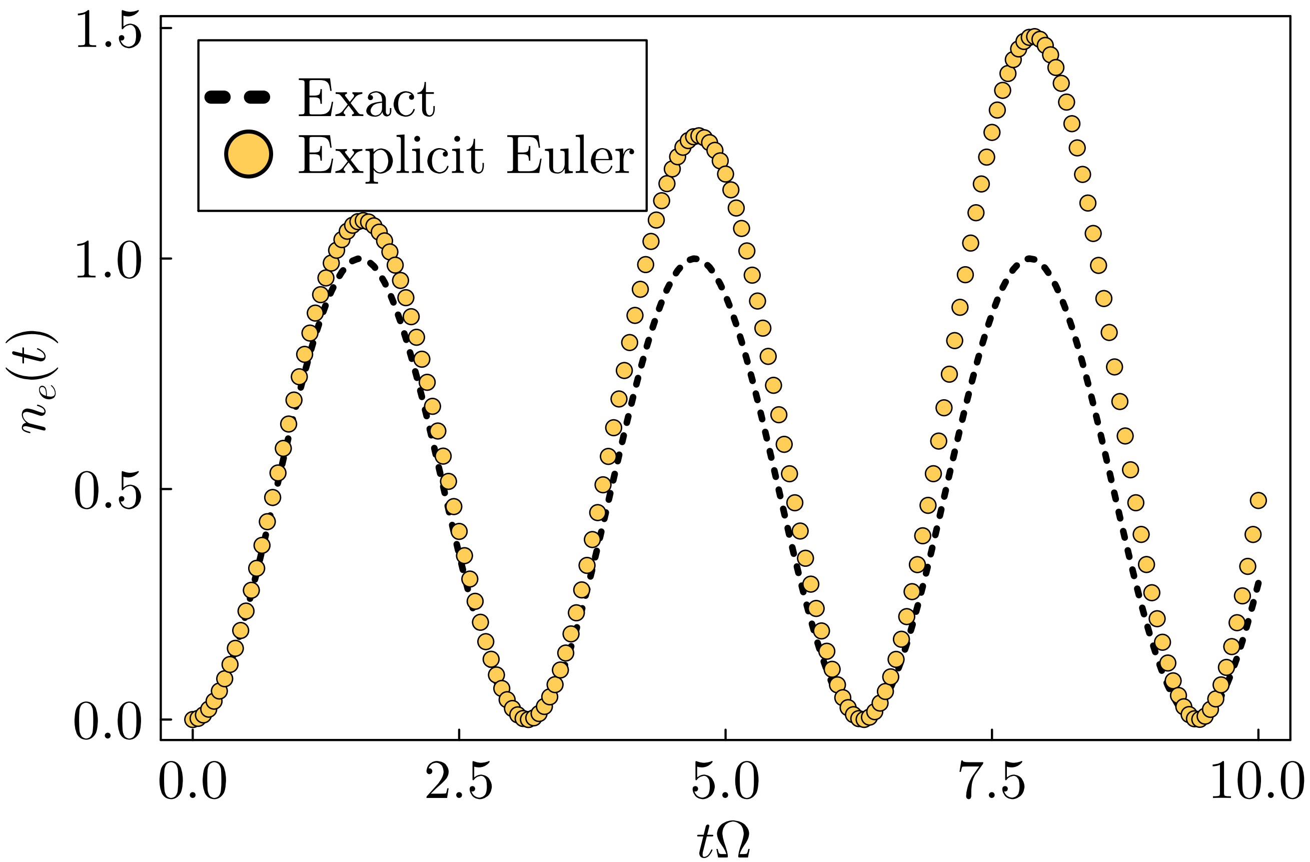
- … very simple example (Rabi oscillations)

$$\hat{H} = \begin{pmatrix} 0 & \Omega \\ \Omega & 0 \end{pmatrix} \qquad \frac{d}{dt}|\psi\rangle = -\mathrm{i}\hat{H}|\psi\rangle \qquad |\psi_0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \begin{matrix} |g\rangle \\ |e\rangle \end{matrix}$$

$$n_e(t) = |\langle\psi(t)|e\rangle|^2$$



Fundamental problem:
Norm keeps increasing!

$$|\psi_{n+1}\rangle = |\psi_n\rangle - \mathrm{i}h\hat{H}\,|\psi_n\rangle$$

$$\langle\psi_{n+1}|\psi_{n+1}\rangle = \langle\psi_n|\psi_n\rangle + h^2\,\langle\psi_n|\,\hat{H}^2\,|\psi_n\rangle$$

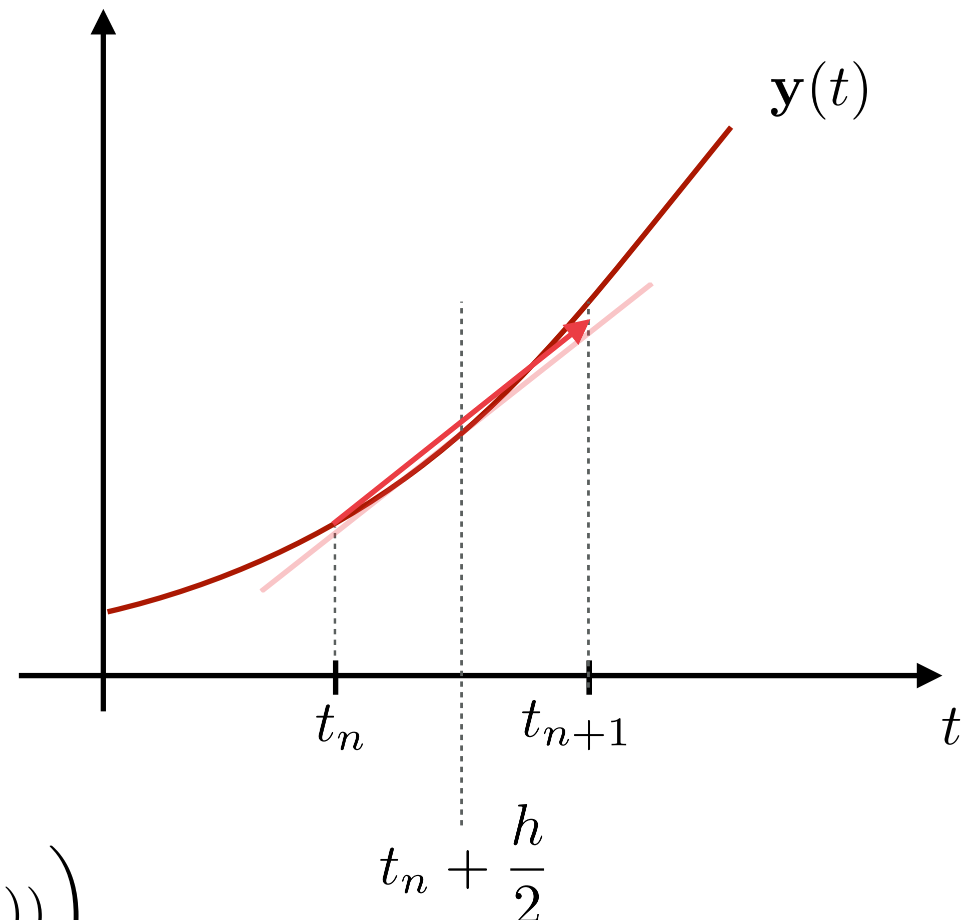
Lecture 3.1 - Runge-Kutta Methods: 2nd order - Midpoint methods

$$\dot{\mathbf{y}}(t) = f(t, \mathbf{y}(t)) \qquad \mathbf{y}(t_n) = \mathbf{y}_n \qquad \textit{Find:} \quad \mathbf{y}_{n+1} \approx \mathbf{y}(t_n + h)$$

- Let's find a better method:

$$\mathbf{y}_{n+1} \approx \mathbf{y}_n + hf\left(t_n + \frac{1}{2}, \frac{1}{2}(\mathbf{y}_n + \mathbf{y}_{n+1})\right)$$

"take slope at middle point"



- Then, in exact Taylor expansion, the error is

$$\begin{aligned}\epsilon_{n+1} &\equiv \mathbf{y}(t_n + h) - \mathbf{y}(t_n) - hf\left(t_n + \frac{h}{2}, \frac{1}{2}(\mathbf{y}(t_n) + \mathbf{y}(t_{n+1}))\right) \\ &= \cdots = 0 + \boxed{\mathcal{O}(h^3)}\end{aligned}$$

(exercise)

- This is called "implicit midpoint method"

Implicit, meaning: The right hand-side has already the solution at n+1, so one generally needs to resolve the equation for the n+1 value or use some iteration.

Lecture 3.1 - Runge-Kutta Methods: 2nd order - Midpoint methods

$$\dot{\mathbf{y}}(t) = f(t, \mathbf{y}(t)) \qquad \mathbf{y}(t_n) = \mathbf{y}_n \qquad \textit{Find:} \quad \mathbf{y}_{n+1} \approx \mathbf{y}(t_n + h)$$

$$\mathbf{y}_{n+1} \approx \mathbf{y}_n + hf\left(t_n + \frac{1}{2}, \frac{1}{2}(\mathbf{y}_n + \mathbf{y}_{n+1})\right)$$

"implicit midpoint method"

- Zero order iteration gives:

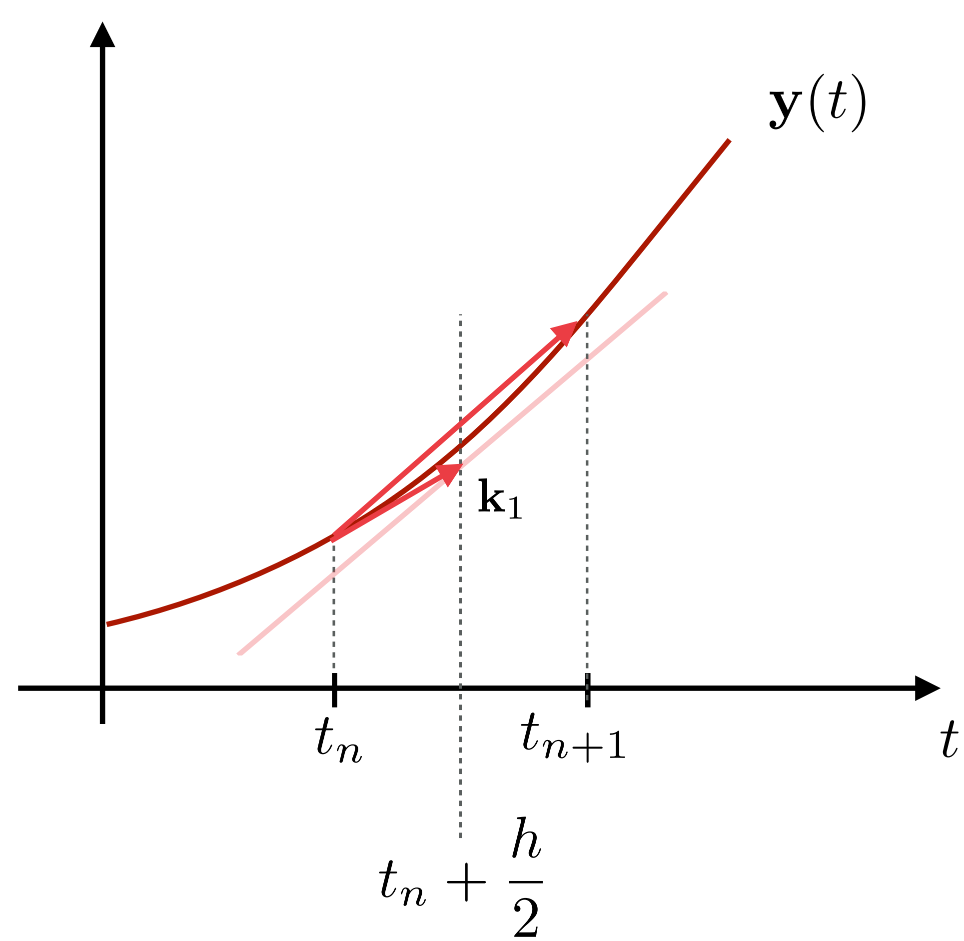
$$\mathbf{y}_{n+1} \approx \mathbf{y}_n + hf\left(t_n + \frac{1}{2}, \mathbf{y}_n\right) \qquad \mathbf{k}_1 \equiv \frac{\mathbf{y}_n + \mathbf{y}_{n+1}}{2} \approx \mathbf{y}_n + \frac{h}{2} f\left(t_n + \frac{1}{2}, \mathbf{y}_n\right)$$

Explicit Euler estimate for mid-point

$$\mathbf{k}_1 = \mathbf{y}_n + \frac{h}{2} f(t_n + \mathbf{y}_n)$$

$$\mathbf{y}_{n+1} \approx \mathbf{y}_n + hf(t_n + \frac{h}{2}, \mathbf{k}_1)$$

"explicit midpoint method"



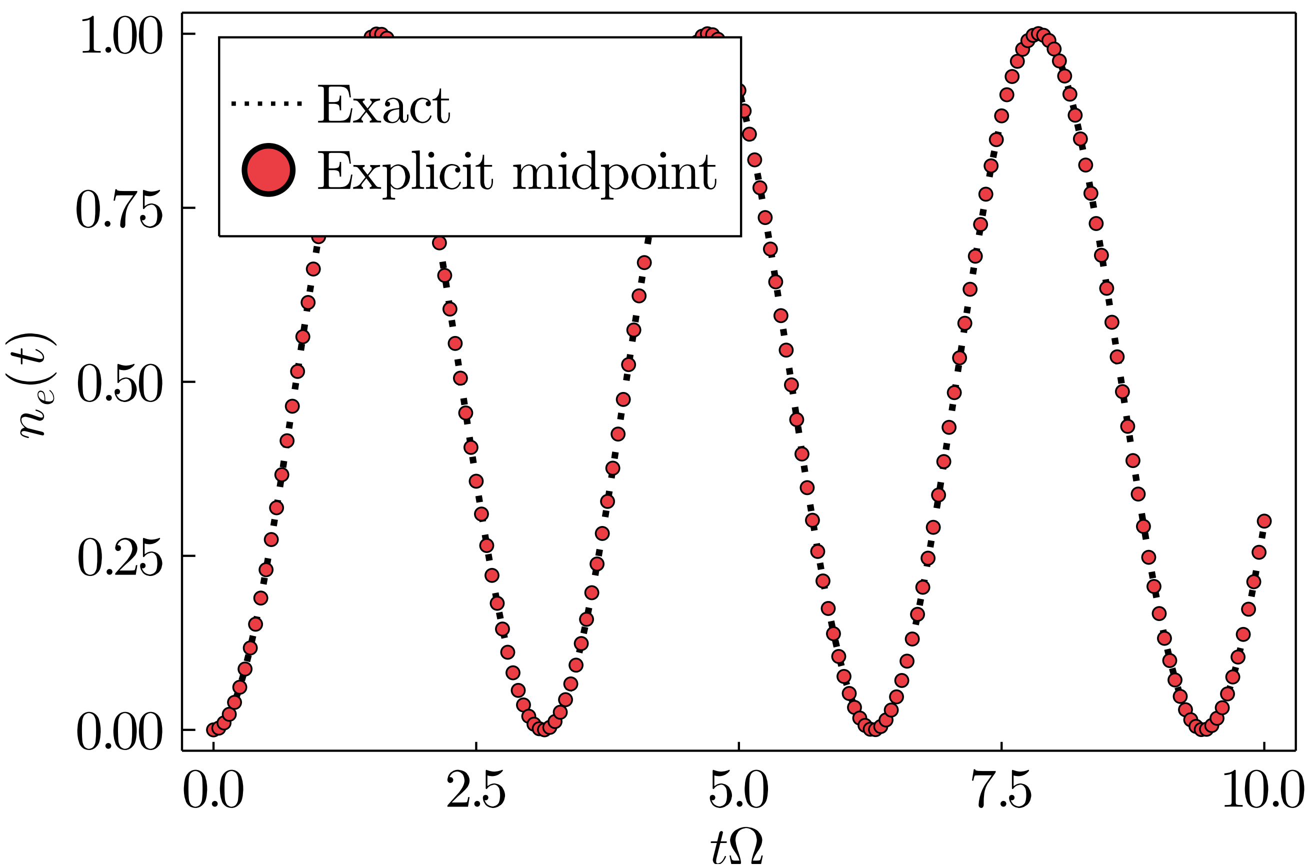
Lecture 3.1 - Runge-Kutta Methods: 2nd order - Midpoint methods

$$\dot{\mathbf{y}}(t) = f(t, \mathbf{y}(t)) \qquad \mathbf{y}(t_n) = \mathbf{y}_n \qquad \textit{Find:} \quad \mathbf{y}_{n+1} \approx \mathbf{y}(t_n + h)$$

- … very simple example (Rabi oscillations)

$$\hat{H} = \begin{pmatrix} 0 & \Omega \\ \Omega & 0 \end{pmatrix} \qquad \frac{d}{dt}|\psi\rangle = -\mathrm{i}\hat{H}|\psi\rangle \qquad |\psi_0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \begin{matrix} |g\rangle \\ |e\rangle \end{matrix}$$

$$n_e(t) = |\langle\psi(t)|e\rangle|^2$$



$$\mathbf{k}_1 = \mathbf{y}_n + \frac{h}{2} f(t_n + \mathbf{y}_n)$$

$$\mathbf{y}_{n+1} \approx \mathbf{y}_n + h f(t_n + \frac{h}{2}, \mathbf{k}_1)$$

"explicit midpoint method"

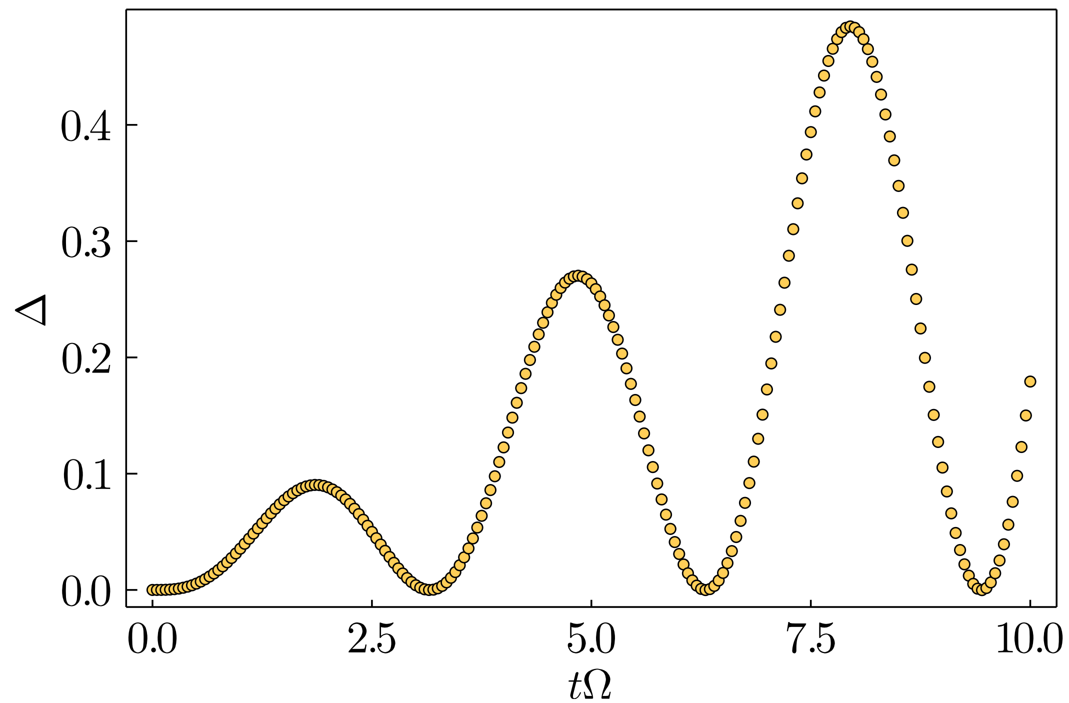
```
function rk2e(H, y, h)
    k1 = y .+ (h/2) .* (-1im .* H * y)
    y += h .* (-1im .* H * k1)
    return y
end
```

Lecture 3.1 - Runge-Kutta Methods: 2nd order

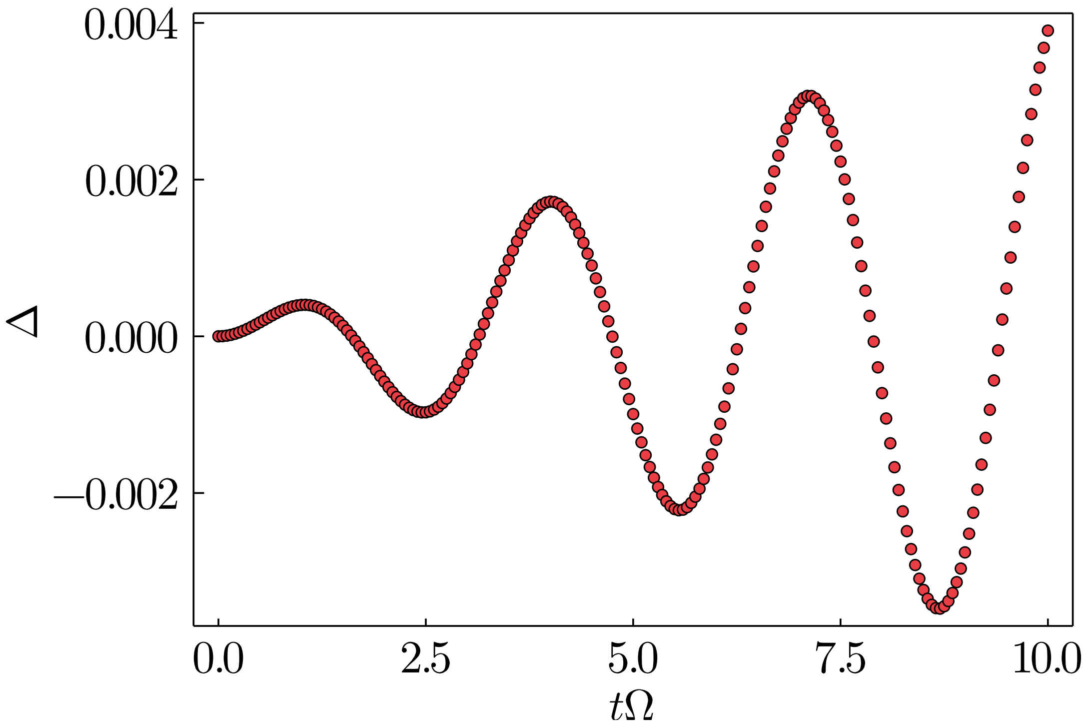
$$\dot{\mathbf{y}}(t) = f(t, \mathbf{y}(t)) \qquad \mathbf{y}(t_n) = \mathbf{y}_n \qquad \textit{Find:} \quad \mathbf{y}_{n+1} \approx \mathbf{y}(t_n + h)$$

- Comparisons $\quad \Delta \equiv n_e(t) - \sin^2(t\Omega)$ $\qquad h\Omega = 0.05$

"explicit Euler"



"explicit midpoint"



Stable!

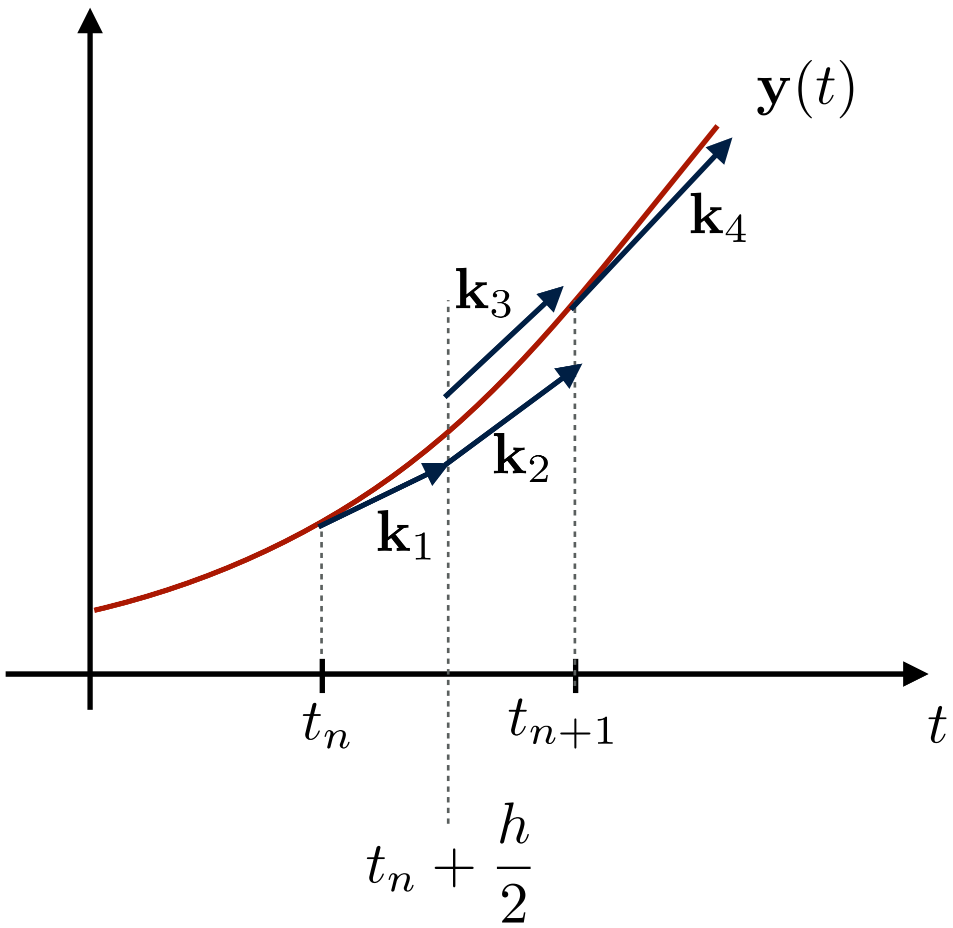
Lecture 3.1 - Runge-Kutta Methods: 4th order

$$\dot{\mathbf{y}}(t) = f(t, \mathbf{y}(t)) \qquad \mathbf{y}(t_n) = \mathbf{y}_n \qquad \textit{Find:} \quad \mathbf{y}_{n+1} \approx \mathbf{y}(t_n + h)$$

- In practice often the most convenient method

$$\mathbf{k}_1 = f(t_n, \mathbf{y}_n)$$
$$\mathbf{k}_2 = f\left(t_n + \frac{h}{2}, \mathbf{y}_n + \frac{h}{2}\mathbf{k}_1\right)$$
$$\mathbf{k}_3 = f\left(t_n + \frac{h}{2}, \mathbf{y}_n + \frac{h}{2}\mathbf{k}_2\right)$$
$$\mathbf{k}_4 = f\left(t_n + h, \mathbf{y}_n + h\mathbf{k}_3\right)$$
$$\mathbf{y}_{n+1} \approx \mathbf{y}_n + \frac{h}{6}(\mathbf{k}_1 + 2\mathbf{k}_2 + 2\mathbf{k}_3 + \mathbf{k}_4)$$

"4th order Runge-Kutta"



- **Remarks:**

  - *Local error* $\epsilon_{n+1} = \mathcal{O}(h^5)$
  - *Note: n-th order = n function evaluations … higher order pays off!*
  - *In practice n=4 is convenient: e.g. 100 steps for plots, typical timescales ~10, time-step ~0.1 ideal*

Lecture 3.1 - Runge-Kutta Methods: 4th order

$$\dot{\mathbf{y}}(t) = f(t, \mathbf{y}(t)) \qquad \mathbf{y}(t_n) = \mathbf{y}_n \qquad \textit{Find:} \quad \mathbf{y}_{n+1} \approx \mathbf{y}(t_n + h)$$

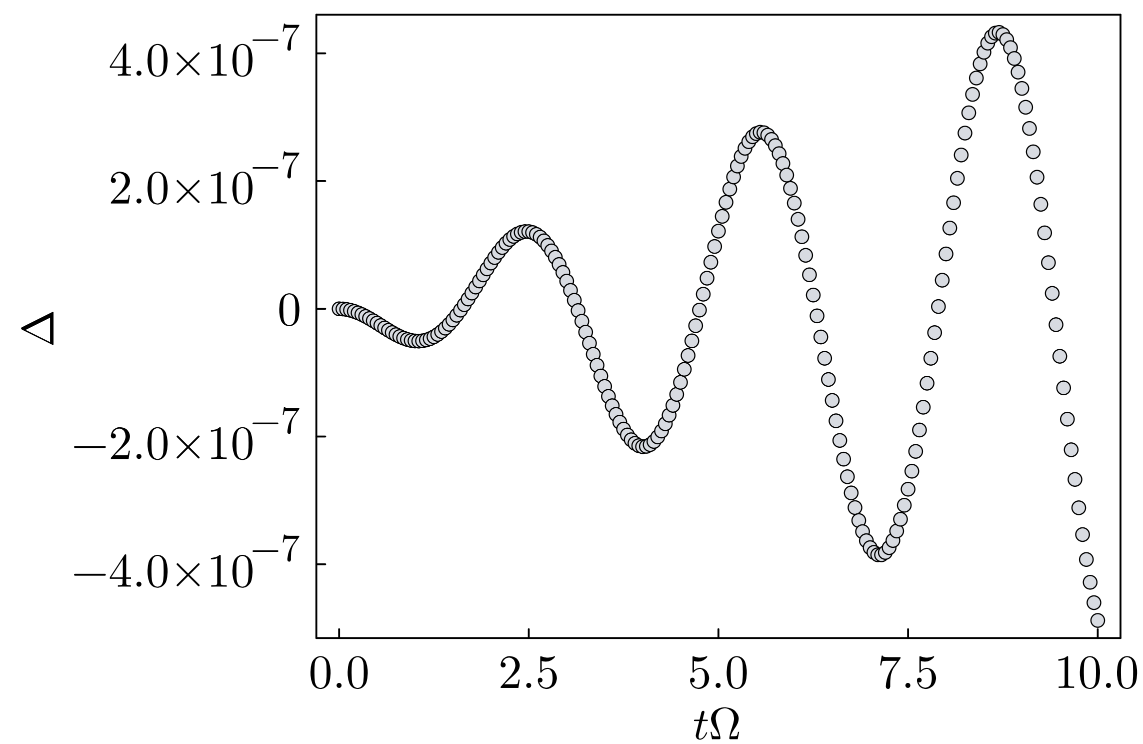
$$\mathbf{k}_1 = f(t_n, \mathbf{y}_n)$$
$$\mathbf{k}_2 = f\left(t_n + \frac{h}{2}, \mathbf{y}_n + \frac{h}{2}\mathbf{k}_1\right)$$
$$\mathbf{k}_3 = f\left(t_n + \frac{h}{2}, \mathbf{y}_n + \frac{h}{2}\mathbf{k}_2\right)$$
$$\mathbf{k}_4 = f\left(t_n + h, \mathbf{y}_n + h\mathbf{k}_3\right)$$
$$\mathbf{y}_{n+1} \approx \mathbf{y}_n + \frac{h}{6}(\mathbf{k}_1 + 2\mathbf{k}_2 + 2\mathbf{k}_3 + \mathbf{k}_4)$$

"4th order Runge-Kutta"

```
function rk4(H, y, h)
    h2 = h/2
    imH = -1im .* H
    k1 = imH * y
    k2 = imH * (y .+ h2 .* k1)
    k3 = imH * (y .+ h2 .* k2)
    k4 = imH * (y .+ h .* k3)
    y += (h/6) .* (k1 .+ 2 .* k2 .+ 2 .* k3 .+ k4)
    return y
end
```

- … very simple example (Rabi oscillations)

$$\Delta \equiv n_e(t) - \sin^2(t\Omega)$$

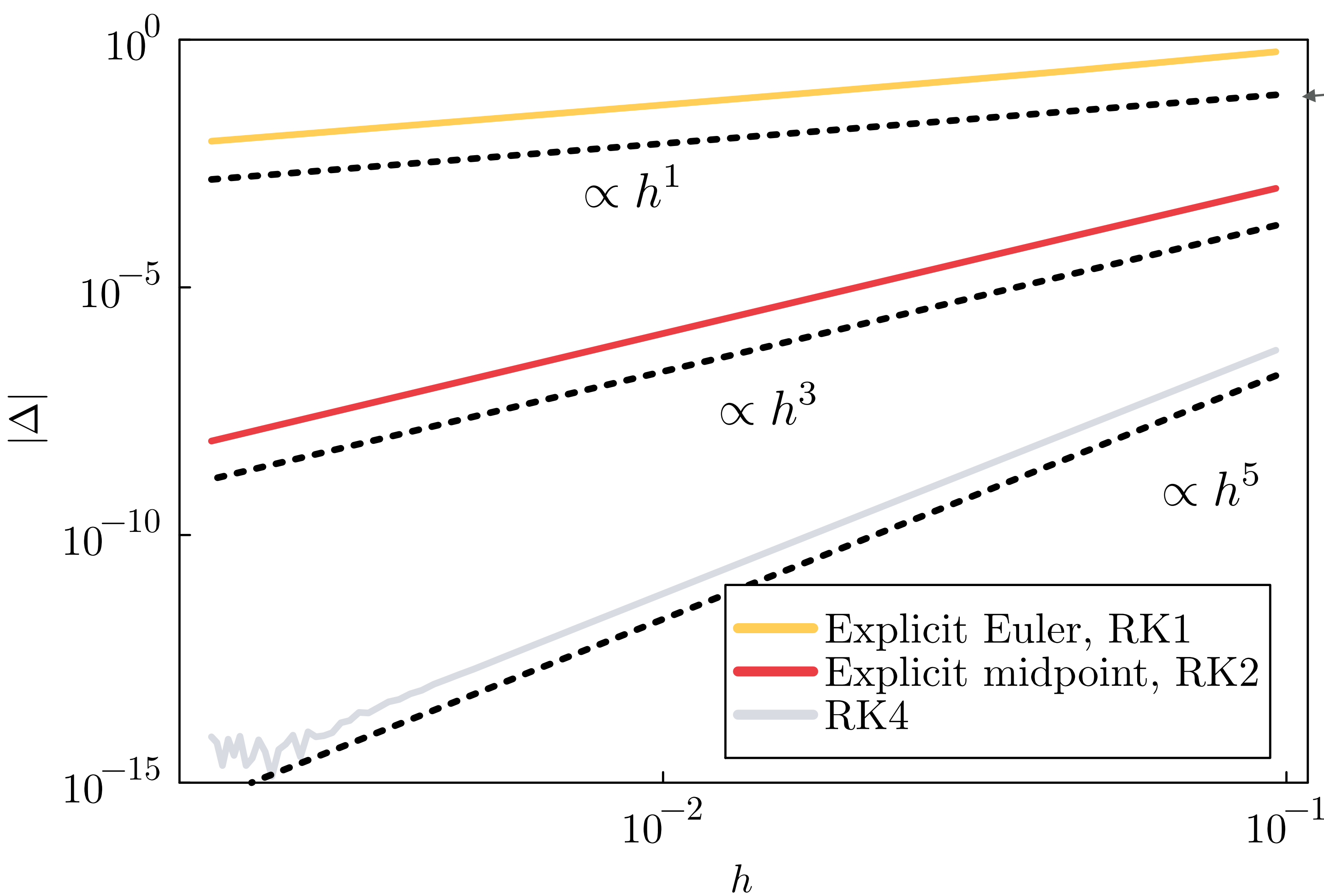


Lecture 3.1 - Runge-Kutta Methods: Sanity checks

- … very simple example (Rabi oscillations) $\hat{H} = \begin{pmatrix} 0 & \Omega \\ \Omega & 0 \end{pmatrix}$ $\frac{d}{dt}|\psi\rangle = -\mathrm{i}\hat{H}|\psi\rangle$ $|\psi_0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \begin{array}{l} |g\rangle \\ |e\rangle \end{array}$

$$\Delta \equiv n_e(t) - \sin^2(t\Omega)$$

- Error at time fixed time, compare methods: $t\Omega = 3\frac{\pi}{2}$ $\sin^2(t\Omega) = 1$



why not? $\propto h^2$

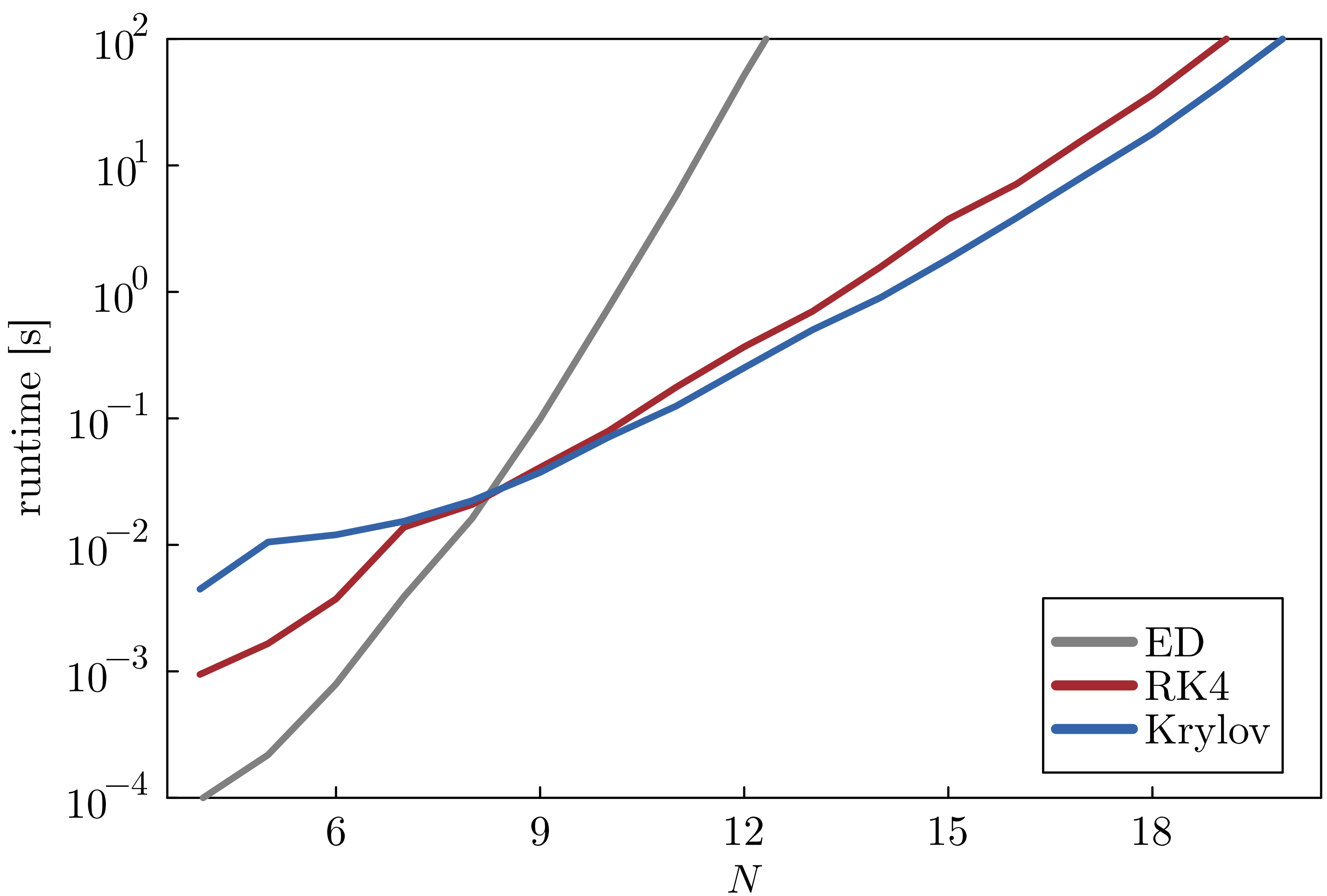
Lecture 3.1 - Comparison: RK4 vs. Krylov

- Evolution of two-spin correlations $\qquad \hat{H}_{\mathrm{TI}} = \sum_{i<j} J_{i,j}\hat{\sigma}_i^z\hat{\sigma}_j^z + h_x \sum_i \hat{\sigma}_i^x \qquad J_{ij} = \frac{J}{|i-j|^\alpha} \qquad \alpha = 1$

- Simulation up to $tJ \leq 5$ *… on Apple M2 Macbook (on battery)* $\qquad |\psi_0\rangle = |\downarrow\uparrow\downarrow\uparrow\downarrow\uparrow\ldots\rangle$

- For fair comparison:

ED	*(no time-step)*	$\left|1 - \| \, |\psi(t)\rangle \, \|\right| < 10^{-14}$
RK4	$\Delta t J = 0.005 \Leftrightarrow$	$\left|1 - \| \, |\psi(t)\rangle \, \|\right| < 10^{-5}$
Krylov	$\Delta t J = 0.1 \Leftrightarrow$	$\left|1 - \| \, |\psi(t)\rangle \, \|\right| < 10^{-13}$



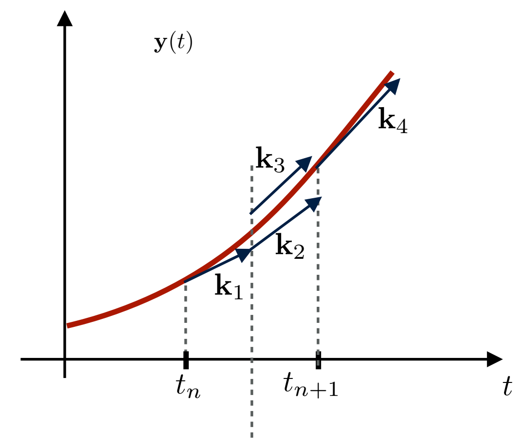
Lecture 3 - Plan for today

Today 50/50: Tutorial style | Theory lecture style

- **Part 3.1:** Introduce Runge-Kutta methods

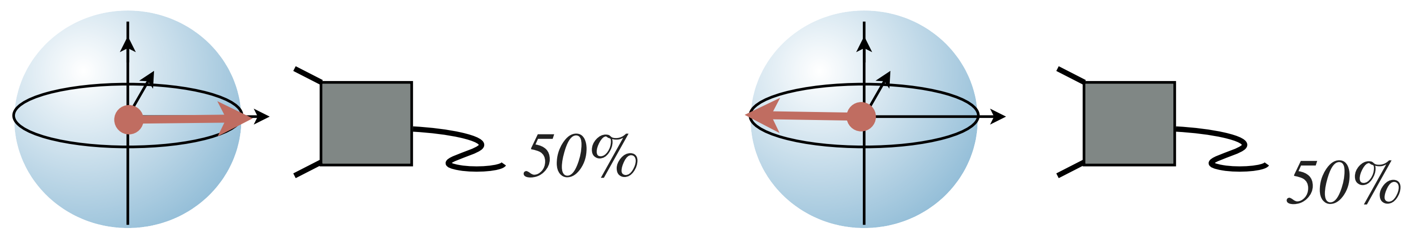
Swiss army knife for solving ODE dynamics

$$\begin{aligned}
\mathbf{k}_1 &= f(t_n, \mathbf{y}_n) \\
\mathbf{k}_2 &= f\left(t_n + \frac{h}{2}, \mathbf{y}_n + \frac{h}{2}\mathbf{k}_1\right) \\
\mathbf{k}_3 &= f\left(t_n + \frac{h}{2}, \mathbf{y}_n + \frac{h}{2}\mathbf{k}_2\right) \\
\mathbf{k}_4 &= f\left(t_n + h, \mathbf{y}_n + h\mathbf{k}_3\right) \\
\mathbf{y}_{n+1} &\approx \mathbf{y}_n + \frac{h}{6}(\mathbf{k}_1 + 2\mathbf{k}_2 + 2\mathbf{k}_3 + \mathbf{k}_4)
\end{aligned}$$



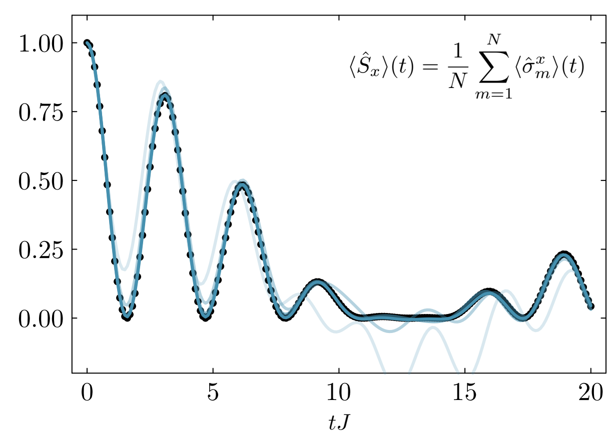
- **Part 3.2:** Back to phase space: The discrete TWA (DTWA) for generic spin-1/2 model dynamics

$$\begin{aligned}
W(+1,+1,-1) &= 1/4 \\
W(-1,+1,-1) &= 1/4 \\
W(+1,-1,-1) &= 1/4 \\
W(-1,-1,-1) &= 1/4
\end{aligned}$$

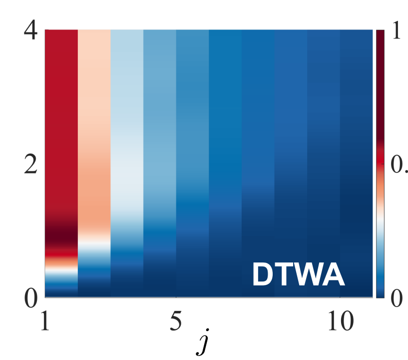


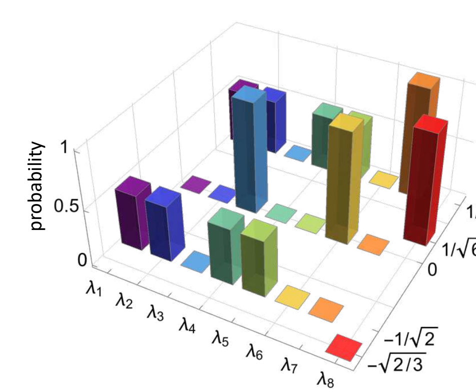
- **Part 3.3:** Set up a DTWA code for Ising model simulations. Understand the approximation better

$$\mathbf{Y} \equiv (\mathbf{Y}_1 \quad \mathbf{Y}_2 \quad \dots \quad \mathbf{Y}_{n_T}) = \begin{pmatrix} x_{1,1} & x_{1,2} & & x_{1,n_T} \\ \vdots & \vdots & & \\ x_{N,1} & x_{N,2} & & x_{N,n_T} \\ y_{1,1} & y_{1,2} & & y_{1,n_T} \\ \vdots & \vdots & \dots & \\ y_{N,1} & y_{N,2} & & y_{N,n_T} \\ z_{1,1} & z_{1,2} & & z_{1,n_T} \\ \vdots & \vdots & & \\ z_{N,1} & z_{N,2} & & z_{N,n_T} \end{pmatrix}$$



- **Part 3.4:** Generalizations to spin > 1/2 models and use case examples





Back to phase space: Lecture 2 - Recap

- We introduced the phase space description of quantum mechanics.

Bopp representation

$$\hat{x} \to x + \frac{\mathrm{i}}{2}\frac{\partial}{\partial p}$$
$$\hat{p} \to p - \frac{\mathrm{i}}{2}\frac{\partial}{\partial x}$$

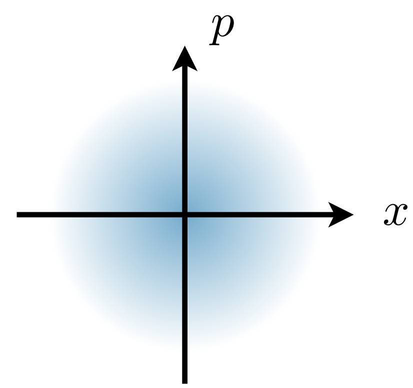
Hilbert space $\Leftrightarrow$ **Phase space**

$$\hat{O} = \int dx dp\, O_W(x,p)\hat{A}(x,p)$$

$$O_W(x,p) = \frac{1}{\mathcal{N}}\,\mathrm{tr}\left[\hat{A}(x,p)\hat{O}\right]$$

- Instead of using matrices on Hilbert space, QM can described by functions of phase space variable (Weyl symbols)
- The transformation can be described by phase-point operators that are **normalized** and **orthogonal**
- The Weyl symbol of the density matrix is the **Wigner function**

A quasi-probability distribution to describe any quantum state. It can have negative values!



$$W(x,p) = \frac{1}{\pi}\mathrm{e}^{-x^2/a^2 - a^2p^2}$$

- Useful alternative picture to look at quantum states!
- Dynamics of Weyl symbols is described by Moyal brackets

  (equivalent to a commutator on phase space)

$$\frac{d}{dt}O_W = \{O_W, H_W\}_{\mathrm{MB}}$$

$$\{O_W, O'_W\}_{\mathrm{MB}} \equiv \frac{2}{\hbar}O_W \sin\left[\frac{\hbar}{2}\boldsymbol{\Lambda}\right] O'_W$$

- Expansion of the Moyal bracket for $\frac{\hbar}{2} \to 0$

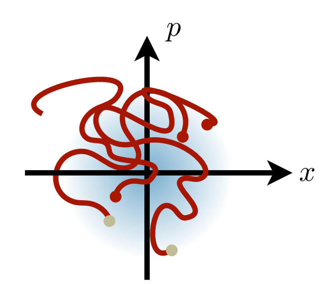
  … leads to the truncated Wigner approximation (**TWA**)

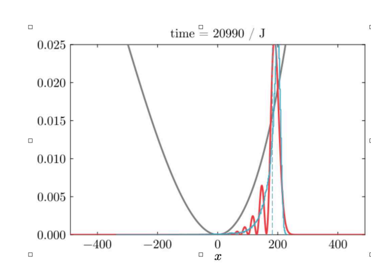
$$\frac{d}{dt}O_W \approx \{O_W, H_W\} - \frac{\hbar^2}{24}\{O_W, H_W\}^3 + \mathcal{O}\left(\frac{\hbar^4}{4!2^4}\right)$$

- TWA implies classical equations for the Weyl symbols, which means that Weyl symbols remain factorized ad all times

$$(\hat{O}_{x^n p^m})_W(t) = (\hat{x})^n_W(t)(\hat{p})^m_W(t)$$

- The TWA is useful for simulating dynamics beyond classical (beyond mean-field): Sample trajectories from (positive) Wigner functions and simulate each trajectory classically. This is exact as long as only quadratic terms are in the Hamiltonian. We tested the concept with anharmonic oscillator evolution.





Extras: Questions from last time

Hilbert space $\Leftrightarrow$ **Phase space**

$$\hat{O} = \int dxdp\, O_W(x,p)\hat{A}(x,p) \qquad O_W(x,p) = \frac{1}{\mathcal{N}}\,\mathrm{tr}\left[\hat{A}(x,p)\hat{O}\right]$$

$$O_W(x,p) = \frac{1}{\mathcal{N}}\mathrm{tr}[\hat{A}(x,p)\hat{O}] = \frac{1}{2\pi}\int dy\, \mathrm{e}^{\mathrm{i}py}\mathrm{tr}(|x+\frac{y}{2}\rangle\langle x-\frac{y}{2}|\,\hat{O}) = \frac{1}{2\pi}\int dy\, \mathrm{e}^{\mathrm{i}py}\langle x-\frac{y}{2}|\,\hat{O}\,|x+\frac{y}{2}\rangle$$

- Not any phase space function describes a quantum state. Therefore it does not guarantee a positive semi-definite density matrix when transforming an arbitrary normalized phase space function.
  The important fact is just that the transformation is unique.

- Counter example:

$$W(x,p) = \delta(x)\delta(p)$$

indeed: $\hat{\rho} = \hat{A}(0,0) = \int dy\, |\frac{y}{2}\rangle\langle -\frac{y}{2}|$

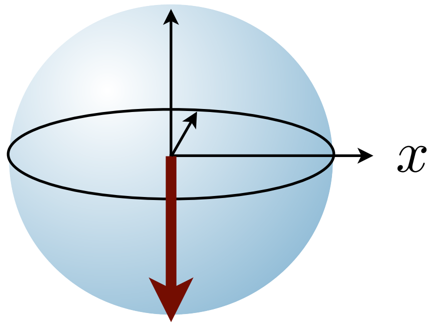
unphysical: violating uncertainty principle

- Phase point operators should be hermitian (since we need Weyl symbols of hermitian operators to be real):

$$O_W(x,p) = \frac{1}{\mathcal{N}}\,\mathrm{tr}\left[\hat{A}(x,p)\hat{O}\right] = O_W(x,p)^* = \frac{1}{\mathcal{N}}\,\mathrm{tr}\left[\hat{A}^\dagger(x,p)\hat{O}\right] \qquad \hat{A}^\dagger(x,p) = \hat{A}(x,p)$$

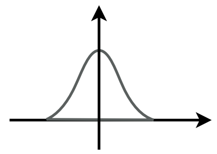
Lecture 3.2 - Phase space for spin-models?

- A single spin-1/2: $\hat{\rho} = (\mathbb{1} + \vec{r}\cdot\vec{\sigma})/2 \qquad \vec{r} = (x, y, z)$



Hilbert space

- We want to use the phase space variables *x, y, z*, **What is the Wigner function?**



- **Idea I:** Re-use results for a two 1D harmonic oscillator *(sketch) … for details see:*

A. Polkovnikov, Ann. Phys., 325, 1790 (2010)

One can also use the complex coherent state phase space: $\hat{x} = \frac{1}{\sqrt{2}}(\hat{a}^\dagger + \hat{a}) \quad \hat{p} = \frac{1}{\sqrt{2}}(\hat{a}^\dagger - \hat{a})$

$\hat{a} \leftrightarrow \alpha \qquad \hat{a}^\dagger \leftrightarrow \alpha^*$

Then use: **Schwinger Bosons**

$$\hat{S}^z = \frac{1}{2}\left(\hat{a}^\dagger\hat{a} - \hat{b}^\dagger\hat{b}\right) \quad \hat{S}^+ = \hat{a}^\dagger\hat{b} \quad \hat{S}^- = \hat{b}^\dagger\hat{a} \qquad \hat{a}^\dagger\hat{a} + \hat{b}^\dagger\hat{b} = 2S$$

$$\hat{S}^x = \frac{1}{2}\left(\hat{S}^+ + \hat{S}^-\right) \quad \hat{S}^y = \frac{1}{2\mathrm{i}}\left(\hat{S}^+ - \hat{S}^-\right)$$

Then, for the spin coherent state $|S_z = -S\rangle$ *… one finds*

$$W(s_x, s_y, s_z) \approx \frac{1}{\pi S}\mathrm{e}^{-(s_x^2+s_y^2)/S}\delta(z-S)$$

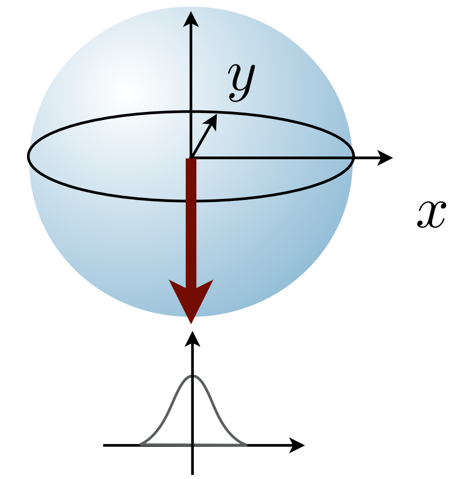
This follows from $|S_z = -S\rangle \leftrightarrow |n_a = 0\rangle$ *(Harmonic oscillator GS)*

$$s_x = \frac{1}{2}(\alpha^*\beta + \beta^*\alpha) \qquad s_y = \frac{1}{2\mathrm{i}}(\alpha^*\beta - \beta^*\alpha)$$

$$|\alpha|^2|\beta|^2 = s_x^2 + s_y^2 \qquad |\beta|^2 \approx 2S$$

$$W(\alpha, \alpha^*) \propto \mathrm{e}^{-2|\alpha|^2} \propto \mathrm{e}^{-(s_x^2+s_y^2)/S}$$

Lecture 3.2 - Phase space for spin-models? … a continuous approach



- Continuous Wigner function for spin-S $$W(s_x, s_y, s_z) \approx \frac{1}{\pi S} \mathrm{e}^{-(s_x^2+s_y^2)/S} \delta(z-S)$$

Normal distribution with width $\propto \sqrt{S/2}$

- Problem: **Very bad for small S and thus for spin-1/2** $\hat{s}_{x,y,z} = \frac{1}{2}\hat{\sigma}_{x,y,z} \qquad \hat{\sigma}^2_{x,y,z} = \mathbb{1}$

Moments for distribution along x

Hilbert space	$\langle \hat{s}_x^1 \rangle = 0$	$\langle \hat{s}_x^2 \rangle = \frac{1}{4}$	$\langle \hat{s}_x^3 \rangle = 0$	$\langle \hat{s}_x^3 \rangle = \frac{1}{16}$	
Phase space	$\overline{s_x^1} = 0$	$\overline{s_x^2} = \frac{1}{4}$	$\overline{s_x^3} = 0$	$\overline{s_x^4} = \frac{3}{16}$	$\cdots$

$$\overline{s_x^n} = \sqrt{\frac{2}{\pi}} \int ds_x\, s_x^n \mathrm{e}^{-2s_x^2} = \frac{1}{2^n} n!! = \frac{1}{2^n} n(n-2)(n-4)\ldots$$

- One may argue that the higher order moments are anyway neglected if we use the TWA, but still this phase space representation is fundamentally flawed, since we don't fulfill our condition for observables

$$\langle \hat{O}_{s_x^n s_y^m s_z^k} \rangle \neq \int ds_x\, ds_y\, ds_y\, W(s_x, s_y, s_z) s_x^n s_y^m s_z^k$$

- Moments for Pauli matrices $\langle (\hat{\sigma}^x)^n \rangle = \begin{cases} 0 & n \,\text{even} \\ 1 & n \,\text{odd} \end{cases}$

… one can show that no continuous distribution exists with such moments!

- **Idea**: Switch to **discrete distributions!**

Lecture 3.2 - Phase space for spin-models? … Wootters' discrete phase space

W. K. Wootters, Annals of Physics 176, 1 (1987)

- A discrete phase space construction — Definition of **discrete phase-point operators:**

$$\hat{A}_\alpha = \hat{A}(x_\alpha, y_\alpha, z_\alpha) = \frac{1}{2}(\mathbb{1} + \mathbf{r}_\alpha \cdot \boldsymbol{\sigma}) = \frac{1}{2}(\mathbb{1} + x_\alpha \hat{\sigma}_x + y_\alpha \hat{\sigma}_y + z_\alpha \hat{\sigma}_z)$$

… and restrict $\quad \begin{array}{l} x_\alpha \in \{-1, 1\} \\ y_\alpha \in \{-1, 1\} \\ z_\alpha \in \{-1, 1\} \end{array}$ $\quad$ ***8 possible combinations***

- **Normalization property:** $\quad \mathrm{tr}[\hat{A}_\alpha(x, y, z)] = 1$ ✔

- **Orthogonality:** $\quad \mathrm{tr}[\hat{A}_\alpha \hat{A}_{\alpha'}] = \frac{1}{4}\mathrm{tr}\left[\mathbb{1} + xx'\mathbb{1} + yy'\mathbb{1} + zz'\mathbb{1}\right] = \frac{1}{2}\left[1 + xx' + yy' + zz'\right]$

In the case $\quad \alpha = \alpha' \quad \mathrm{tr}[\hat{A}_\alpha \hat{A}_{\alpha'}] = 2$

In the case $\quad xx' + yy' + zz' = -1 \quad \mathrm{tr}[\hat{A}_\alpha \hat{A}_{\alpha'}] = 0$

Proper phase space transformation!

$$O_W(\alpha) = \frac{1}{\mathcal{N}} \mathrm{tr}\left[\hat{A}_\alpha \hat{O}\right] \qquad \mathcal{N} = 2$$

- This implies, that for a good discrete phase space we need to select **4 different** discrete values

… two equivalent choices

$$\begin{aligned} r_1 &= (+1, +1, +1) \\ r_2 &= (+1, -1, -1) \\ r_3 &= (-1, +1, -1) \\ r_4 &= (-1, -1, +1) \end{aligned}$$

or

$$\begin{aligned} r_1 &= (-1, -1, -1) \\ r_2 &= (-1, +1, +1) \\ r_3 &= (+1, -1, +1) \\ r_4 &= (+1, +1, -1) \end{aligned}$$

✔

Lecture 3.2 - Phase space for spin-models? … Wootters' discrete phase space

W. K. Wootters, Annals of Physics 176, 1 (1987)

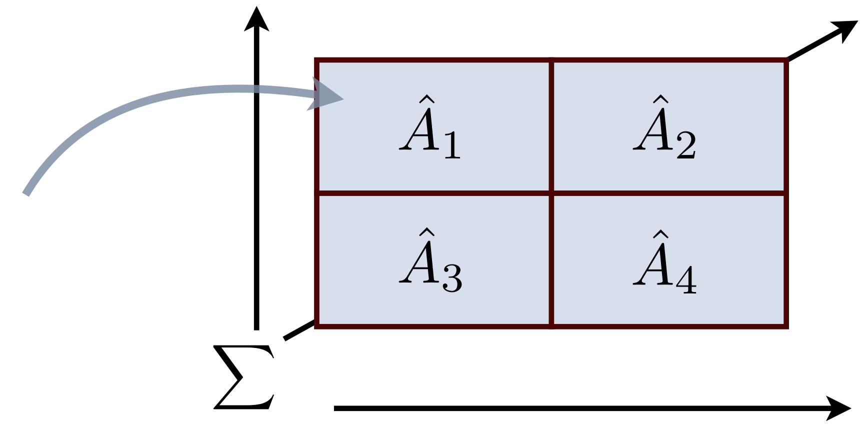
- Also the projection property can be translated to the discrete phase space:

$$\hat{A}_\alpha = \frac{1}{2}(\mathbb{1} + x_\alpha \hat{\sigma}_x + y_\alpha \hat{\sigma}_y + z_\alpha \hat{\sigma}_z)$$

$$r_1 = (+1, +1, +1)$$
$$r_2 = (+1, -1, -1)$$
$$r_3 = (-1, +1, -1)$$
$$r_4 = (-1, -1, +1)$$

map to matrix:

$$\alpha = 1 \leftrightarrow (1,1)$$
$$\alpha = 2 \leftrightarrow (1,2)$$
$$\alpha = 3 \leftrightarrow (2,1)$$
$$\alpha = 4 \leftrightarrow (2,2)$$



… then, e.g. summation along horizontal/ vertical/diagonal lines:

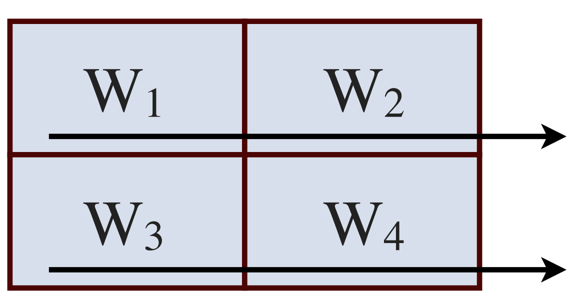
Horizontal	*Vertical*	*Diagonal*
$\hat{A}_1 + \hat{A}_2 = \mathbb{1} + \hat{\sigma}^x$	$\hat{A}_3 + \hat{A}_1 = \mathbb{1} + \hat{\sigma}^y$	$\hat{A}_1 + \hat{A}_4 = \mathbb{1} + \hat{\sigma}^z$
$\hat{A}_3 + \hat{A}_4 = \mathbb{1} - \hat{\sigma}^x$	$\hat{A}_4 + \hat{A}_2 = \mathbb{1} - \hat{\sigma}^y$	$\hat{A}_3 + \hat{A}_2 = \mathbb{1} - \hat{\sigma}^z$

$$\mathbb{1} \pm \hat{\sigma}^{x,y,z}$$

*are the **projectors** on the two eigenstates of $\hat{\sigma}^{x,y,z}$ with eigenvalues ± 1!*

- This implies that Wigner function sums correspond to positive probabilities for the outcomes of measuring x, y, and z

$$W(\alpha) = \frac{1}{2}\mathrm{tr}\left[\hat{A}_\alpha \hat{\rho}\right]$$



$$W_1 + W_2 = p(x = +1)$$
$$W_3 + W_4 = p(x = -1)$$

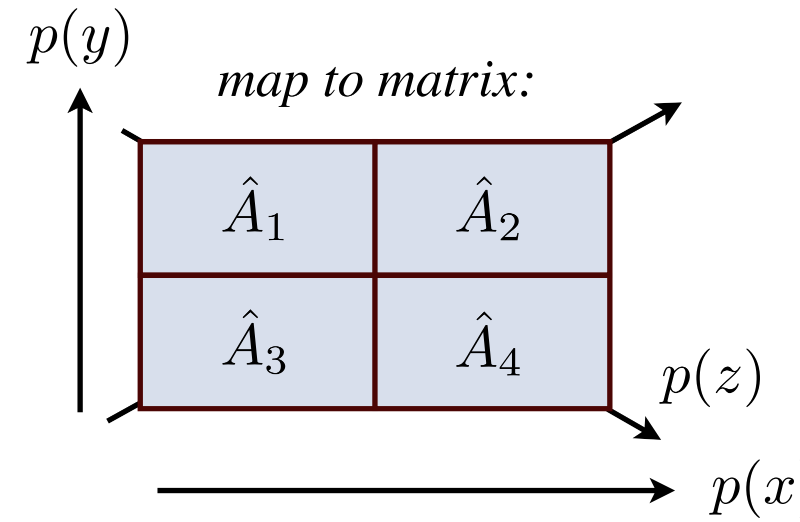
…. for details, see Annals of Physics 176, 1 (1987)

Lecture 3.2 - Phase space for spin-models? … Wootters' discrete phase space

W. K. Wootters, Annals of Physics 176, 1 (1987)

$$\hat{A}_\alpha = \frac{1}{2}(\mathbb{1} + x_\alpha \hat{\sigma}_x + y_\alpha \hat{\sigma}_y + z_\alpha \hat{\sigma}_z)$$

$$r_1 = (+1, +1, +1)$$
$$r_2 = (+1, -1, -1)$$
$$r_3 = (-1, +1, -1)$$
$$r_4 = (-1, -1, +1)$$



- Example Wigner functions *(exercise)*

$|\downarrow\rangle \quad \hat{\sigma}^z |\downarrow\rangle = -1 |\downarrow\rangle$

$$W = \begin{array}{|c|c|}\hline 0 & 0.5 \\ \hline 0.5 & 0 \\ \hline\end{array}$$

$|+\rangle = (|\downarrow\rangle + |\uparrow\rangle)/\sqrt{2}$

$$W = \begin{array}{|c|c|}\hline 0.5 & 0.5 \\ \hline 0 & 0 \\ \hline\end{array}$$

$|\psi\rangle = \frac{\sqrt{3}}{2} |\downarrow\rangle + \frac{1}{2} |\uparrow\rangle$

$$W \approx \begin{array}{|c|c|}\hline 0.6 & 0.3 \\ \hline -0.1 & 0.2 \\ \hline\end{array}$$

$\hat{\rho} = \mathbb{1}/2$

$$W = \begin{array}{|c|c|}\hline 0.25 & 0.25 \\ \hline 0.25 & 0.25 \\ \hline\end{array}$$

- **Remark:** Negative values are again possible, only the marginal distributions are positive, all elements always sum up to one.
- **Remark:** Interesting aspect when sampling from this Wigner function. E.g. in the case of the spin-down state, when picking one of the two phase points, the *x* and the *y* components are anti-correlated. It is like there is a hidden variable. Furthermore this depends on the choice of phase point operators. When choosing the other set, the *x* and *y* coordinates become correlated.
- **Remark:** The natural phase space variables correspond here to the indices on the axis! In the following we will be still interested in a phase space where the phase space variables correspond to *x*, *y*, and *z*, which is slightly different.

Lecture 3.2 - The discrete TWA (DTWA) - sampling

JS, A. Pikovski, and Ana Maria Rey, Phys. Rev. X 5, 011022 (2015)

- We want to perform simulations on the basis of the phase space variables = Weyl symbols

$$(\hat{\sigma}_x)_W = x \qquad (\hat{\sigma}_y)_W = y \qquad (\hat{\sigma}_z)_W = z$$

- We will actually not define the Wigner-Weyl transformation, it is actually *not* identical to the one defined by Wootters

For more recent discussions see:
B. Zhu, A. M. Rey, and JS, New J. Phys. 21, 082001 (2019)
D. Mink, D. Petrosyan, and M. Fleischhauer, Phys. Rev. Research 4, 043136 (2022)

- **Starting point:** Definition of a good phase space = We have a probability distribution exactly reproducing all observables that are constructible from the phase space variables:

$$\langle \hat{O}_{x^n y^m z^l} \rangle = \sum_{x,y,z=\pm 1} W(x,y,z) x^n y^m z^l$$

(symmetrized)

- **Specify probability distribution for** $|\downarrow\rangle$ *(all other initial pure states can be derived from a basis rotation)*

- This state is perfectly described by:

$$W(+1,+1,-1) = 1/4$$
$$W(-1,+1,-1) = 1/4$$
$$W(+1,-1,-1) = 1/4$$
$$W(-1,-1,-1) = 1/4$$

$$W = 0$$

…for other configurations

Lecture 3.2 - The discrete TWA (DTWA) - sampling

- **Specify probability distribution for** $|\downarrow\rangle$

$$\langle \hat{O}_{x^n y^m z^l}\rangle = \sum_{x,y,z=\pm 1} W(x,y,z)x^n y^m z^l$$

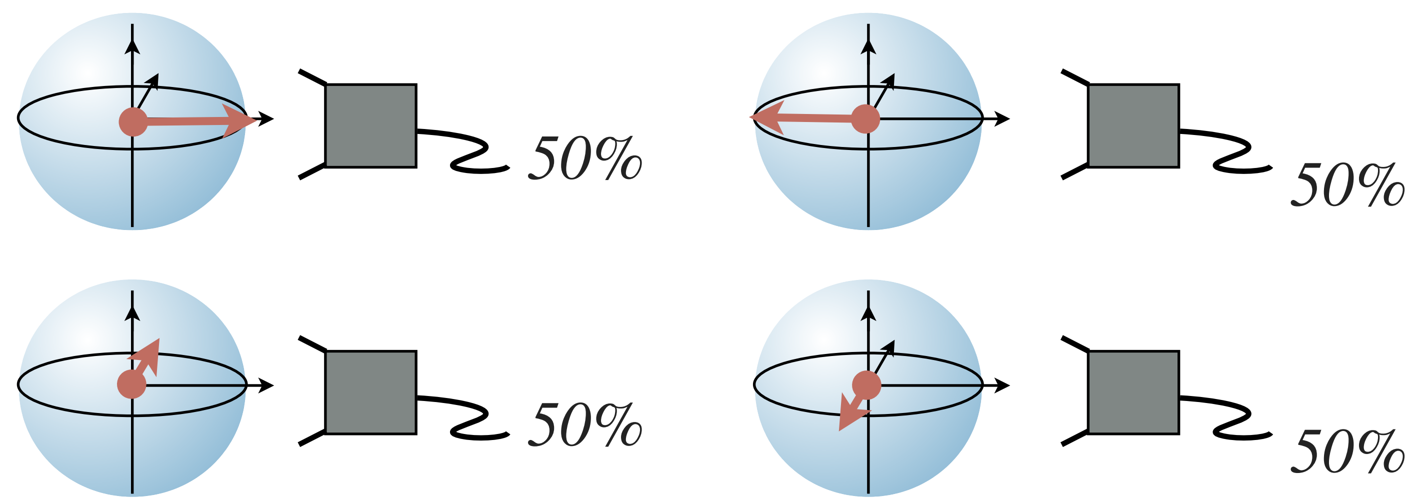
$$W(+1,+1,-1) = 1/4$$
$$W(-1,+1,-1) = 1/4$$
$$W(+1,-1,-1) = 1/4$$
$$W(-1,-1,-1) = 1/4$$

Intuitively clear from the measurement statistics $z = -1$

$$W(+1,+1,-1) = 1/4$$

… then measure x component:

… or measure y component:



- Checks: $\langle \hat{O}_z\rangle = \langle \hat{\sigma}_z\rangle = \sum_{x,y,z=\pm 1} W(x,y,z)z = 4(1/4)(-1) = -1$ ✓

$$\langle \hat{O}_x\rangle = \langle \hat{\sigma}_x\rangle = 2(1/4)(-1) + 2(1/4)(+1) = 0$$ ✓

$$\langle \hat{O}_{x^m}\rangle = (1/2)(+1)^m + (1/2)(-1)^m = m \mod 2$$ ✓ *(all moments correct!)*

$$\langle \hat{O}_{xy}\rangle = (1/4)(1) + (1/4)(-1) + (1/4)(-1) + (1/4)(+1) = 0$$ ✓ $\hat{O}_{xy} = 0$

- General proof can be made for arbitrary discrete spaces *B. Zhu, A. M. Rey, and JS, New J. Phys. 21, 082001 (2019)*

Lecture 3.2 - The discrete TWA (DTWA)

- Equivalently, for a system of *N* spins and any **product state** perfectly described by a Wigner function $W_i(x_i, y_i, z_i)$

$$\langle \hat{O}_{\prod_i x_i^n y_i^m z_i^l} \rangle = \prod_i \langle \hat{O}_{x_i^n y_i^m z_i^l} \rangle = \prod_{i=1}^{N} \sum_{x_i, y_i, z_i = \pm 1} W_i(x_i, y_i, z_j) x_i^n y_i^m z_i^l$$

… perfectly describes all possible observables

- Simple example for *N=2*:

$$|\psi\rangle = |\downarrow\rangle \otimes |\leftarrow\rangle \qquad |\leftarrow\rangle = \frac{1}{\sqrt{2}}(|\downarrow\rangle - |\uparrow\rangle)$$

$$\hat{O}_{z_1 x_2^3} = \hat{\sigma}_z \otimes \hat{\sigma}_x^3 = \hat{\sigma}_z \otimes \hat{\sigma}_x \qquad \langle \hat{O}_{x_1 z_1} \rangle = +1$$

$$W_1(+1,+1,-1) = 1/4$$
$$W_1(-1,+1,-1) = 1/4$$
$$W_1(+1,-1,-1) = 1/4$$
$$W_1(-1,-1,-1) = 1/4$$

$$W_2(-1,+1,+1) = 1/4$$
$$W_2(-1,-1,+1) = 1/4$$
$$W_2(-1,+1,-1) = 1/4$$
$$W_2(-1,-1,-1) = 1/4$$

$$\left(\sum_{x_1, y_1, z_1 = \pm 1} W_1(x_1, y_1, z_1) z_1 \right) \left(\sum_{x_2, y_2, z_2 = \pm 1} W_2(x_2, y_2, z_2) x_2^3 \right)$$
$$= \frac{1}{4}(-1-1-1-1)\frac{1}{4}(-1-1-1-1)) = +1$$

✔

- General proof can be made for arbitrary discrete spaces *B. Zhu, A. M. Rey, and JS, New J. Phys. 21, 082001 (2019)*

Lecture 3.2 - The discrete TWA (DTWA) - Equations of motion

- We now use the fact that the TWA approximation is equivalent to the fact that all Weyl symbols remain factorized.

$$\left(\hat{O}_{\prod_i x_i^n y_i^m z_i^l}\right)_W (t) \approx \prod_i x_i(t)^n y_i(t)^m z_i(t)^l$$

- We can now derive the DTWA equations of motion from **Heisenberg equations of motion** on phase space, enforcing **factorization**
- Let's specify a two-body spin-model Hamiltonian

$$\hat{H} = \hat{H}_1 + \hat{H}_2 = \sum_i \mathbf{b}_i \cdot \boldsymbol{\sigma}_i + \frac{1}{2}\sum_{ij}\left(V_{ij}^{xx}\hat{\sigma}_i^x\hat{\sigma}_j^x + V_{ij}^{yy}\hat{\sigma}_i^y\hat{\sigma}_j^y + V_{ij}^{zz}\hat{\sigma}_i^z\hat{\sigma}_j^z\right)$$

$$\mathbf{b}_i \cdot \boldsymbol{\sigma}_i = b_i^x\hat{\sigma}_i^x + b_i^y\hat{\sigma}_i^y + b_i^z\hat{\sigma}_i^z \qquad V_{ii}^{\alpha\alpha} = 0 \quad V_{ij}^{\alpha\alpha} = V_{ji}^{\alpha\alpha}$$

- Single-body terms:

using: $(x,y,z) = (1,2,3)$

$$\frac{d}{dt}\hat{\sigma}_m^x = \mathrm{i}\left[\hat{H}_1, \hat{\sigma}_m^x\right] = \mathrm{i}b_m^y\left[\hat{\sigma}_m^y, \hat{\sigma}_m^x\right] + \mathrm{i}b_m^z\left[\hat{\sigma}_m^z, \hat{\sigma}_m^x\right] = 2b_m^y\hat{\sigma}_m^z - 2b_m^z\hat{\sigma}_m^y \qquad \left[\hat{\sigma}^\alpha, \hat{\sigma}^\beta\right] = 2\mathrm{i}\sum_\gamma \epsilon_{\alpha\beta\gamma}\hat{\sigma}^\gamma$$

- On phase space: **No factorization necessary — DTWA exact**

Levi-Civita tensor

$$\epsilon_{123} = \epsilon_{312} = \epsilon_{231} = 1$$
$$\epsilon_{321} = \epsilon_{132} = \epsilon_{213} = -1$$

0 otherwise

$$\left(\frac{d}{dt}\hat{\sigma}_m^x\right)_W = \frac{d}{dt}x_m = 2b_m^y(\hat{\sigma}_m^z)_W - 2b_m^z(\hat{\sigma}_m^y)_W = 2b_m^y z_m - 2b_m^z y_m$$

Lecture 3.2 - The discrete TWA (DTWA) - Equations of motion

$$\hat{H} = \hat{H}_1 + \hat{H}_2 = \sum_i \mathbf{b}_i \cdot \boldsymbol{\sigma}_i + \frac{1}{2}\sum_{ij}\left(V_{ij}^{xx}\hat{\sigma}_i^x\hat{\sigma}_j^x + V_{ij}^{yy}\hat{\sigma}_i^y\hat{\sigma}_j^y + V_{ij}^{zz}\hat{\sigma}_i^z\hat{\sigma}_j^z\right)$$

$$\mathbf{b}_i \cdot \boldsymbol{\sigma}_i = b_i^x\hat{\sigma}_i^x + b_i^y\hat{\sigma}_i^y + b_i^z\hat{\sigma}_i^z$$

$$V_{ii}^{\alpha\alpha} = 0 \qquad V_{ij}^{\alpha\alpha} = V_{ji}^{\alpha\alpha}$$

- Single-body terms: $\dfrac{d}{dt}\hat{\sigma}_m^x = \mathrm{i}\left[\hat{H}_1, \hat{\sigma}_m^x\right] = \mathrm{i}\left[\hat{\sigma}_m^y, \hat{\sigma}_m^x\right] + \left[\hat{\sigma}_m^z, \hat{\sigma}_m^x\right] = 2b_m^y\hat{\sigma}_m^z - 2b_m^z\hat{\sigma}_m^y$

$$\frac{d}{dt}x_m = 2b_m^y z_m - 2b_m^z y_m$$

- **Remark:** These are indeed identical to fully classical spin equations (alternative derivation)

Poisson bracket for spin-dynamics

$$\dot{\alpha}_m = \{\alpha_m, H_C\} = 2\sum_\beta \epsilon_{\alpha\beta\gamma}\gamma_m\frac{\partial H_C}{\partial\beta_m} \qquad H_C(x_m, y_m, z_m) = b_m^x x_m + b_m^y y_m + b_m^z z_m$$

$$\dot{x}_m = \{x_m, H_C\} = 2\epsilon_{xyz}z_m\frac{\partial H_C}{\partial y_m} + 2\epsilon_{xzy}y_m\frac{\partial H_C}{\partial z_m} = 2z_m b_m^y - 2y_m b_m^z \checkmark$$

- **Other equations:**

$$\frac{d}{dt}y_m = -2b_m^x z_m + 2b_m^z x_m$$

$$\frac{d}{dt}z_m = 2b_m^x y_m - 2b_m^y x_m$$

(exercise)

$(x, y, z) = (1, 2, 3)$

Levi-Civita tensor

$\epsilon_{123} = \epsilon_{312} = \epsilon_{231} = 1$

$\epsilon_{321} = \epsilon_{132} = \epsilon_{213} = -1$

0 otherwise

Lecture 3.2 - The discrete TWA (DTWA) - Equations of motion

$$\hat{H} = \hat{H}_1 + \hat{H}_2 = \sum_i \mathbf{b}_i \cdot \boldsymbol{\sigma}_i + \frac{1}{2}\sum_{ij}\left(V_{ij}^{xx}\hat{\sigma}_i^x\hat{\sigma}_j^x + V_{ij}^{yy}\hat{\sigma}_i^y\hat{\sigma}_j^y + V_{ij}^{zz}\hat{\sigma}_i^z\hat{\sigma}_j^z\right)$$

$$\mathbf{b}_i \cdot \boldsymbol{\sigma}_i = b_i^x\hat{\sigma}_i^x + b_i^y\hat{\sigma}_i^y + b_i^z\hat{\sigma}_i^z$$

$$V_{ii}^{\alpha\alpha} = 0 \qquad V_{ij}^{\alpha\alpha} = V_{ji}^{\alpha\alpha}$$

- Two-body terms:

$$\frac{d}{dt}\hat{\sigma}_m^x = \mathrm{i}\left[\hat{H}_2, \hat{\sigma}_m^x\right]$$

$$= \frac{\mathrm{i}}{2}\left(\sum_j V_{mj}^{yy}[\hat{\sigma}_m^y, \hat{\sigma}_m^x]\hat{\sigma}_j^y + \sum_i V_{im}^{yy}\hat{\sigma}_i^y[\hat{\sigma}_m^y, \hat{\sigma}_m^x] + \sum_j V_{ij}^{zz}[\hat{\sigma}_m^z, \hat{\sigma}_m^x]\hat{\sigma}_j^z + \sum_i V_{mj}^{zz}\hat{\sigma}_i^z[\hat{\sigma}_m^z, \hat{\sigma}_m^x]\right)$$

$V_{ij}^{\alpha\alpha} = V_{ji}^{\alpha\alpha}$

$$= -\sum_j V_{mj}^{yy}(-\hat{\sigma}_m^z\hat{\sigma}_j^y - \hat{\sigma}_j^y\hat{\sigma}_m^z) - \sum_j V_{mj}^{zz}(\hat{\sigma}_m^y\hat{\sigma}_j^z + \hat{\sigma}_j^z\hat{\sigma}_m^y)$$

$V_{ii}^{\alpha\alpha} = 0$

$$= 2\sum_j V_{mj}^{yy}\hat{\sigma}_m^z\hat{\sigma}_j^y - 2\sum_j V_{mj}^{zz}\hat{\sigma}_m^y\hat{\sigma}_j^z$$

using: $(x, y, z) = (1, 2, 3)$

$$\left[\hat{\sigma}^\alpha, \hat{\sigma}^\beta\right] = 2\mathrm{i}\sum_\gamma \epsilon_{\alpha\beta\gamma}\hat{\sigma}^\gamma$$

Levi-Civita tensor

$$\epsilon_{123} = \epsilon_{312} = \epsilon_{231} = 1$$

$$\epsilon_{321} = \epsilon_{132} = \epsilon_{213} = -1$$

0 otherwise

- In phase space: **with factorization (now really an approximation)**

$$\frac{d}{dt}x_m \approx 2\sum_j V_{mj}^{yy}(\hat{\sigma}_m^z)_W(\hat{\sigma}_j^y)_W - 2\sum_j V_{mj}^{zz}(\hat{\sigma}_m^y)_W(\hat{\sigma}_j^z)_W$$

$$= z_m\Big(2\sum_j V_{mj}^{yy}y_j\Big) - y_m\Big(2\sum_j V_{mj}^{zz}z_j\Big)$$

Lecture 3.2 - The discrete TWA (DTWA) - Equations of motion

$$\hat{H} = \hat{H}_1 + \hat{H}_2 = \sum_i \mathbf{b}_i \cdot \boldsymbol{\sigma}_i + \frac{1}{2}\sum_{ij}\left(V_{ij}^{xx}\hat{\sigma}_i^x\hat{\sigma}_j^x + V_{ij}^{yy}\hat{\sigma}_i^y\hat{\sigma}_j^y + V_{ij}^{zz}\hat{\sigma}_i^z\hat{\sigma}_j^z\right)$$

$$\mathbf{b}_i \cdot \boldsymbol{\sigma}_i = b_i^x\hat{\sigma}_i^x + b_i^y\hat{\sigma}_i^y + b_i^z\hat{\sigma}_i^z$$

$$V_{ii}^{\alpha\alpha} = 0 \qquad V_{ij}^{\alpha\alpha} = V_{ji}^{\alpha\alpha}$$

- Two-body terms:

$$\frac{d}{dt}x_m \approx z_m\big(2\sum_j V_{mj}^{yy}y_j\big) - y_m\big(2\sum_j V_{mj}^{zz}z_j\big)$$

$$\frac{d}{dt}y_m \approx z_m\big(2\sum_j V_{mj}^{xx}x_j\big) - x_m\big(2\sum_j V_{mj}^{zz}z_j\big)$$ *(exercise)*

$$\frac{d}{dt}z_m \approx x_m\big(2\sum_j V_{mj}^{yy}y_j\big) - y_m\big(2\sum_j V_{mj}^{xx}x_j\big)$$ *(exercise)*

- **Remark:** These are fully identical to mean-field equations, i.e. when considering equations for $x_m \equiv \langle\hat{\sigma}_m^x\rangle$

… assuming a product state at all times

$$\frac{d}{dt}x_m \approx z_m\big(2\underbrace{\sum_j V_{mj}^{yy}y_j}_{\text{“mean-field”} \,\parallel\, y}\big) - y_m\big(2\underbrace{\sum_j V_{mj}^{zz}z_j}_{\text{“mean-field”} \,\parallel\, z}\big)$$

- The mean-fields created by the other spins lead to a classical precession of spin *m*   *Equations are non-linear!*

Lecture 3.2 - The discrete TWA (DTWA) - Equations of motion

$$\hat{H} = \hat{H}_1 + \hat{H}_2 = \sum_i \mathbf{b}_i \cdot \boldsymbol{\sigma}_i + \frac{1}{2}\sum_{ij}\left(V_{ij}^{xx}\hat{\sigma}_i^x\hat{\sigma}_j^x + V_{ij}^{yy}\hat{\sigma}_i^y\hat{\sigma}_j^y + V_{ij}^{zz}\hat{\sigma}_i^z\hat{\sigma}_j^z\right)$$

$$\mathbf{b}_i \cdot \boldsymbol{\sigma}_i = b_i^x\hat{\sigma}_i^x + b_i^y\hat{\sigma}_i^y + b_i^z\hat{\sigma}_i^z$$

$$V_{ii}^{\alpha\alpha} = 0 \qquad V_{ij}^{\alpha\alpha} = V_{ji}^{\alpha\alpha}$$

- Two-body terms:

$$\frac{d}{dt}x_m \approx z_m\left(2\sum_j V_{mj}^{yy}y_j\right) - y_m\left(2\sum_j V_{mj}^{zz}z_j\right)$$

$$\frac{d}{dt}y_m \approx z_m\left(2\sum_j V_{mj}^{xx}x_j\right) - x_m\left(2\sum_j V_{mj}^{zz}z_j\right)$$

$$\frac{d}{dt}z_m \approx x_m\left(2\sum_j V_{mj}^{yy}y_j\right) - y_m\left(2\sum_j V_{mj}^{xx}x_j\right)$$

- **Remark:** Note that all equations can also again be derived from the full classical ansatz, e.g.

$$\dot{\alpha}_m = \{\alpha_m, H_C\} = 2\sum_\beta \epsilon_{\alpha\beta\gamma}\gamma_m\frac{\partial H_C}{\partial\beta_m} \qquad H_C(\{x_i, y_i, z_i\}) = \sum_{ij}V_{ij}^{zz}z_iz_j$$

$$\begin{aligned}\dot{x}_m &= 2\epsilon_{xzy}y_m\frac{\partial H_C}{\partial z_m} + 2\epsilon_{xyz}z_m\frac{\partial H_C}{\partial y_m} \\ &= -2y_m\frac{1}{2}\left(\sum_i V_{im}^{zz}z_j + \sum_j V_{mj}^{zz}z_i\right) = -y_m\left(2\sum_j V_{mj}^{zz}\right) \quad \checkmark\end{aligned}$$

$$(x, y, z) = (1, 2, 3)$$

Levi-Civita tensor

$$\epsilon_{123} = \epsilon_{312} = \epsilon_{231} = 1$$

$$\epsilon_{321} = \epsilon_{132} = \epsilon_{213} = -1$$

0 otherwise

Lecture 3.2 - The discrete TWA (DTWA) - Equations of motion

$$\hat{H} = \hat{H}_1 + \hat{H}_2 = \sum_i \mathbf{b}_i \cdot \boldsymbol{\sigma}_i + \frac{1}{2}\sum_{ij}\left(V_{ij}^{xx}\hat{\sigma}_i^x\hat{\sigma}_j^x + V_{ij}^{yy}\hat{\sigma}_i^y\hat{\sigma}_j^y + V_{ij}^{zz}\hat{\sigma}_i^z\hat{\sigma}_j^z\right)$$

$$\mathbf{b}_i \cdot \boldsymbol{\sigma}_i = b_i^x\hat{\sigma}_i^x + b_i^y\hat{\sigma}_i^y + b_i^z\hat{\sigma}_i^z$$

$$V_{ii}^{\alpha\alpha} = 0 \qquad V_{ij}^{\alpha\alpha} = V_{ji}^{\alpha\alpha}$$

- Full equation of motion for Weyl symbols in DTWA

$$\frac{d}{dt}x_m = z_m\left(2b_m^y + 2\sum_j V_{mj}^{yy}y_j\right) + y_m\left(2b_m^z - 2\sum_j V_{mj}^{zz}z_j\right)$$

$$\frac{d}{dt}y_m = z_m\left(-2b_m^x + 2\sum_j V_{mj}^{xx}x_j\right) + x_m\left(2b_m^z - 2\sum_j V_{mj}^{zz}z_j\right)$$

$$\frac{d}{dt}z_m = x_m\left(-2b_m^y + 2\sum_j V_{mj}^{yy}y_j\right) + y_m\left(-2b_m^x - 2\sum_j V_{mj}^{xx}x_j\right)$$

precession due to external fields and mean-fields of other spins

- **Remark:** Here all was derived for Pauli matrices, for spin operators $s_m^x = \frac{1}{2}x_m$

- In the following we will use the DTWA to solve dynamics in an **Ising model** (without fields)

$$\hat{H} = \frac{1}{2}\sum_{ij}V_{ij}^{zz}\hat{\sigma}_i^z\hat{\sigma}_j^z$$

$$\frac{d}{dt}x_m = -y_m\left(2\sum_j V_{mj}^{zz}z_j\right)$$

$$\frac{d}{dt}y_m = x_m\left(2\sum_j V_{mj}^{zz}z_j\right)$$

$$\frac{d}{dt}z_m = 0$$

$$V_{ij}^{xx} = V_{ij}^{yy} = 0$$

$$\mathbf{b}_i = 0$$

(magnetization conserved)

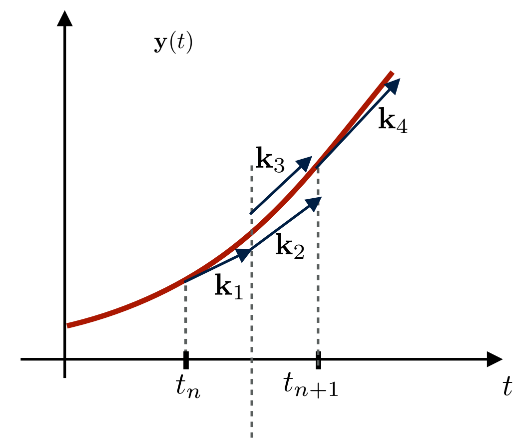
Lecture 3 - Plan for today

Today 50/50: Tutorial style | Theory lecture style

- **Part 3.1:** Introduce Runge-Kutta methods

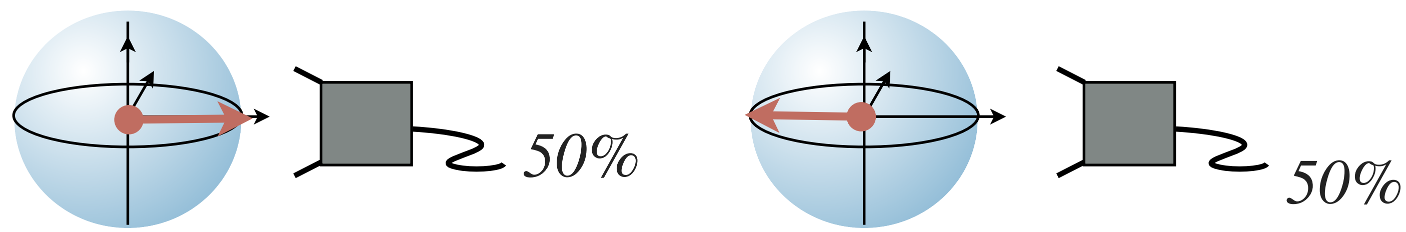
Swiss army knife for solving ODE dynamics

$$
\begin{aligned}
\mathbf{k}_1 &= f(t_n, \mathbf{y}_n)\\
\mathbf{k}_2 &= f\left(t_n + \frac{h}{2}, \mathbf{y}_n + \frac{h}{2}\mathbf{k}_1\right)\\
\mathbf{k}_3 &= f\left(t_n + \frac{h}{2}, \mathbf{y}_n + \frac{h}{2}\mathbf{k}_2\right)\\
\mathbf{k}_4 &= f\left(t_n + h, \mathbf{y}_n + h\mathbf{k}_3\right)\\
\mathbf{y}_{n+1} &\approx \mathbf{y}_n + \frac{h}{6}(\mathbf{k}_1 + 2\mathbf{k}_2 + 2\mathbf{k}_3 + \mathbf{k}_4)
\end{aligned}
$$



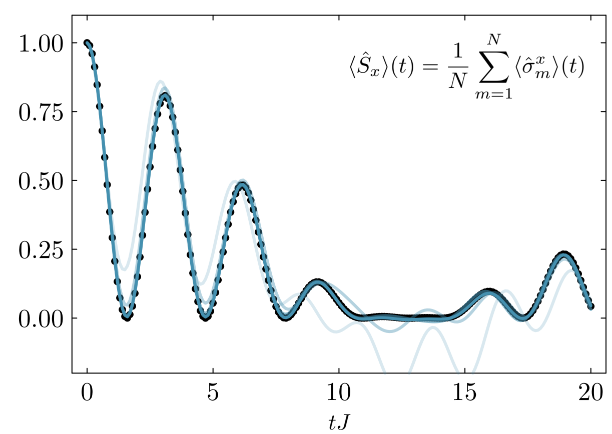
- **Part 3.2:** Back to phase space: The discrete TWA (DTWA) for generic spin-1/2 model dynamics

$$
\begin{aligned}
W(+1,+1,-1) &= 1/4\\
W(-1,+1,-1) &= 1/4\\
W(+1,-1,-1) &= 1/4\\
W(-1,-1,-1) &= 1/4
\end{aligned}
$$

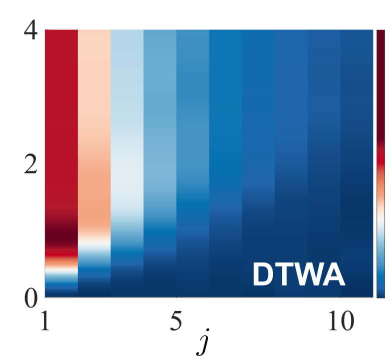


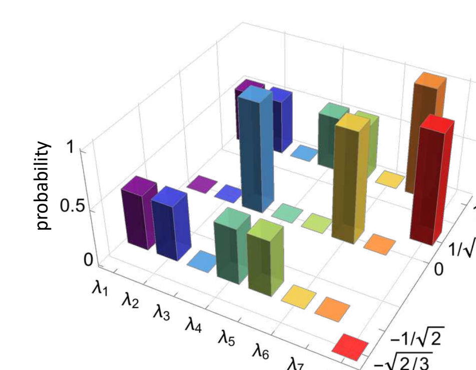
- **Part 3.3:** Set up a DTWA code for Ising model simulations. Understand the approximation better

$$
\mathbf{Y} \equiv (\mathbf{Y}_1 \quad \mathbf{Y}_2 \quad \dots \quad \mathbf{Y}_{n_T}) = \begin{pmatrix}
x_{1,1} & x_{1,2} & & x_{1,n_T}\\
\vdots & \vdots & & \\
x_{N,1} & x_{N,2} & & x_{N,n_T}\\
y_{1,1} & y_{1,2} & & y_{1,n_T}\\
\vdots & \vdots & \dots & \\
y_{N,1} & y_{N,2} & & y_{N,n_T}\\
z_{1,1} & z_{1,2} & & z_{1,n_T}\\
\vdots & \vdots & & \\
z_{N,1} & z_{N,2} & & z_{N,n_T}
\end{pmatrix}
$$



- **Part 3.4:** Generalizations to spin > 1/2 models and use case examples





Lecture 3.3 - DTWA for Ising model

- As a test case, let's compute DTWA dynamics for the following many-body problem

Ising Hamiltonian: $\hat{H} = \frac{1}{2}\sum_{ij=1}^{N} V_{ij}^{zz}\hat{\sigma}_i^z\hat{\sigma}_j^z \qquad V_{ij}^{zz} = \frac{J}{|i-j|^3}$ *Initial state:* $|\psi\rangle = \bigotimes_{i=1}^{N} |\rightarrow\rangle_i$

$$|\rightarrow\rangle_i = \frac{1}{\sqrt{2}}(|\downarrow\rangle + |\uparrow\rangle)$$

This model is simple enough to allow for an semi-analytical solution to compare with!

- Observable: $\langle\hat{S}_x\rangle(t) = \frac{1}{N}\sum_{m=1}^{N}\langle\hat{\sigma}_m^x\rangle(t)$

Analytical solution

$$\langle\hat{\sigma}_m^x\rangle(t) = \prod_{i\neq m}\cos(2tV_{im}^{zz})$$

I. J. Lowe and R. E. Norberg, Phys. Rev. 107, 46 (1957)

(easy to prove from Heisenberg equations of motion)

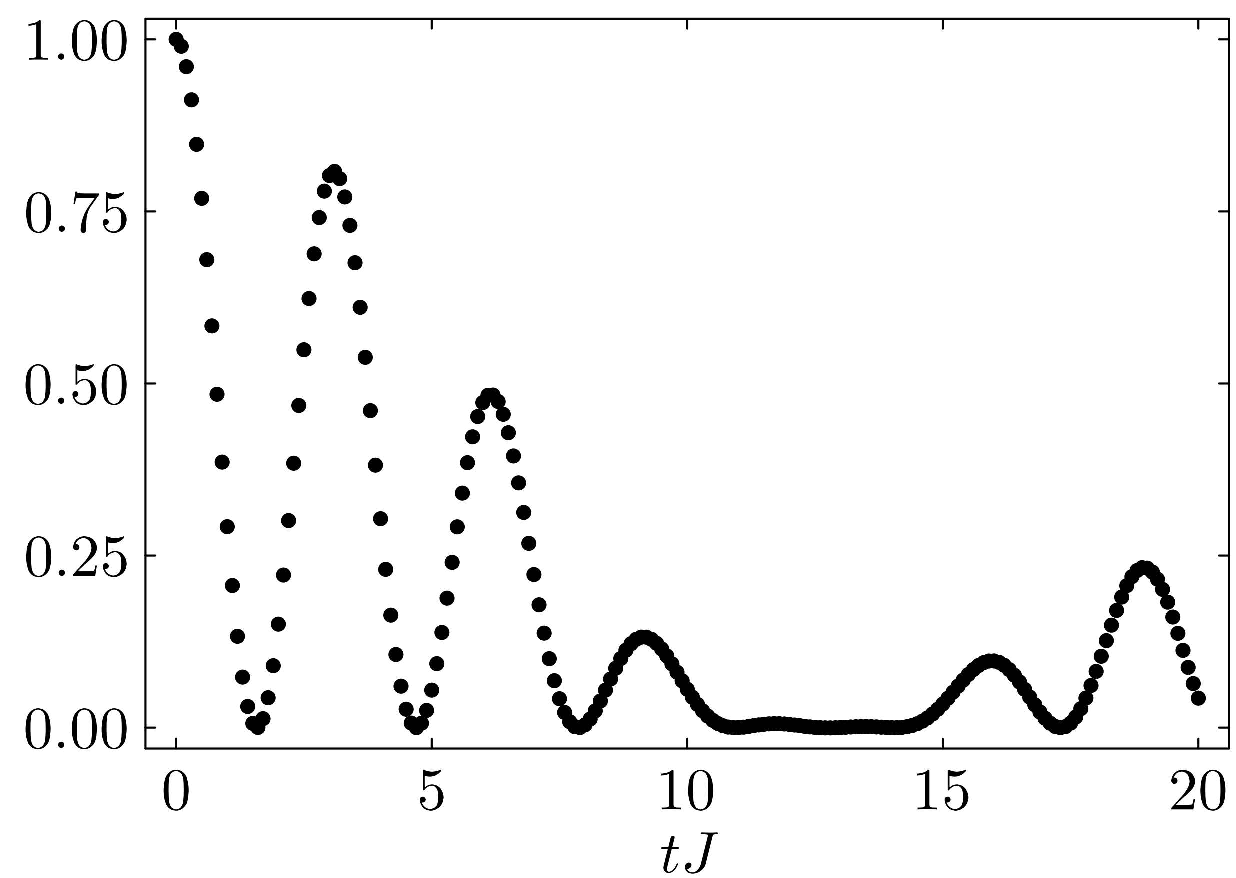
- Expectation:

```
N = 100
imat = repeat(1:N, 1, N)
Vij = 1 ./ abs.(imat - imat') .^3
Vij[diagind(Vij)] .= 0


dt = 0.1
tran = 0:0.01:20
Sx = Vector()

for tt in tran
    push!(Sx,  sum(prod(cos.(tt .* Vij); dims=1))/N)
end

plot(tran, Sx)
```



Lecture 3.3 - DTWA for Ising model

- As a test case, let's compute DTWA dynamics for the following many-body problem

Ising Hamiltonian: $\hat{H} = \frac{1}{2}\sum_{ij=1}^{N} V_{ij}^{zz}\hat{\sigma}_i^z\hat{\sigma}_j^z \qquad V_{ij}^{zz} = \frac{J}{|i-j|^3}$ *Initial state:* $|\psi\rangle = \bigotimes_{i=1}^{N} |{\rightarrow}\rangle_i$

- Constructing the state-vector for (D)TWA

single trajectory

$$\mathbf{Y}_\eta \equiv \begin{pmatrix}\mathbf{x}\\ \mathbf{y}\\ \mathbf{z}\end{pmatrix} = \begin{pmatrix} x_1 \\ \vdots \\ x_N \\ y_1 \\ \vdots \\ y_N \\ z_1 \\ \vdots \\ z_N \end{pmatrix}$$

… still makes sense to group multiple trajectories into one state:

n_T trajectories

$$\mathbf{Y} \equiv \begin{pmatrix}\mathbf{Y}_1 & \mathbf{Y}_2 & \dots & \mathbf{Y}_{n_T}\end{pmatrix} = \begin{pmatrix} x_{1,1} & x_{1,2} & & x_{1,n_T} \\ \vdots & \vdots & & \\ x_{N,1} & x_{N,2} & & x_{N,n_T} \\ y_{1,1} & y_{1,2} & & y_{1,n_T} \\ \vdots & \vdots & \dots & \\ y_{N,1} & y_{N,2} & & y_{N,n_T} \\ z_{1,1} & z_{1,2} & & z_{1,n_T} \\ \vdots & \vdots & & \\ z_{N,1} & z_{N,2} & & z_{N,n_T} \end{pmatrix}$$

All trajectories independent from each other

Trivial parallelization, general advantage of TWA!

$N \times n_T$ *matrix*

Lecture 3.3 - DTWA for Ising model

- As a test case, let's compute DTWA dynamics for the following many-body problem

Ising Hamiltonian: $\hat{H} = \frac{1}{2}\sum_{ij=1}^{N} V_{ij}^{zz}\hat{\sigma}_i^z\hat{\sigma}_j^z$ $\quad V_{ij}^{zz} = \frac{J}{|i-j|^3}$ $\quad$ *Initial state:* $|\psi\rangle = \bigotimes_{i=1}^{N} |{\rightarrow}\rangle_i$

- Samples for the initial state:

$$W(1,+1,+1) = 1/4$$
$$W(1,-1,+1) = 1/4$$
$$W(1,+1,-1) = 1/4$$
$$W(1,-1,-1) = 1/4$$

$$\mathbf{Y} \equiv \begin{pmatrix} \mathbf{Y}_1 & \mathbf{Y}_2 & \dots & \mathbf{Y}_{n_T} \end{pmatrix} = \begin{pmatrix} +1 & +1 & & +1 \\ \vdots & \vdots & & \\ +1 & +1 & & +1 \\ \pm1 & \pm1 & & \pm1 \\ \vdots & \vdots & \dots & \\ \pm1 & \pm1 & & \pm1 \\ \pm1 & \pm1 & & \pm1 \\ \vdots & \vdots & & \\ \pm1 & \pm1 & & \pm1 \end{pmatrix}$$

select all with 50%

```julia
# DTWA
N = 3
nt = 10
rng = MersenneTwister(1907)
Y = [ones(N, nt); rand(rng, -1:2:1, 2*N, nt)]
```

```
julia> Y
9x10 Matrix{Float64}:
  1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0
  1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0
  1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0
 -1.0   1.0  -1.0   1.0   1.0  -1.0  -1.0  -1.0  -1.0  -1.0
 -1.0  -1.0  -1.0   1.0   1.0  -1.0   1.0   1.0  -1.0   1.0
 -1.0   1.0  -1.0   1.0   1.0   1.0  -1.0  -1.0   1.0   1.0
  1.0   1.0  -1.0  -1.0   1.0   1.0   1.0   1.0   1.0   1.0
 -1.0  -1.0   1.0   1.0  -1.0  -1.0  -1.0   1.0   1.0  -1.0
 -1.0  -1.0  -1.0   1.0   1.0  -1.0  -1.0   1.0  -1.0  -1.0
```

$N = 3, n_T = 10$

Lecture 3.3 - DTWA for Ising model

- As a test case, let's compute DTWA dynamics for the following many-body problem

Ising Hamiltonian: $\hat{H} = \frac{1}{2}\sum_{ij=1}^{N} V_{ij}^{zz}\hat{\sigma}_i^z\hat{\sigma}_j^z$ $\quad V_{ij}^{zz} = \frac{J}{|i-j|^3}$ $\quad$ *Initial state:* $|\psi\rangle = \bigotimes_{i=1}^{N} |{\rightarrow}\rangle_i$

$$\mathbf{Y} \equiv \begin{pmatrix} \mathbf{Y}_1 & \mathbf{Y}_2 & \dots & \mathbf{Y}_{n_T} \end{pmatrix}$$

```
julia> Y
9x1 Matrix{Float64}:
 1.0
 1.0
 1.0
 0.0
 0.0
 0.0
 0.0
 0.0
 0.0
```

- **Remarks:**

We can easily cross-check TWA results with ordinary mean-field solutions

```
# mean-field
N = 3
nt = 1
Y = [ones(N, nt); zeros(2*N, nt)]
```

We can easily cross-check against with the continuous Gaussian sampling:

$$W(x,y,z) \approx \frac{1}{\pi}\mathrm{e}^{-(y^2+z^2)/S}\delta(x-\frac{1}{2})$$

```
# CTWA
N = 100
nt = 1000
rng = MersenneTwister(1907)
Y = [ones(N, nt); randn(rng, 2*N, nt)]
```

```
julia> Y
9x10 Matrix{Float64}:
  1.0         1.0         1.0          1.0       …  1.0        1.0        1.0       1.0
  1.0         1.0         1.0          1.0          1.0        1.0        1.0       1.0
  1.0         1.0         1.0          1.0          1.0        1.0        1.0       1.0
 -0.229775    0.605765    0.322977    -0.020384    -0.889596  -0.657218  -0.689025  0.626106
 -0.218955   -0.0749984   0.355384    -0.564143     0.710167  -0.189217   0.600977  0.492251
 -0.729395   -0.656307   -0.00221271   0.426511  … -1.27996    1.31126    0.657482  0.506242
  0.0153071  -0.684092    0.378696     0.836102    -0.48824   -0.973533  -1.21143   0.947317
 -2.02646     0.128265   -1.04281      0.960508     0.239302  -0.349364   0.459254  0.748061
 -0.457312    0.254755   -0.547085     0.201716     0.169882   0.436504   0.390963  0.294559
```

Lecture 3.3 - DTWA for Ising model

- As a test case, let's compute DTWA dynamics for the following many-body problem

Ising Hamiltonian: $\hat{H} = \frac{1}{2}\sum_{ij=1}^{N} V_{ij}^{zz}\hat{\sigma}_i^z\hat{\sigma}_j^z$ $\quad V_{ij}^{zz} = \frac{J}{|i-j|^3}$ $\quad$ *Initial state:* $|\psi\rangle = \bigotimes_{i=1}^{N} |\rightarrow\rangle_i$

$$\mathbf{Y} \equiv (\mathbf{Y}_1 \quad \mathbf{Y}_2 \quad \dots \quad \mathbf{Y}_{n_T})$$

```
using Statistics
```

- **Observables:**

$$\mathbf{Y} \equiv (\mathbf{Y}_1 \quad \mathbf{Y}_2 \quad \dots \quad \mathbf{Y}_{n_T}) = \begin{pmatrix} x_{1,1} & x_{1,2} & & x_{1,n_T} \\ \vdots & \vdots & & \\ x_{N,1} & x_{N,2} & & x_{N,n_T} \\ y_{1,1} & y_{1,2} & & y_{1,n_T} \\ \vdots & \vdots & \dots & \\ y_{N,1} & y_{N,2} & & y_{N,n_T} \\ z_{1,1} & z_{1,2} & & z_{1,n_T} \\ \vdots & \vdots & & \\ z_{N,1} & z_{N,2} & & z_{N,n_T} \end{pmatrix}$$

$\frac{1}{n_T}\sum \dots \approx \langle\hat{\sigma}_1^x\rangle$

```
mean(Y[1, :])
```

$\frac{1}{n_T}\sum \dots \approx \langle\hat{\sigma}_1^y\rangle$

```
mean(Y[N+1, :])
```

$\frac{1}{n_T}\sum \dots \approx \langle\hat{\sigma}_1^z\rangle$

```
mean(Y[2*N+1, :])
```

- **Remark:** Error bars due to statistical error:
  Standard error of the mean from sample standard deviation: $\langle\hat{\sigma}_1^z\rangle \pm$ `std(Y[1, :]) / sqrt(nt)`

- **Remark:** Correlation functions also simple $\langle\hat{\sigma}_1^x\hat{\sigma}_N^z\rangle \approx$ `mean(Y[1, :] .* Y[N, :])`

Lecture 3.3 - DTWA for Ising model

- As a test case, let's compute DTWA dynamics for the following many-body problem

Ising Hamiltonian: $\hat{H} = \frac{1}{2}\sum_{ij=1}^{N} V_{ij}^{zz}\hat{\sigma}_i^z\hat{\sigma}_j^z$ $\quad V_{ij}^{zz} = \frac{J}{|i-j|^3}$ $\quad$ *Initial state:* $|\psi\rangle = \bigotimes_{i=1}^{N} |{\rightarrow}\rangle_i$

$$\mathbf{Y} \equiv \begin{pmatrix} \mathbf{Y}_1 & \mathbf{Y}_2 & \dots & \mathbf{Y}_{n_T} \end{pmatrix}$$

- **Observable:** $\langle \hat{S}_x \rangle(t) = \frac{1}{N}\sum_{m=1}^{N} \langle \hat{\sigma}_m^x \rangle(t)$

$$\mathbf{Y} \equiv \begin{pmatrix} \mathbf{Y}_1 & \mathbf{Y}_2 & \dots & \mathbf{Y}_{n_T} \end{pmatrix} = \begin{pmatrix} x_{1,1} & x_{1,2} & & x_{1,n_T} \\ \vdots & \vdots & & \\ x_{N,1} & x_{N,2} & & x_{N,n_T} \\ y_{1,1} & y_{1,2} & & y_{1,n_T} \\ \vdots & \vdots & \dots & \\ y_{N,1} & y_{N,2} & & y_{N,n_T} \\ z_{1,1} & z_{1,2} & & z_{1,n_T} \\ \vdots & \vdots & & \\ z_{N,1} & z_{N,2} & & z_{N,n_T} \end{pmatrix}$$

Very simple:

```
Sx = mean(1:N, :)
dSx = std(1:N, :) / sqrt(nt)
```

Lecture 3.3 - DTWA for Ising model

- As a test case, let's compute DTWA dynamics for the following many-body problem

Ising Hamiltonian: $\hat{H} = \frac{1}{2}\sum_{ij=1}^{N} V_{ij}^{zz}\hat{\sigma}_i^z\hat{\sigma}_j^z$ $\quad V_{ij}^{zz} = \frac{J}{|i-j|^3}$ $\quad$ *Initial state:* $|\psi\rangle = \bigotimes_{i=1}^{N} |\rightarrow\rangle_i$

$$\mathbf{Y} \equiv \begin{pmatrix} \mathbf{Y}_1 & \mathbf{Y}_2 & \dots & \mathbf{Y}_{n_T} \end{pmatrix}$$

- **ODE for evolution:**

$$\frac{d}{dt}x_m = -y_m\big(2\sum_j V_{mj}^{zz} z_j\big)$$
$$\frac{d}{dt}y_m = x_m\big(2\sum_j V_{mj}^{zz} z_j\big)$$
$$\frac{d}{dt}z_m = 0$$

$$\frac{d}{dt}\mathbf{Y} = f_{\text{Ising}}(\mathbf{Y})$$

```
function f_Ising(Y, Vij, N)

    xran = 1:N
    yran = (N+1):(2*N)
    zran = (2*N+1):(3*N)

    dY = zeros(size(Y))

    @views mfs = Vij * Y[zran, :]  # mean-fields (N x nt)
    @views dY[xran, :] = - mfs .* Y[yran, :]
    @views dY[yran, :] = mfs .* Y[xran, :]

    return dY

end
```

Lecture 3 - Tutorial - DTWA for Ising model

- As a test case, let's compute DTWA dynamics for the following many-body problem

Ising Hamiltonian: $\hat{H} = \frac{1}{2}\sum_{ij=1}^{N} V_{ij}^{zz}\hat{\sigma}_i^z\hat{\sigma}_j^z$ $\quad V_{ij}^{zz} = \frac{J}{|i-j|^3}$ $\quad$ *Initial state:* $|\psi\rangle = \bigotimes_{i=1}^{N} |\rightarrow\rangle_i$

$$\mathbf{Y} \equiv \begin{pmatrix} \mathbf{Y}_1 & \mathbf{Y}_2 & \dots & \mathbf{Y}_{n_T} \end{pmatrix}$$

- **Solve ODE with RK4**

$$\frac{d}{dt}x_m = -y_m\left(2\sum_j V_{mj}^{zz} z_j\right)$$
$$\frac{d}{dt}y_m = x_m\left(2\sum_j V_{mj}^{zz} z_j\right)$$
$$\frac{d}{dt}z_m = 0$$

$$\frac{d}{dt}\mathbf{Y} = f_{\text{Ising}}(\mathbf{Y})$$

```
function rk4_Ising(Y, Vij, h, N)

    f(Y) = f_Ising(Y, Vij, N)

    h2 = h/2
    k1 = f(Y)
    k2 = f(Y .+ h2 .* k1)
    k3 = f(Y .+ h2 .* k2)
    k4 = f(Y .+ h .* k3)
    Y += (h/6) .* (k1 .+ 2 .* k2 .+ 2 .* k3 .+ k4)

    return Y
end
```

Lecture 3.3 - DTWA for Ising model

- As a test case, let's compute DTWA dynamics for the following many-body problem

$$\textit{Ising Hamiltonian:} \quad \hat{H} = \frac{1}{2}\sum_{ij=1}^{N} V_{ij}^{zz}\hat{\sigma}_i^z\hat{\sigma}_j^z \qquad V_{ij}^{zz} = \frac{J}{|i-j|^3} \qquad \textit{Initial state:} \quad |\psi\rangle = \bigotimes_{i=1}^{N} |\rightarrow\rangle_i$$

$$\mathbf{Y} \equiv \begin{pmatrix} \mathbf{Y}_1 & \mathbf{Y}_2 & \dots & \mathbf{Y}_{n_T} \end{pmatrix}$$

- **Full code:**

```
# DTWA
N = 100
nt = 10000
rng = MersenneTwister(1907)
Y = [ones(N, nt); rand(rng, -1:2:1, 2*N, nt)]

dt = 0.1
tran = 0:0.01:20
Sx_dtwa = Vector()

for tt in tran

    push!(Sx_dtwa, mean(Y[1:N, :])) # evaluate
    Y = rk4_Ising(Y, Vij, dt, N) # evolve

end

p = plot(tran, Sx_dtwa)
```

Lecture 3.3 - DTWA for Ising model

- As a test case, let's compute DTWA dynamics for the following many-body problem

Ising Hamiltonian: $\hat{H} = \frac{1}{2}\sum_{ij=1}^{N} V_{ij}^{zz}\hat{\sigma}_i^z\hat{\sigma}_j^z$ $\quad V_{ij}^{zz} = \frac{J}{|i-j|^3}$ $\quad$ *Initial state:* $|\psi\rangle = \bigotimes_{i=1}^{N} |\rightarrow\rangle_i$

- **Mean-field:**

```
# mean-field
N = 100
nt = 1
Y = [ones(N, nt); zeros(2*N, nt)]
```

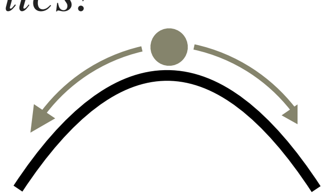
$$\langle \hat{S}_x\rangle(t) = \frac{1}{N}\sum_{m=1}^{N}\langle\hat{\sigma}_m^x\rangle(t)$$

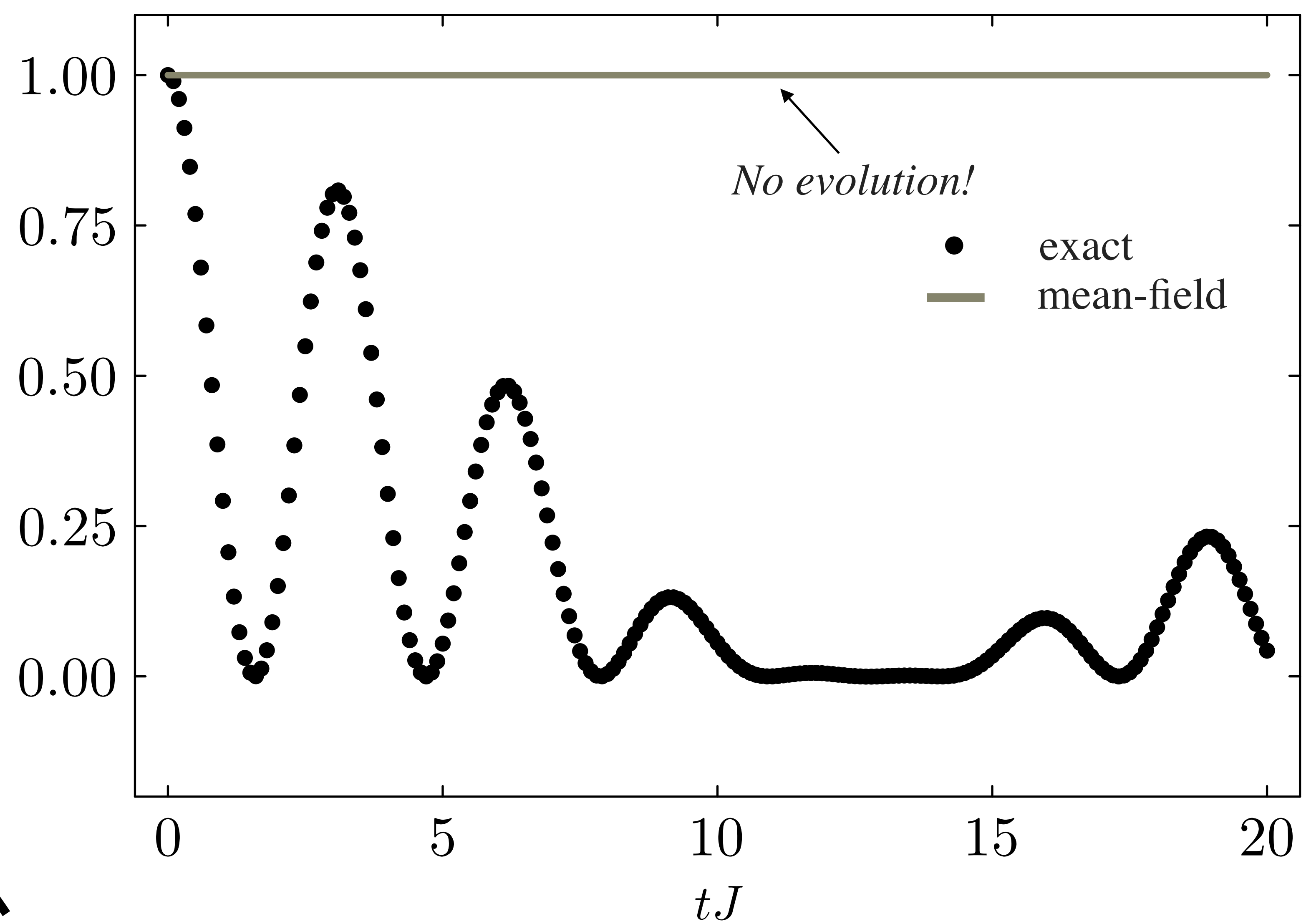
$$\frac{d}{dt}x_m = -y_m\big(2\sum_j V_{mj}^{zz}z_j\big)$$
$$\frac{d}{dt}y_m = x_m\big(2\sum_j V_{mj}^{zz}z_j\big)$$
$$\frac{d}{dt}z_m = 0$$

No mean-field!

$$\big(2\sum_j V_{mj}^{zz}z_j\big) = 0$$

Quantum fluctuations are needed to tip off the dynamics!





Lecture 3.3 - DTWA for Ising model

- As a test case, let's compute DTWA dynamics for the following many-body problem

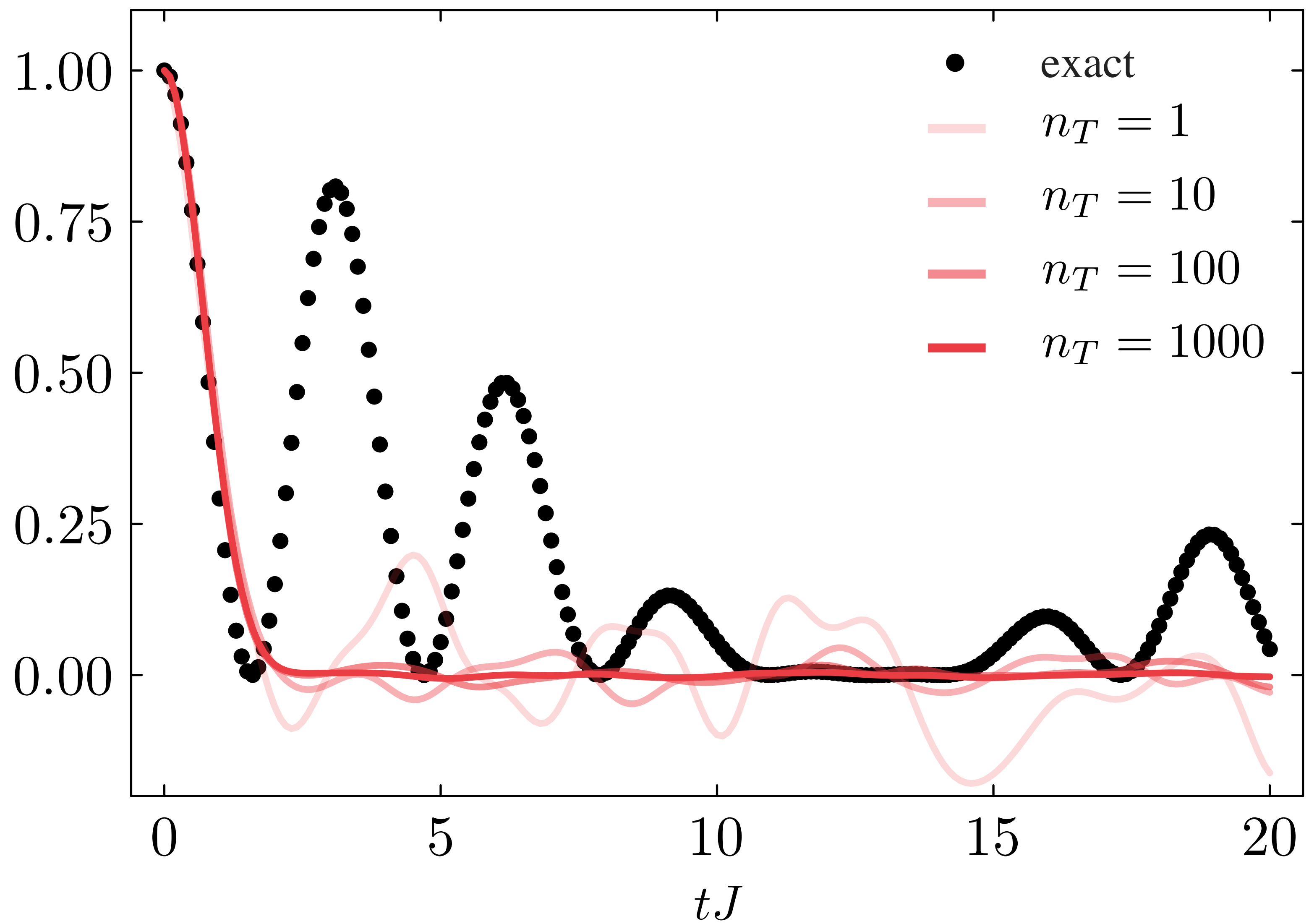
Ising Hamiltonian: $\hat{H} = \frac{1}{2}\sum_{ij=1}^{N} V_{ij}^{zz}\hat{\sigma}_i^z\hat{\sigma}_j^z$ $\quad V_{ij}^{zz} = \frac{J}{|i-j|^3}$ $\quad$ *Initial state:* $|\psi\rangle = \bigotimes_{i=1}^{N} |\rightarrow\rangle_i$

- **Gaussian noise**

```
# CTWA
N = 100
nt = 1000
rng = MersenneTwister(1907)
Y = [ones(N, nt); randn(rng, 2*N, nt)]
```

$$\langle \hat{S}_x\rangle(t) = \frac{1}{N}\sum_{m=1}^{N}\langle\hat{\sigma}_m^x\rangle(t)$$

$$\frac{d}{dt}x_m = -y_m\big(2\sum_j V_{mj}^{zz} z_j\big)$$
$$\frac{d}{dt}y_m = x_m\big(2\sum_j V_{mj}^{zz} z_j\big)$$
$$\frac{d}{dt}z_m = 0$$



Exact for short times, but no revivals

Lecture 3.3 - DTWA for Ising model

- As a test case, let's compute DTWA dynamics for the following many-body problem

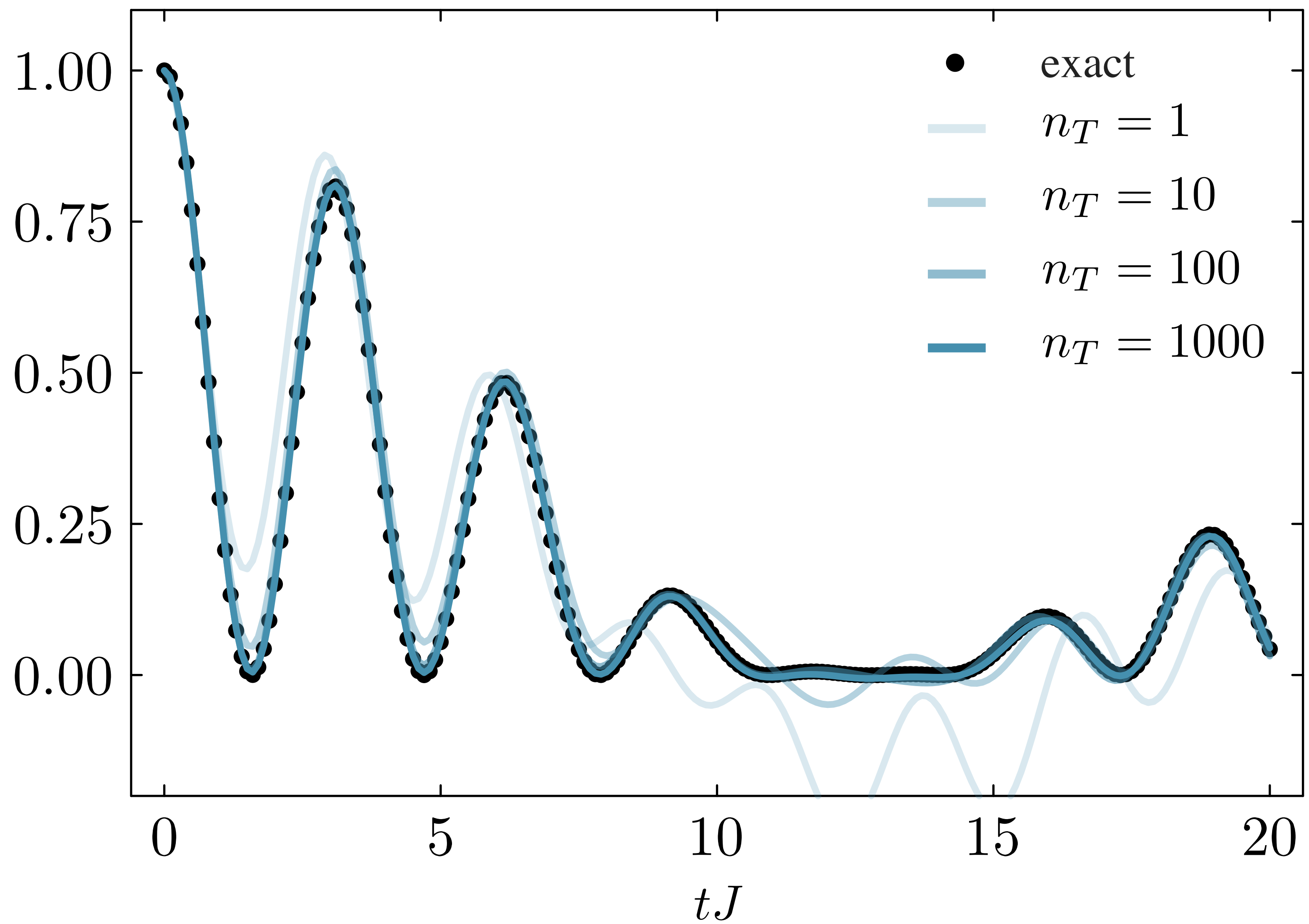
Ising Hamiltonian: $\hat{H} = \frac{1}{2}\sum_{ij=1}^{N} V_{ij}^{zz}\hat{\sigma}_i^z\hat{\sigma}_j^z$ $\quad V_{ij}^{zz} = \frac{J}{|i-j|^3}$ $\quad$ *Initial state:* $|\psi\rangle = \bigotimes_{i=1}^{N} |\rightarrow\rangle_i$

- **Discrete noise**

```
# DTWA
N = 100
nt = 1000
rng = MersenneTwister(1907)
Y = [ones(N, nt); rand(rng, -1:2:1, 2*N, nt)]
```

$$\langle\hat{S}_x\rangle(t) = \frac{1}{N}\sum_{m=1}^{N}\langle\hat{\sigma}_m^x\rangle(t)$$

$$\frac{d}{dt}x_m = -y_m\left(2\sum_j V_{mj}^{zz}z_j\right)$$
$$\frac{d}{dt}y_m = x_m\left(2\sum_j V_{mj}^{zz}z_j\right)$$
$$\frac{d}{dt}z_m = 0$$



DTWA is exact!

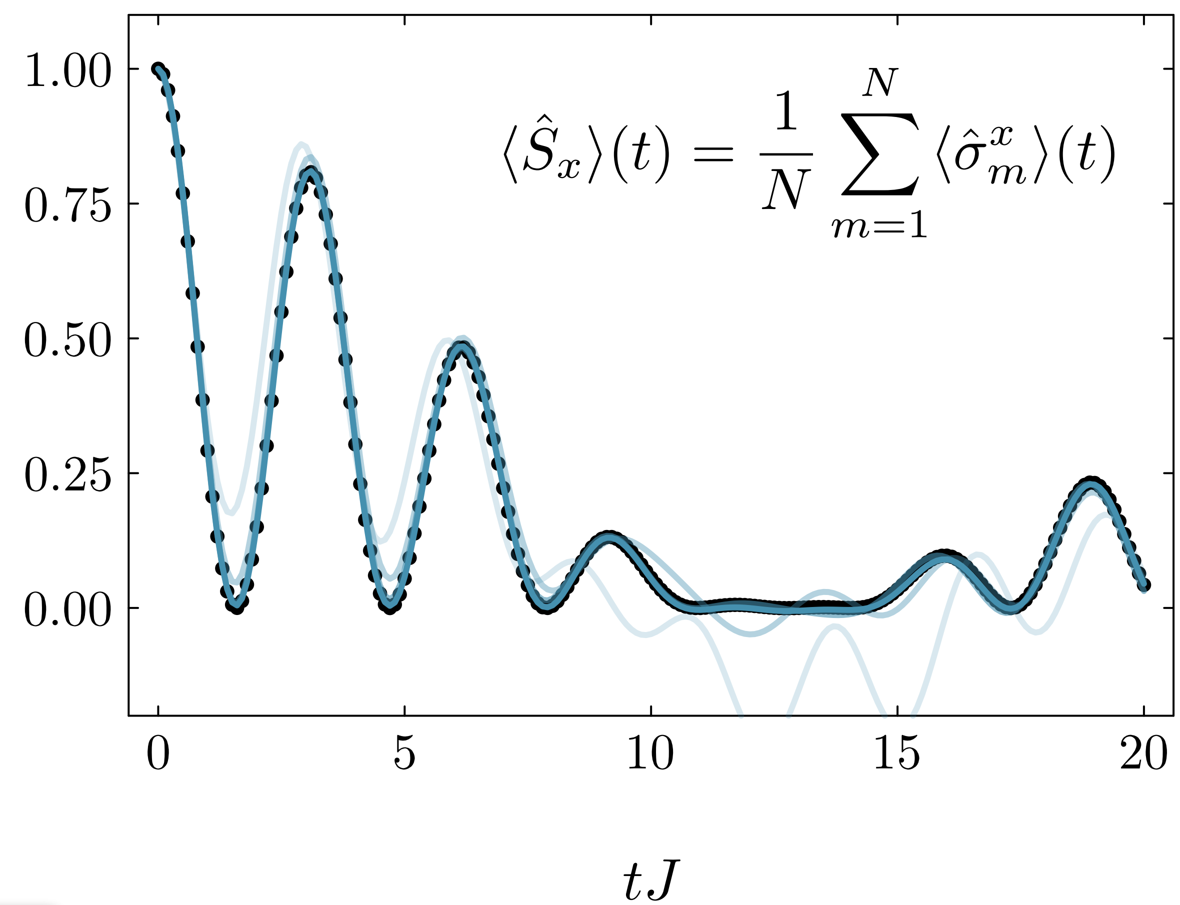
Lecture 3.3 - DTWA for Ising model

- As a test case, let's compute DTWA dynamics for the following many-body problem

Ising Hamiltonian: $\hat{H} = \frac{1}{2}\sum_{ij=1}^{N} V_{ij}^{zz}\hat{\sigma}_i^z\hat{\sigma}_j^z$ $\quad V_{ij}^{zz} = \frac{J}{|i-j|^3}$ $\quad$ *Initial state:* $|\psi\rangle = \bigotimes_{i=1}^{N} |\rightarrow\rangle_i$

- **Remark:** Naively, in retrospect it's obvious that the DTWA is exact for the Ising model: The Hamiltonian is classical in the sense that it only contains commuting terms. Then, all quantum evolution comes from the **initial state only**. We showed before that all quantum fluctuations of the initial state are perfectly captured by the sampling.

- **Remark:** One can also easily proof that the DTWA is exact for the Ising model:



Identity (Wikipedia)

$$\prod_{k=1}^{n}\cos\theta_k = \frac{1}{2^n}\sum_{e\in S}\cos(e_1\theta_1+\cdots+e_n\theta_n)$$

$$\text{where } e = (e_1,\ldots,e_n) \in S = \{1,-1\}^n$$

Analytical solution

$$\langle\hat{\sigma}_m^x\rangle(t) = \prod_{i\neq m}\cos(2tV_{im}^{zz})$$

+ analytical expression for classical solution

(exercise)

- **Remark:** Of course, for more complicated models and observables, the DTWA is not exact! … but it can still give excellent predictions!

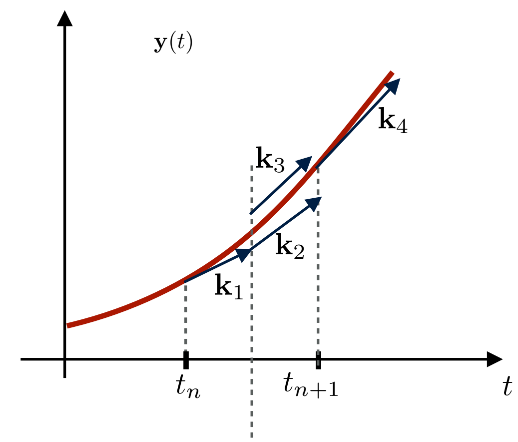
Lecture 3 - Plan for today

Today 50/50: Tutorial style | Theory lecture style

- **Part 3.1:** Introduce Runge-Kutta methods

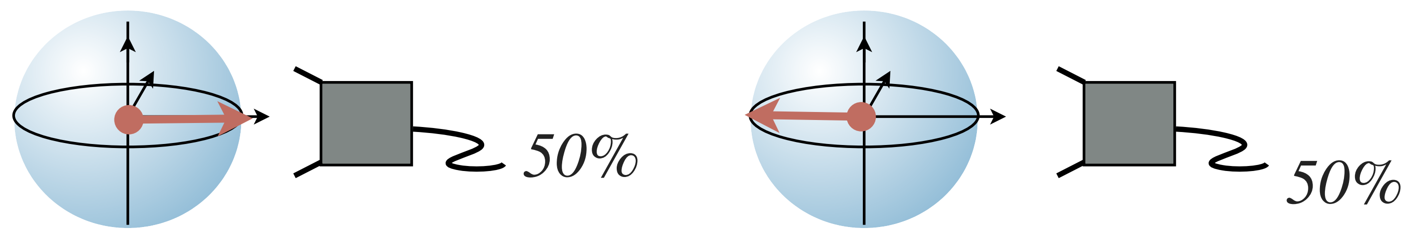
Swiss army knife for solving ODE dynamics

$$\begin{aligned}
\mathbf{k}_1 &= f(t_n, \mathbf{y}_n) \\
\mathbf{k}_2 &= f\left(t_n + \frac{h}{2}, \mathbf{y}_n + \frac{h}{2}\mathbf{k}_1\right) \\
\mathbf{k}_3 &= f\left(t_n + \frac{h}{2}, \mathbf{y}_n + \frac{h}{2}\mathbf{k}_2\right) \\
\mathbf{k}_4 &= f\left(t_n + h, \mathbf{y}_n + h\mathbf{k}_3\right) \\
\mathbf{y}_{n+1} &\approx \mathbf{y}_n + \frac{h}{6}(\mathbf{k}_1 + 2\mathbf{k}_2 + 2\mathbf{k}_3 + \mathbf{k}_4)
\end{aligned}$$



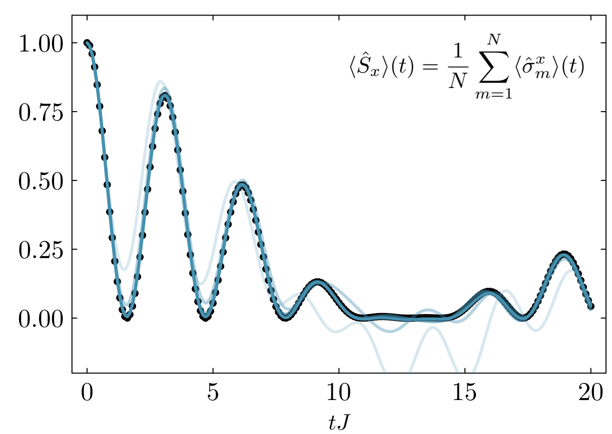
- **Part 3.2:** Back to phase space: The discrete TWA (DTWA) for generic spin-1/2 model dynamics

$$\begin{aligned}
W(+1,+1,-1) &= 1/4 \\
W(-1,+1,-1) &= 1/4 \\
W(+1,-1,-1) &= 1/4 \\
W(-1,-1,-1) &= 1/4
\end{aligned}$$

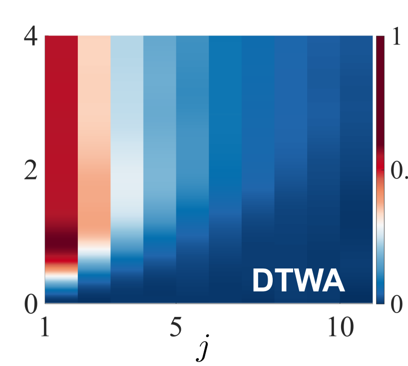


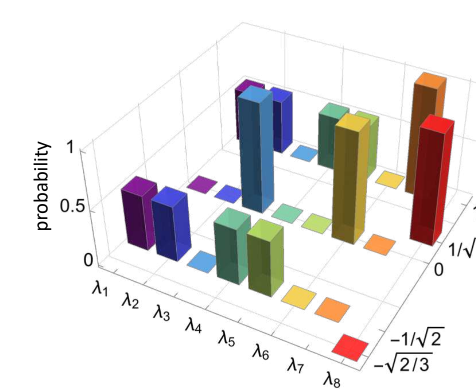
- **Part 3.3:** Set up a DTWA code for Ising model simulations. Understand the approximation better

$$\mathbf{Y} \equiv (\mathbf{Y}_1 \quad \mathbf{Y}_2 \quad \dots \quad \mathbf{Y}_{n_T}) = \begin{pmatrix} x_{1,1} & x_{1,2} & & x_{1,n_T} \\ \vdots & \vdots & & \\ x_{N,1} & x_{N,2} & & x_{N,n_T} \\ y_{1,1} & y_{1,2} & & y_{1,n_T} \\ \vdots & \vdots & \dots & \\ y_{N,1} & y_{N,2} & & y_{N,n_T} \\ z_{1,1} & z_{1,2} & & z_{1,n_T} \\ \vdots & \vdots & & \\ z_{N,1} & z_{N,2} & & z_{N,n_T} \end{pmatrix}$$



- **Part 3.4:** Generalizations to spin > 1/2 models and use case examples

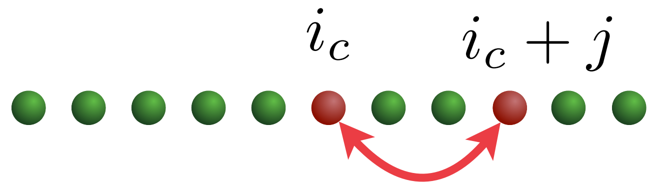




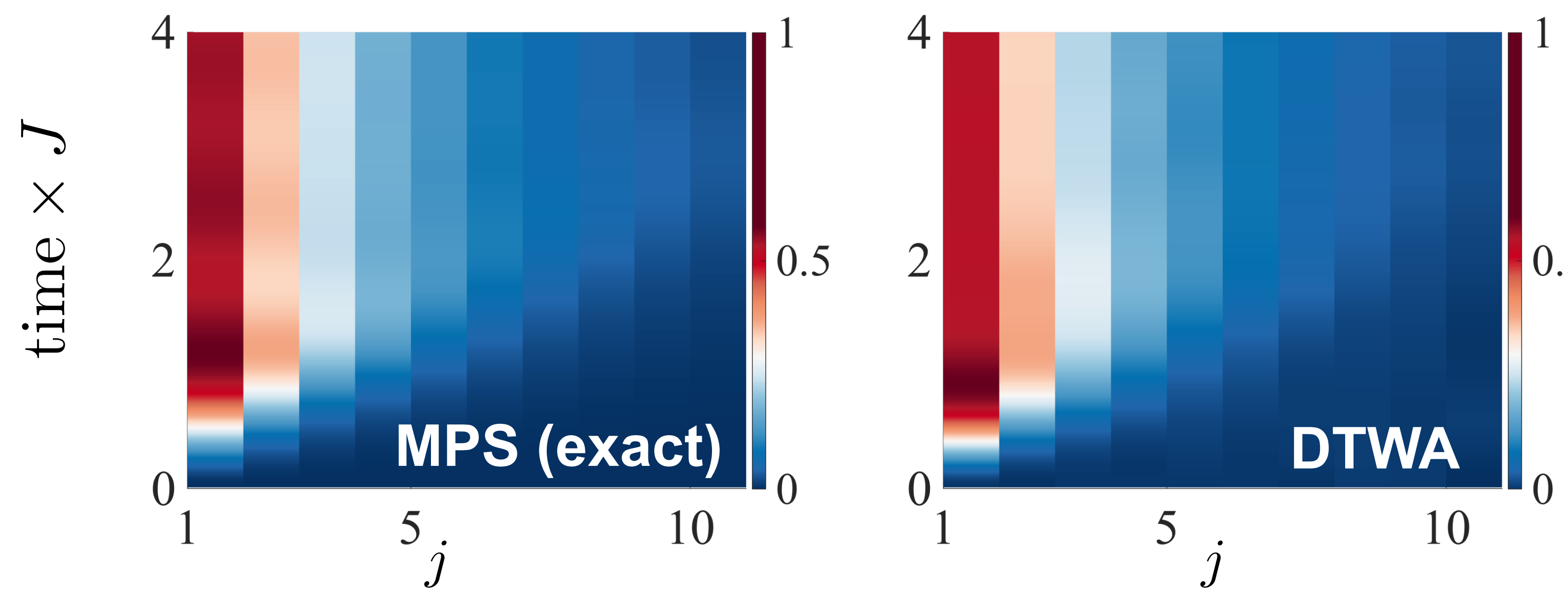
Lecture 3.4 - DTWA application examples

$$H = \frac{1}{2}\sum_{i \neq j} J_{ij}^{\perp}(\sigma_i^x \sigma_j^x + \sigma_i^y \sigma_j^y) \qquad J_{ij}^{\perp} = \frac{J}{|i-j|^3}$$

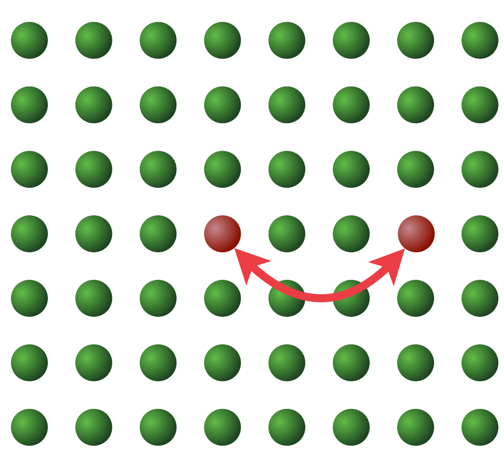
- **One dimension (XY model):**



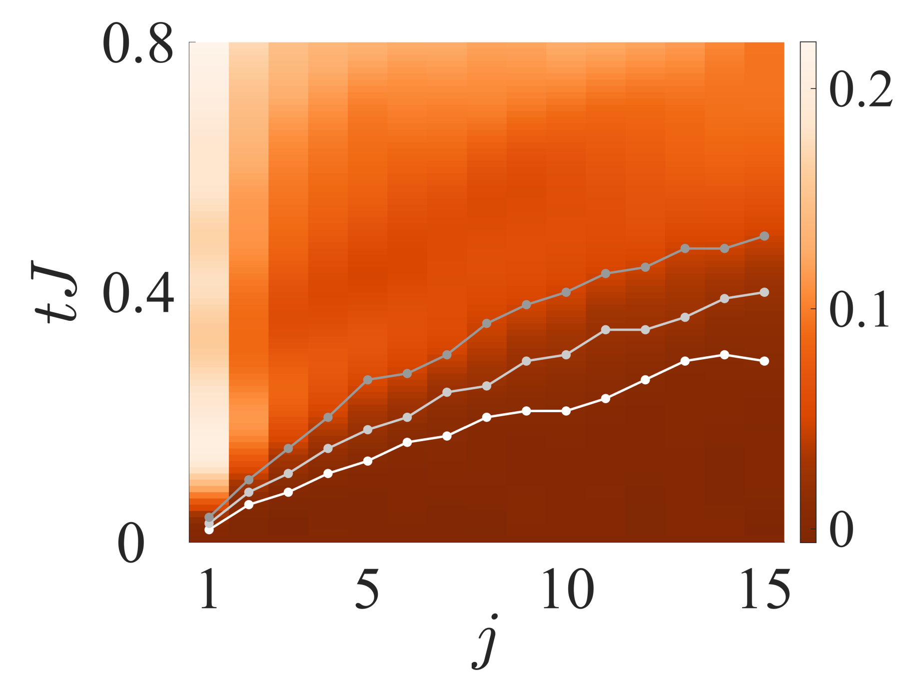
$$\mathcal{C}_j^{yy} \equiv \langle \hat{\sigma}_{i_c}^y \hat{\sigma}_{i_c+j}^y \rangle - \langle \hat{\sigma}_{i_c}^y \rangle \langle \hat{\sigma}_{i_c+j}^y \rangle$$



- **Two dimensions:**



up to 10 000 spins!



JS, A. Pikovski, and Ana Maria Rey,
New J. Phys. 17, 065009 (2015)

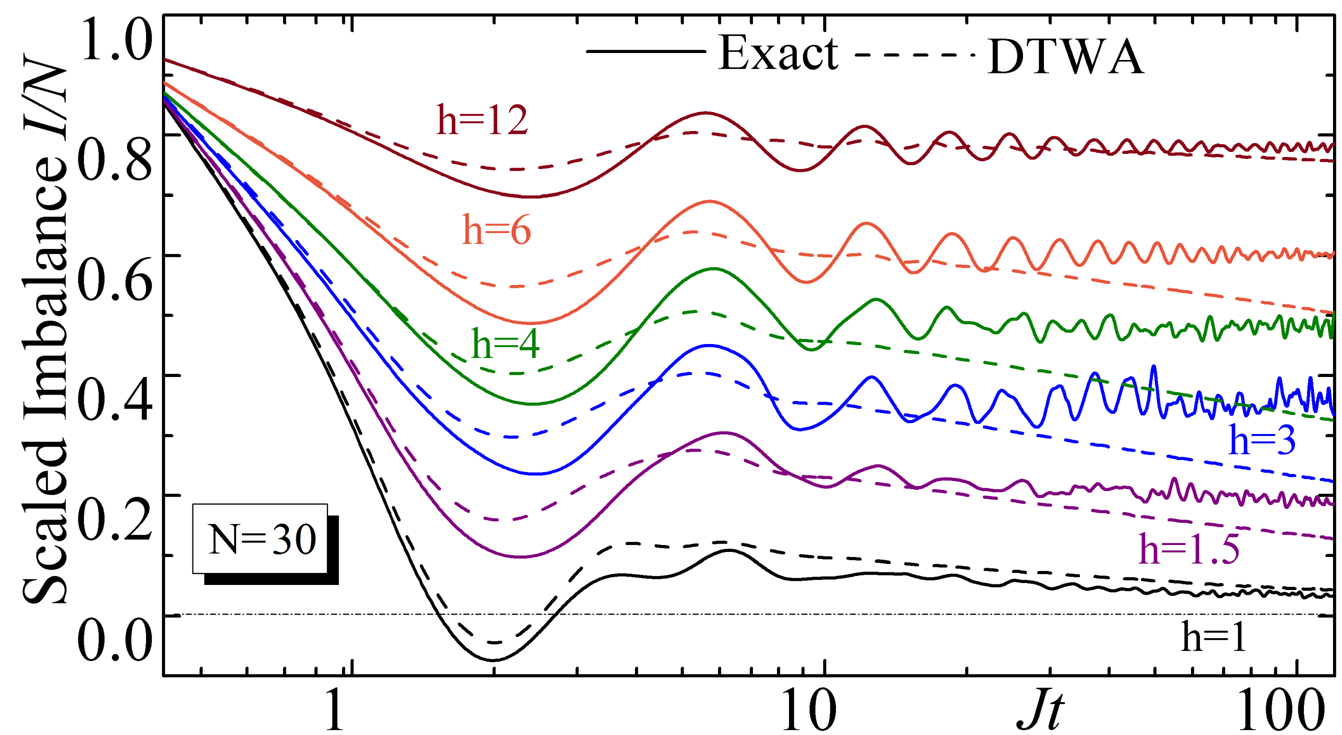
Lecture 3.4 - DTWA application examples

- Thermalization dynamics in disordered Heisenberg chain:

$$\hat{H} = J \sum_{i=1}^{N-1} \hat{\mathbf{s}}_i \cdot \hat{\mathbf{s}}_{i+1} + \sum_{i=1}^{N} h_i \hat{s}_i^z$$

O. L. Acevado, et al. Phys. Rev. A 96, 033604 (2017)

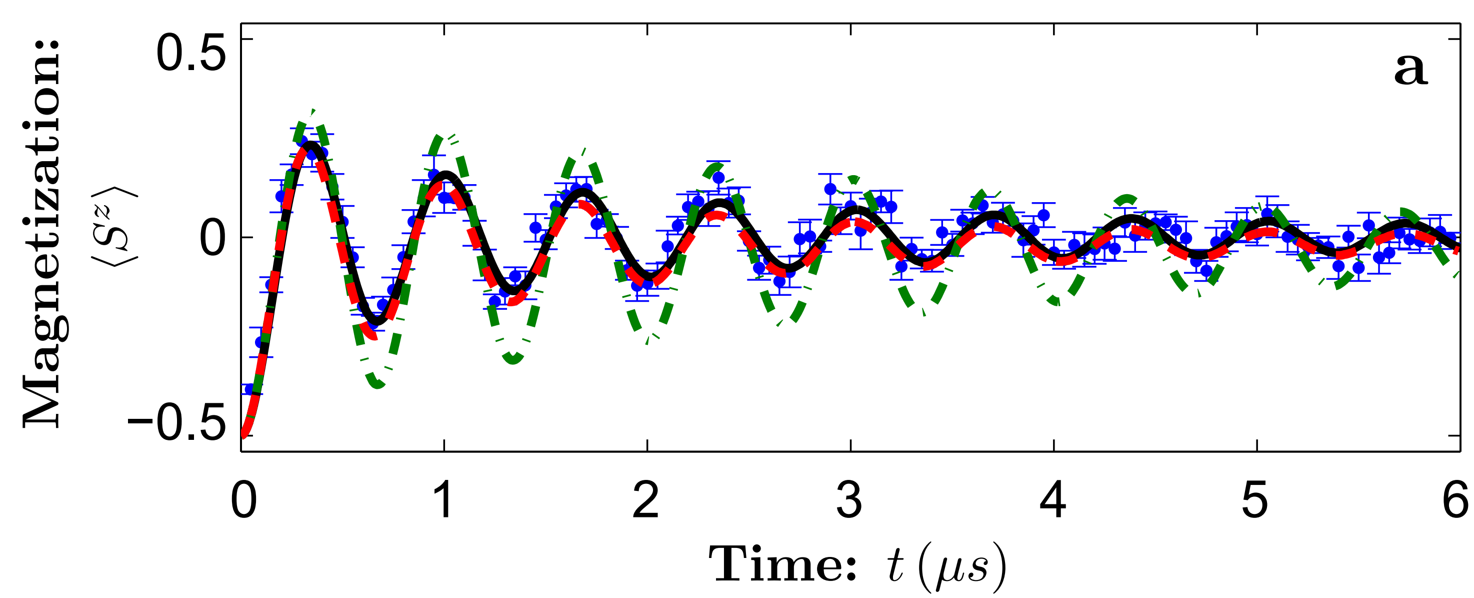
$$|\psi_0\rangle = |\downarrow\uparrow \ldots \downarrow\uparrow\rangle$$



- Modelling a Rydberg atom experiment in Heidelberg

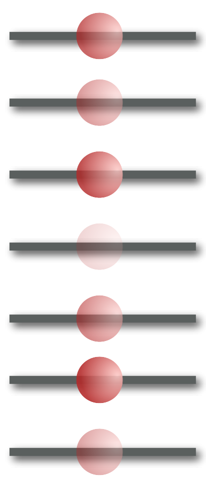
A. Piñeiro Orioli, et al. Phys. Rev. Lett. 120, 063601 (2018)

green: mean-field, red: DTWA

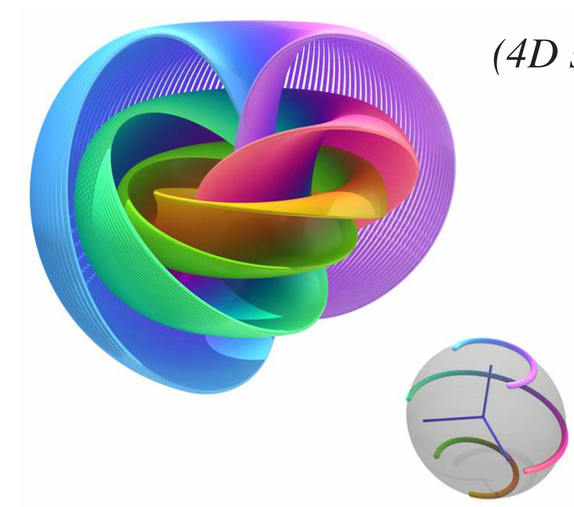


Lecture 3.4 - Spin > 1/2 models - The GDTWA

- Generalization to coupled D-level systems



$$\hat{\rho} = \frac{1}{2}\left(\mathbb{1} + \boldsymbol{\lambda}\cdot\hat{\boldsymbol{\Lambda}}\right) \quad \Leftrightarrow$$



(4D sphere projection from wikipedia)

$$\hat{\boldsymbol{\Lambda}} = (\hat{\Lambda}_1, \hat{\Lambda}_2, \ldots, \hat{\Lambda}_{48})$$

Generalized Gell-Mann matrices

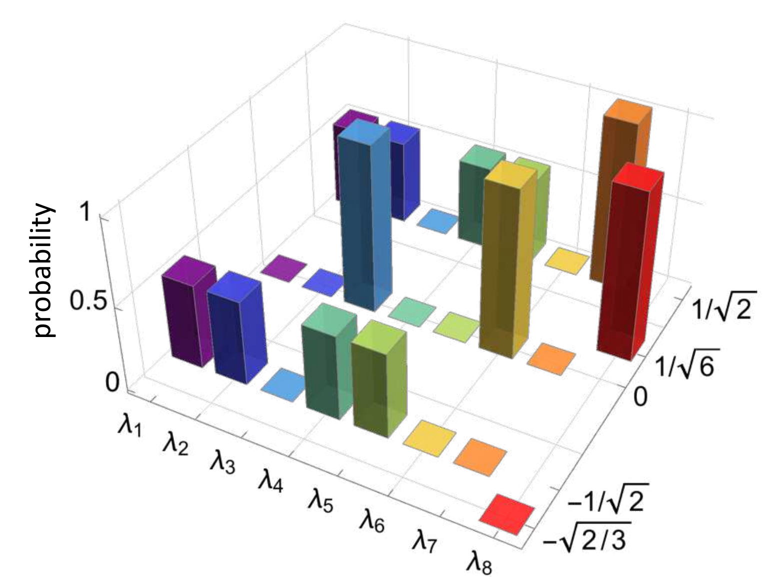
R. A. Bertlmann and P. Krammer, J. Phys. A: Math. Theor. 41, 235303 (2008).

48D "Hyper-Bloch-sphere" components as phase space!

$$\boldsymbol{\lambda} = (\lambda_1, \lambda_2, \lambda_3, \lambda_4, \ldots, \lambda_{48})$$

Classical mean-field equations: $$\frac{d}{dt}\boldsymbol{\lambda}_i = \boldsymbol{M}[\boldsymbol{\lambda}_{j\neq i}]\boldsymbol{\lambda}_i$$

- We can find exact discrete distributions for our initial states

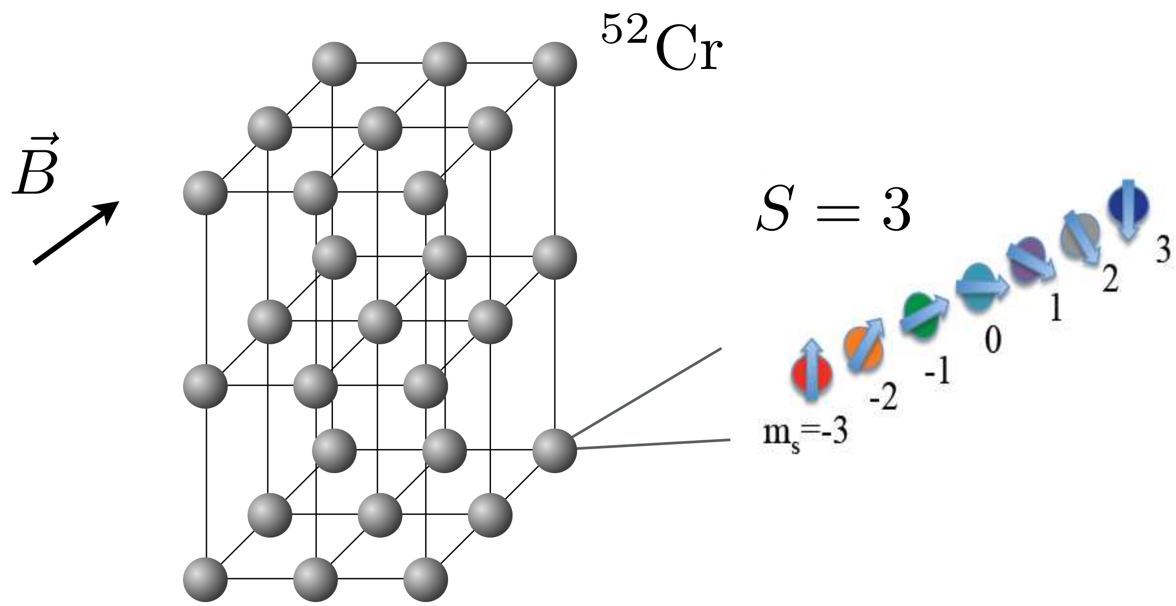


Generalized DTWA (GDTWA)

B. Zhu, A. M. Rey, and JS, *New J. Phys. 21, 082001 (2019)*

Lecture 3.4 - DTWA application examples - the GDTWA

- **Experiment** (Paris Nord): Chromium atoms trapped in (anisotropic) 3D optical lattice:



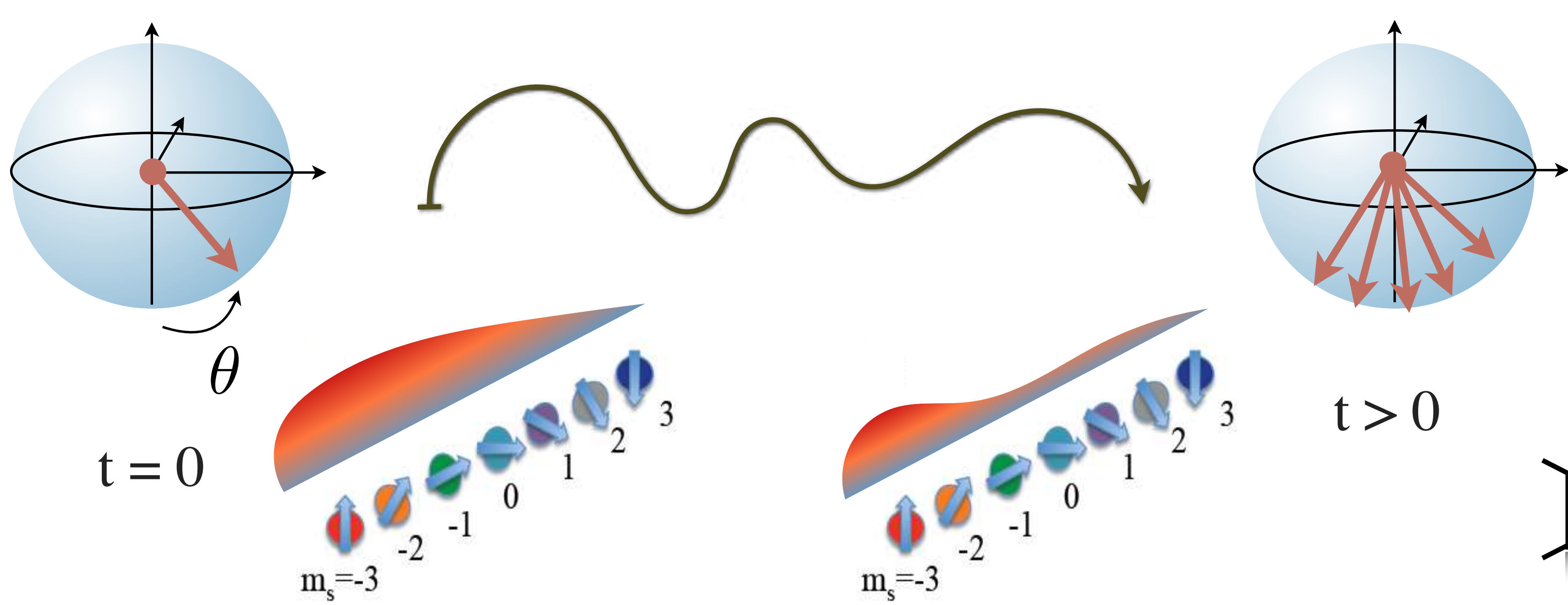
Magnetic dipole-dipole couplings

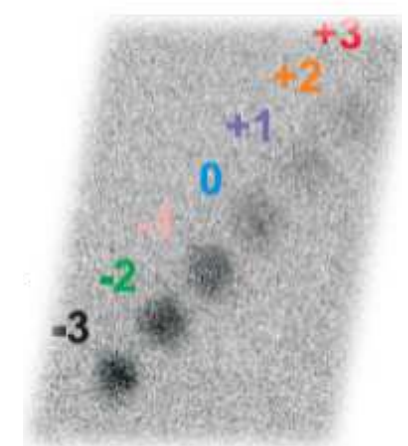
Spin S = 3 operators

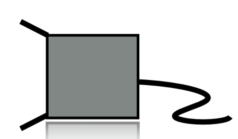
$$\hat{H} = \sum_{i>j} V_{ij} \left[\hat{S}_i^z \hat{S}_j^z - \frac{1}{2} \left(\hat{S}_i^x \hat{S}_j^x + \hat{S}_i^y \hat{S}_j^y \right) \right]$$

$$V_{i,j} \equiv \frac{\mu_0 (g\mu_B)^2}{4\pi} \left(\frac{1 - 3\cos^2 \phi_{(i,j)}}{r^3_{(i,j)}} \right)$$

- Time evolution after initial tilt:







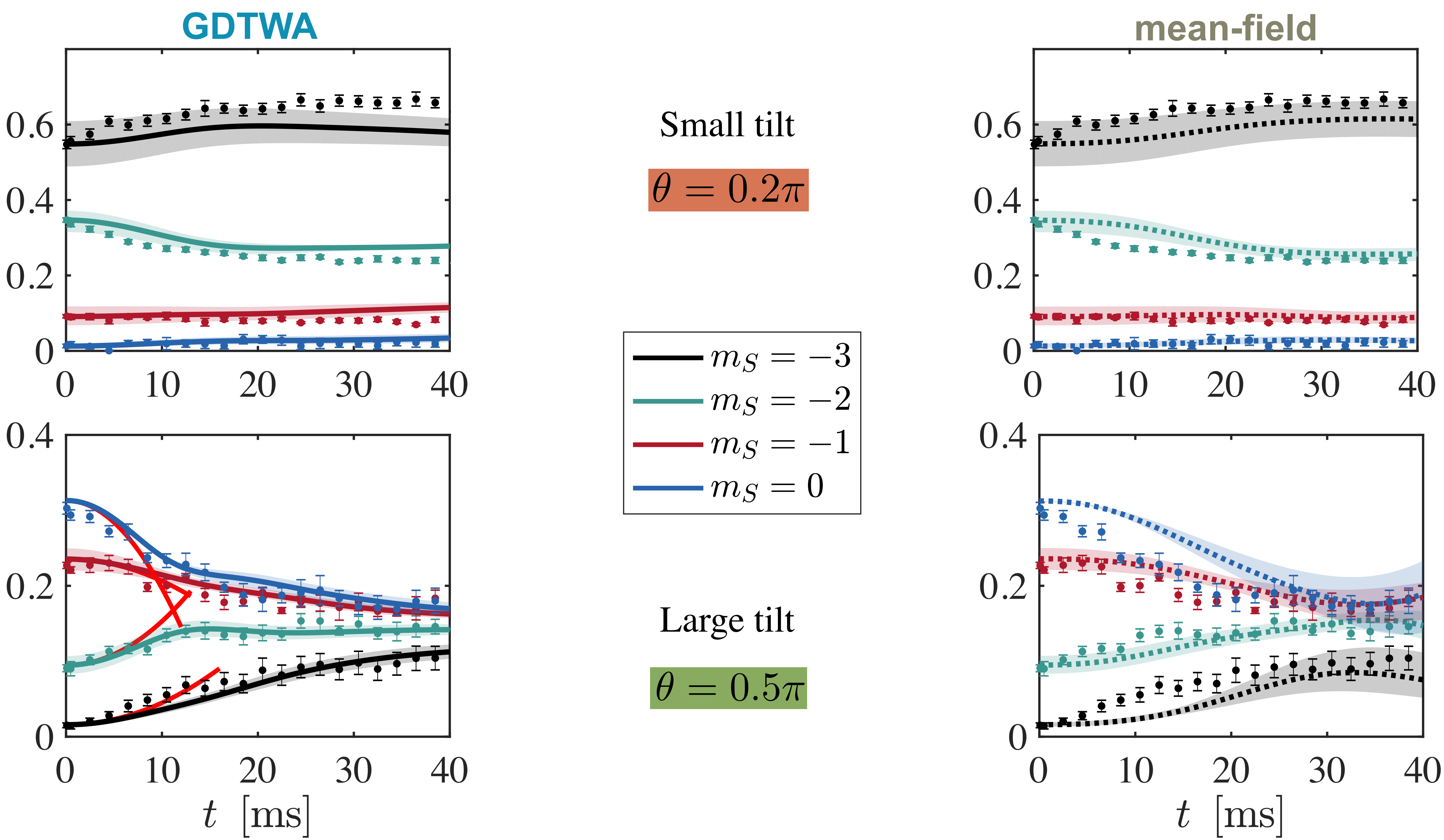
Measure Zeeman state populations

Measure evolution for different tilt angles

$$\theta = 0.2\pi, 0.3\pi, 0.4\pi, 0.5\pi$$

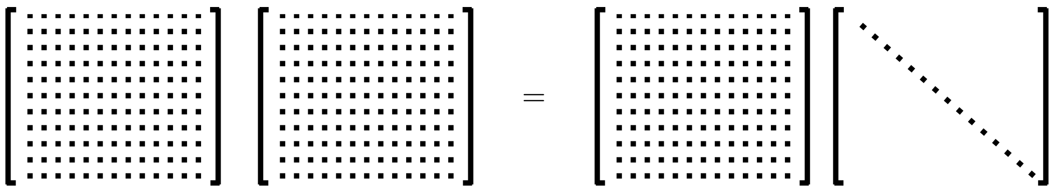
Lecture 3.4 - DTWA application examples - the GDTWA

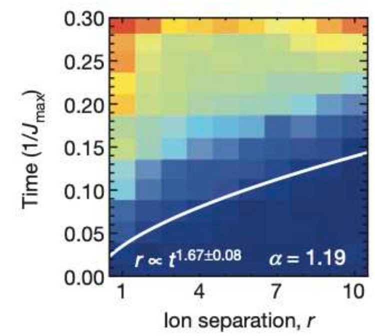
S. Lepoutre, JS, L. Gabardos, B. Zhu, B. Naylor, E. Maréchal, O. Gorceix, A. M. Rey, L. Vernac, and B. Laburthe-Tolra, Nat. Comm. 10, 1714 (2019)

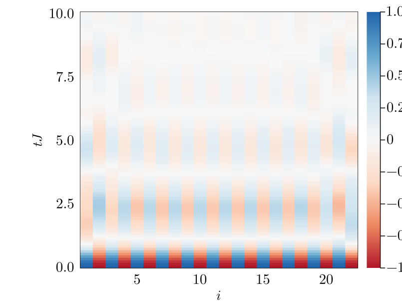


Full recap

- We covered some basics on fundamental numerical tools for solving ODEs (Runge-Kutta) or linear Schrödinger equations (Krylov space).







- With some easy tricks, without advanced stuff, ~20-30 spins are easily doable as laptop science

- We introduced the phase space description of quantum mechanics.

Hilbert space $\Longleftrightarrow$ **Phase space**

$$\hat{O} = \int dx dp\, O_W(x,p)\hat{A}(x,p)$$

$$O_W(x,p) = \frac{1}{\mathcal{N}}\,\mathrm{tr}\left[\hat{A}(x,p)\hat{O}\right]$$

Bopp representation

$$\hat{x} \to x + \frac{\mathrm{i}}{2}\frac{\partial}{\partial p}$$

$$\hat{p} \to p - \frac{\mathrm{i}}{2}\frac{\partial}{\partial x}$$

- We introduced the phase space description of quantum mechanics.

- Dynamics of Weyl symbols is described by Moyal brackets

  (equivalent to a commutator on phase space)

$$\frac{d}{dt}O_W = \{O_W, H_W\}_{\mathrm{MB}}$$

$$\{O_W, O'_W\}_{\mathrm{MB}} \equiv \frac{2}{\hbar}O_W \sin\left[\frac{\hbar}{2}\mathbf{\Lambda}\right] O'_W$$

- Expansion of the Moyal bracket for $\frac{\hbar}{2} \to 0$

$$\frac{d}{dt}O_W \approx \{O_W, H_W\} - \frac{\hbar^2}{24}\{O_W, H_W\}^3 + \mathcal{O}\left(\frac{\hbar^4}{4!2^4}\right)$$

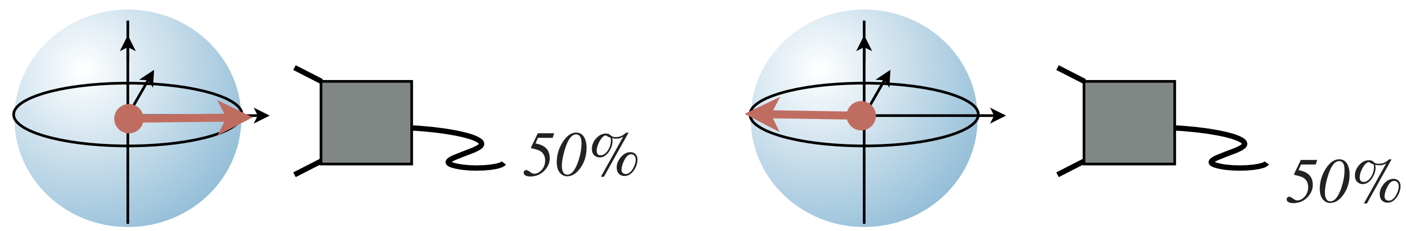
- TWA implies classical equations for the Weyl symbols, which means that Weyl symbols remain factorized ad all times

$$(\hat{O}_{x^n p^m})_W(t) = (\hat{x})^n_W(t)(\hat{p})^m_W(t)$$

Full recap

- We discussed phase space approximations for spins. Continuous Wigner functions are simply not good for models with small spin S=1/2. Instead, **discrete Wigner functions** can perfectly reproduce all possible measurements for any spin-observable on product spin states (assuming some restrictions on states).

$$
\begin{aligned}
W(+1,+1,-1) &= 1/4\\
W(-1,+1,-1) &= 1/4\\
W(+1,-1,-1) &= 1/4\\
W(-1,-1,-1) &= 1/4
\end{aligned}
$$



$$\langle \hat{O}_{\prod_i x_i^n y_i^m z_i^l} \rangle = \prod_i \langle \hat{O}_{x_i^n y_i^m z_i^l} \rangle = \prod_{i=1}^{N} \sum_{x_i, y_i, z_i = \pm 1} W_i(x_i, y_i, z_j) x_i^n y_i^m z_i^l$$

JS, A. Pikovski, and Ana Maria Rey, Phys. Rev. X 5, 011022 (2015)

B. Zhu, A. M. Rey, and JS, New J. Phys. 21, 082001 (2019)

- Using this discrete sampling in combination with the TWA is called the **discrete TWA (DTWA)** for spin-1/2 models. For models with arbitrary local discrete levels (e.g. for multi-level atoms) it is known as **generalized DTWA (GDTWA)**.

- DTWA codes are very easy to write and we demonstrated the simulation idea for a long-range Ising model.

- In general (G)DTWA can given excellent predictions when compared to other methods. It has been used to describe results for far-from-equilibrium dynamics in several cold atom experiments, also in limits where no other methods worked (3D and long-range models).