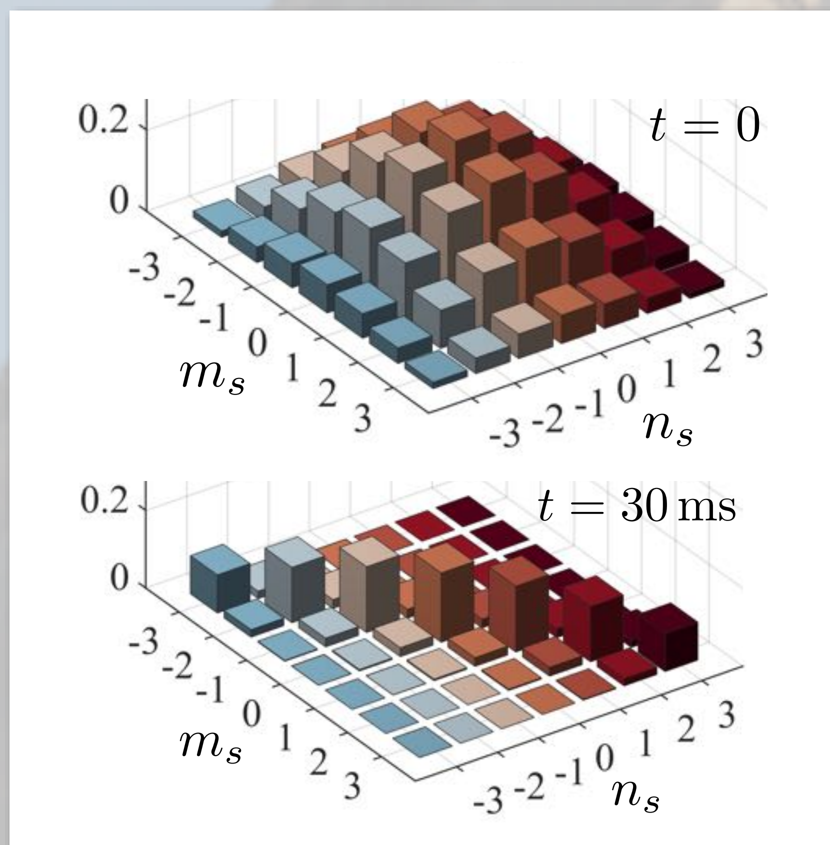
Numerical simulations of ultra-cold atom experiments: Applications to molecular polaritonics?

Johannes Schachenmayer



"A generalized phase space approach for solving quantum spin dynamics", arXiv:1905.08782

"Out-of-equilibrium quantum magnetism and thermalization in a spin-3 many-body dipolar lattice system", Nat. Comm. 10, 1714 (2019)

Collaborators - Theory & Experiment

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IPCMS

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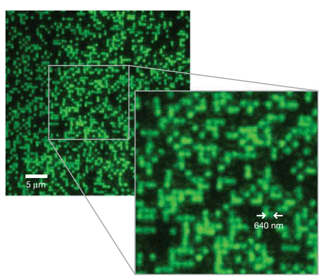
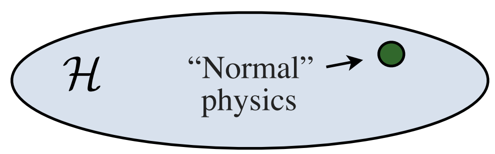
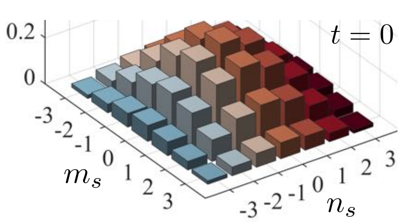
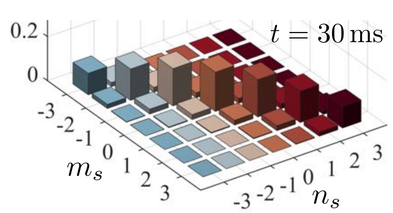
Outline





Overview:
Ultra-cold atom physics and numerical simulations



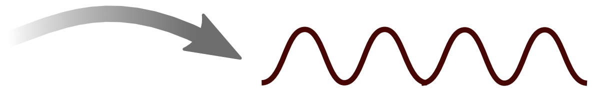


Semi-classical phase-space method:
The generalized discrete truncated Wigner approximation

Ultra-cold atoms in optical lattices

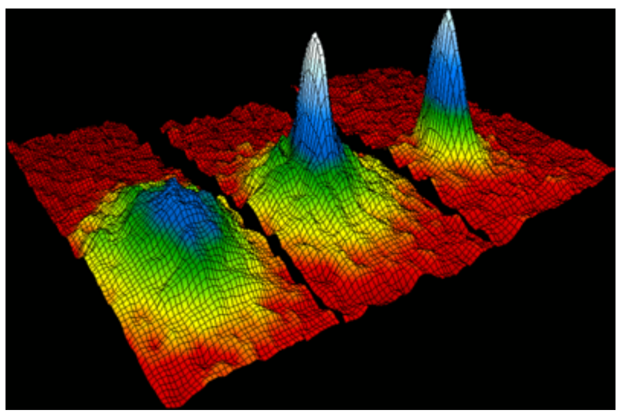
Ultra-Cold gases

Standing laser wave



Optical Lattice

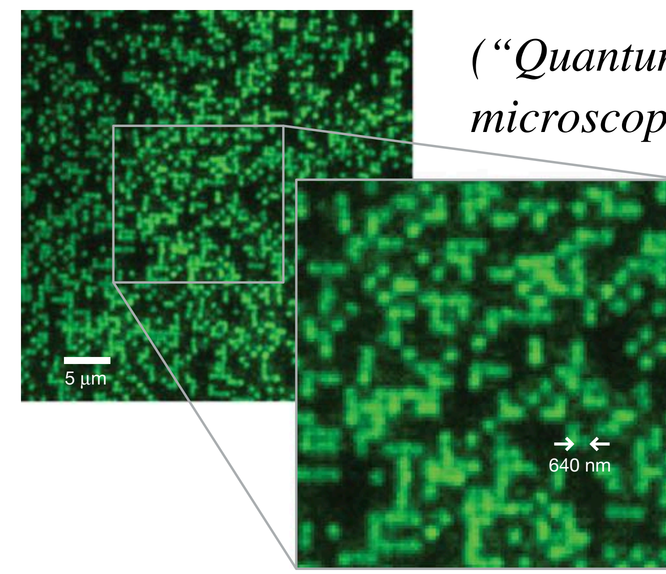
- *Weakly interacting* (Bosons/Fermions)



(First BEC in 1995)

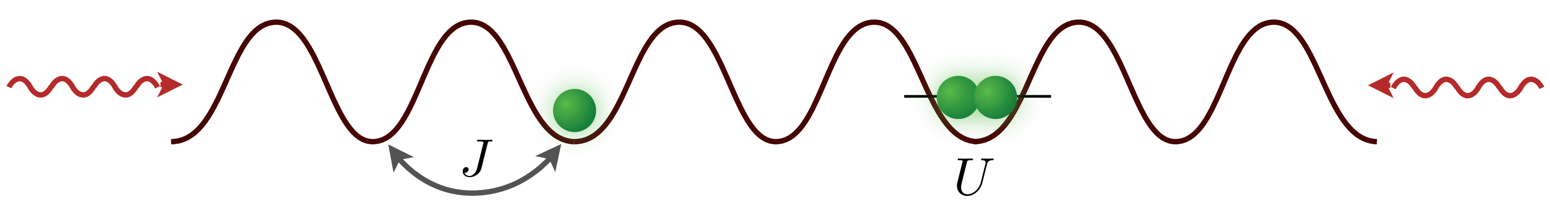
- *Strongly interacting* lattice models

(Optical lattices ~2002)



("Quantum gas microscopes" ~2009)

- e.g.: Bose-Hubbard model $\hat{H} = -J \sum_{\langle i,j \rangle} \hat{b}_i^\dagger \hat{b}_j + \frac{U}{2} \sum_i \hat{n}_i (\hat{n}_i - 1)$



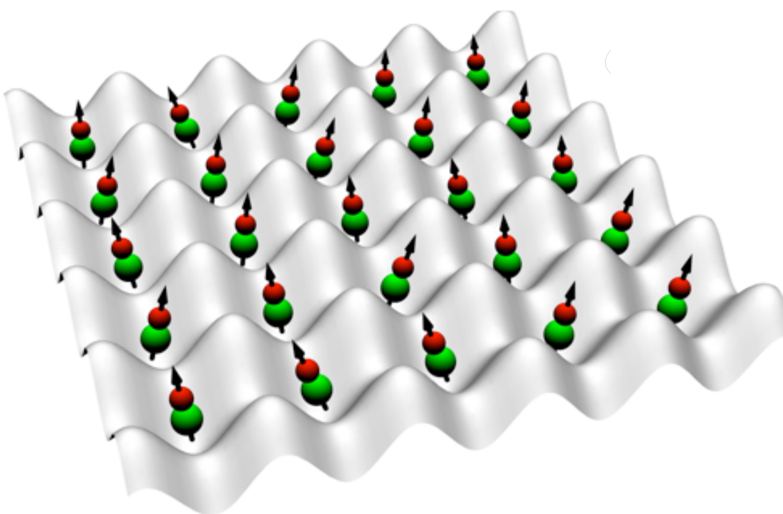
Experiments: *Munich, Harvard/MIT, Zürich, Innsbruck, Glasgow, Paris, JILA, Innsbruck, Hamburg, Okazaki, Pisa, Florence, Oxford, Cambridge, Austin, Chicago, Penn State, Kyoto, Toronto, Stony Brook, Illinois, ...*

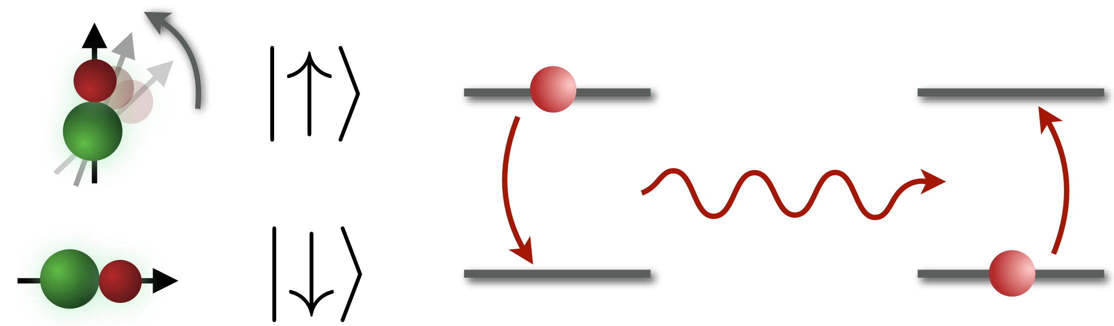
- Idea: Emulating models for condensed matter?

Spin-models with ultra-cold atoms

- Polar molecules in optical lattices

(Experiment: 2013 Boulder, Theory: 2006 Innsbruck) KRb





Spin exchange interaction

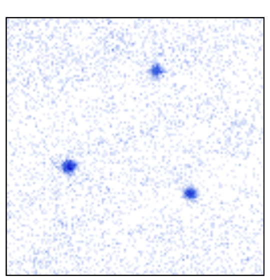
XY **Ising**

- Quantum spin-models

$$\hat{H} = \frac{1}{2}\sum_{i\neq j}\left[J_{ij}^{\perp}(\hat{\sigma}_i^x\hat{\sigma}_j^x + \hat{\sigma}_i^y\hat{\sigma}_j^y) + J_{ij}^z\hat{\sigma}_i^z\hat{\sigma}_j^z\right]$$

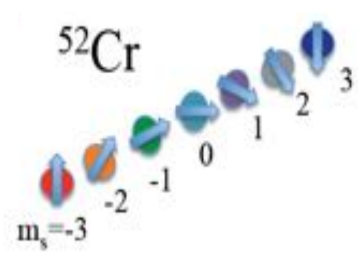
- Also:

Rydberg atoms



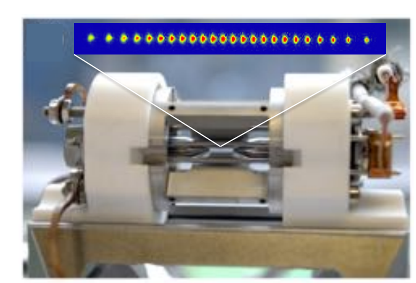
Munich, Paris,
Strasbourg (S. Whitlock), Okazaki, …

Magnetic atoms



Paris, Innsbruck, Stuttgart, …

Trapped ions



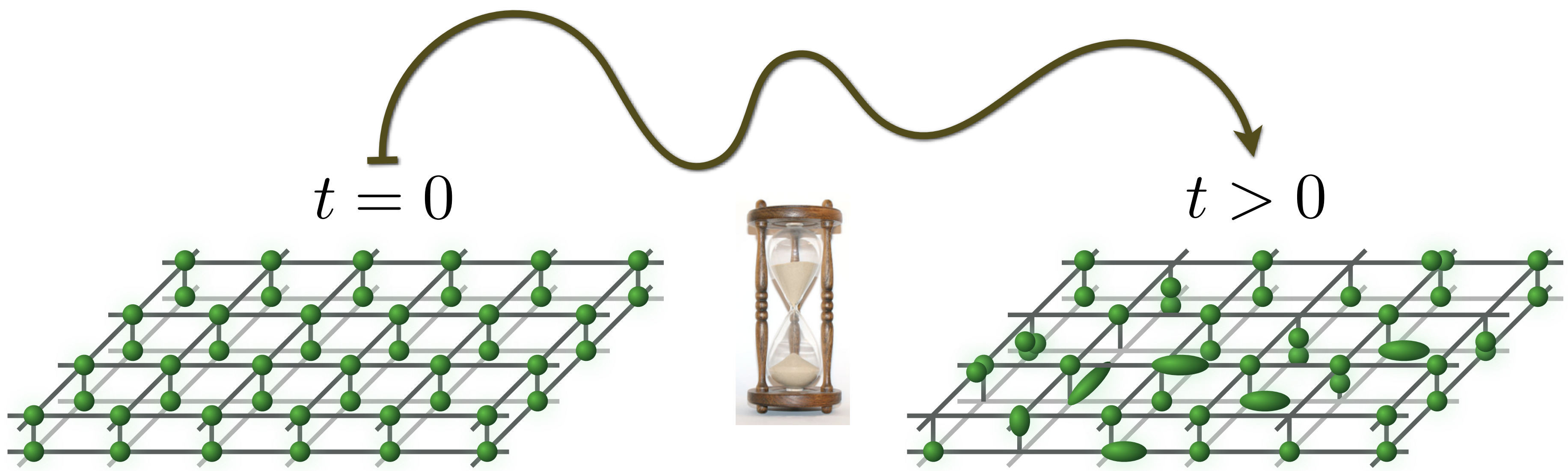
Innsbruck, Maryland, Boulder, …

…

Non-equilibrium dynamics in quantum many-body models

- Ultra-cold atom experiments are: **Well-isolated, controllable,** and have **low interaction energies**

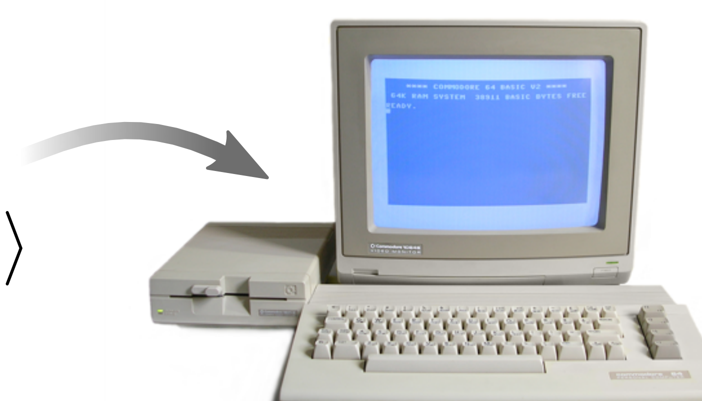
Experimental access to non-equilibrium dynamics in many-body models!



- Our interest:

Numerical simulations on computers?

$e^{-it\hat{H}}|\psi_0\rangle$

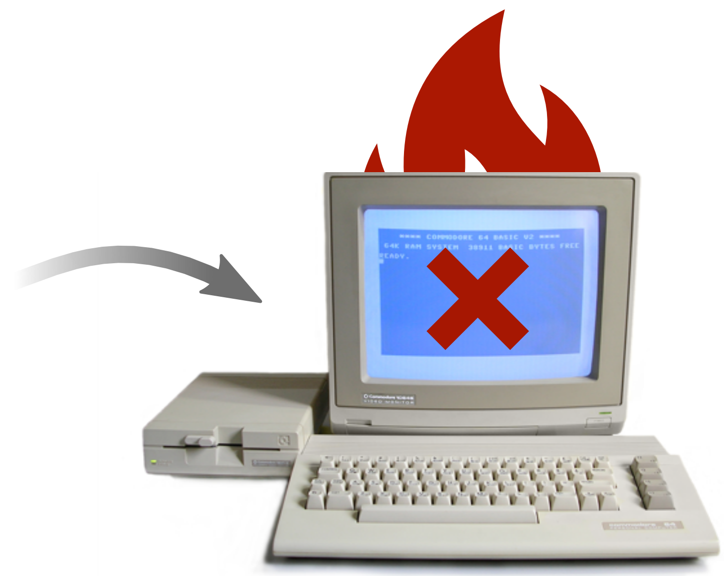


- Why?

Fundamental question

When do simulations on classical computers become **impossible**?

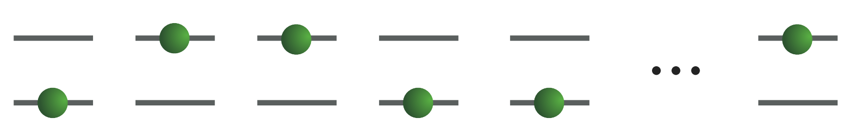
$e^{-\mathrm{i}t\hat{H}}|\psi_0\rangle$



Hilbert space

$|\psi\rangle \in \mathcal{H}$

$\dim(\mathcal{H}) = 2^N$

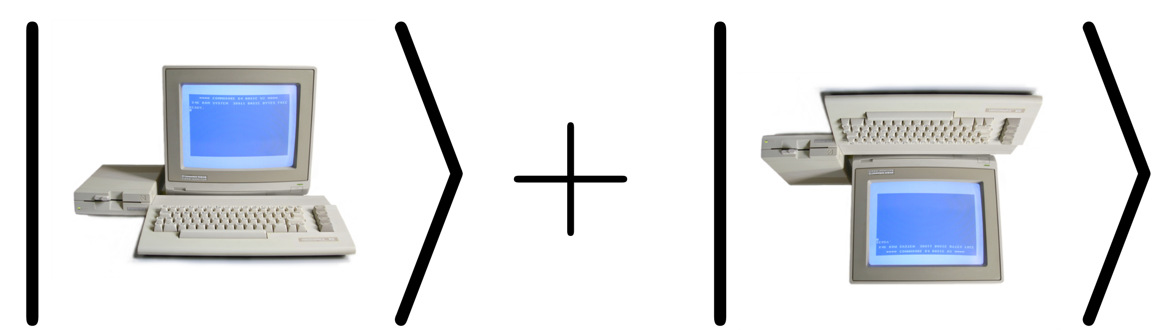


1 ... *N = 300*

$\sim 10^{82}$ gigabyte

Atoms in universe: $\sim 10^{80}$

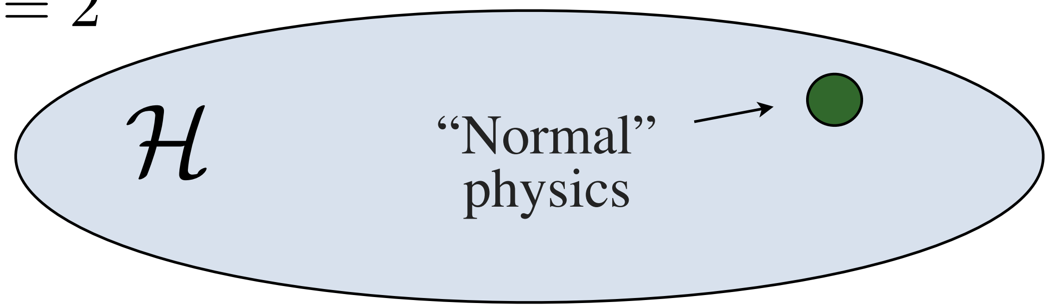
- When do we need a quantum computer?



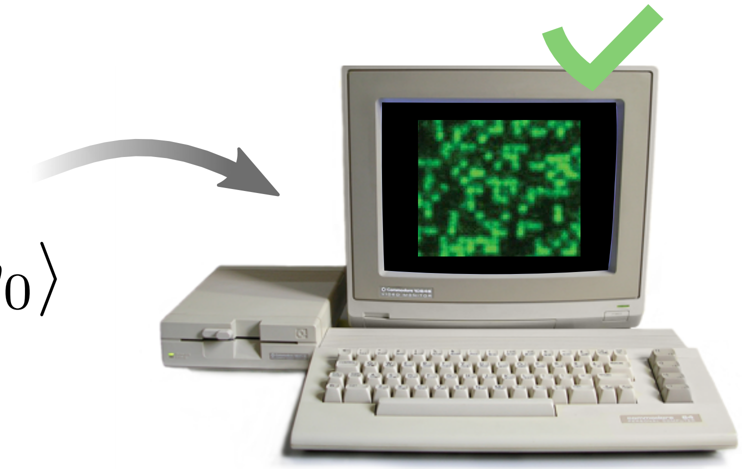
Matrix product states

- Most of the time a classical computer is just fine!

$$\dim(\mathcal{H}) = 2^N$$



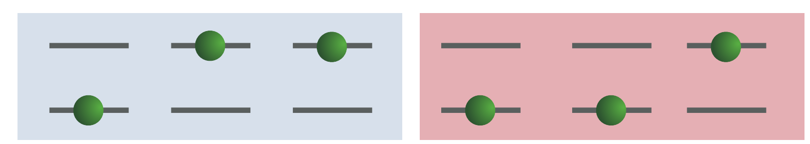
$$e^{-it\hat{H}}|\psi_0\rangle$$



- Bipartite entanglement:

$|\psi_A\rangle$ $|\psi_B\rangle$

$$|\psi\rangle =$$



Product state $|\psi\rangle = |\psi_A\rangle|\psi_B\rangle$

Entangled state $|\psi\rangle \neq |\psi_A\rangle|\psi_B\rangle$

Matrix product state

$D \times D$ *matrix*

$$|\psi_{\mathrm{PS}}\rangle \approx |\psi_1\rangle|\psi_2\rangle \ldots |\psi_N\rangle$$

$$|\psi_{\mathrm{MPS}}\rangle \approx \left(|\psi_1^{11}\rangle \quad |\psi_1^{12}\rangle\right) \begin{pmatrix} |\psi_2^{11}\rangle & |\psi_2^{12}\rangle \\ |\psi_2^{21}\rangle & |\psi_2^{22}\rangle \end{pmatrix} \begin{pmatrix} |\psi_3^{11}\rangle & |\psi_3^{12}\rangle \\ |\psi_3^{21}\rangle & |\psi_3^{22}\rangle \end{pmatrix} \ldots \begin{pmatrix} |\psi_N^{11}\rangle \\ |\psi_N^{21}\rangle \end{pmatrix}$$

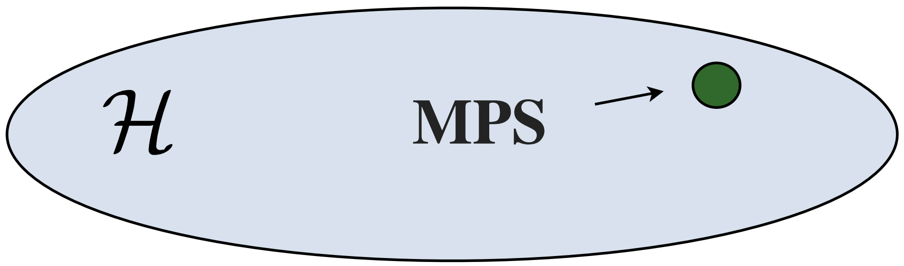
*2N parameters, **no** entanglement*

*$2ND^2$ parameters, **some** entanglement, **exact** if not much entanglement*

- **Fundamental question:** *In the dynamics, how does entanglement build-up?*
- [Our contributions: *Phys. Rev. Lett. 109, 020505 (2012), Phys. Rev. X 3, 031015 (2013), Phys. Rev. A 93, 053620 (2016)*]

Problem: Higher dimensions?

- MPS (more general "tensor network state") methods have been extensively studied and used:

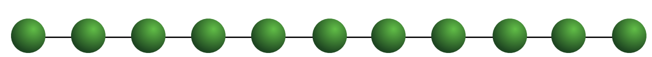


Algorithms: (t-)DMRG, TEBD, TDVP, …

S. R. White,, Phys. Rev. Lett. 69, 2863 (1992)
G. Vidal, Phys. Rev. Lett. 93, 040502 (2004)
S. R. White et al., Phys. Rev. Lett. 93, 076401 (2004)
A. J. Daley et al., J. Stat. Mech P04005 (2004)

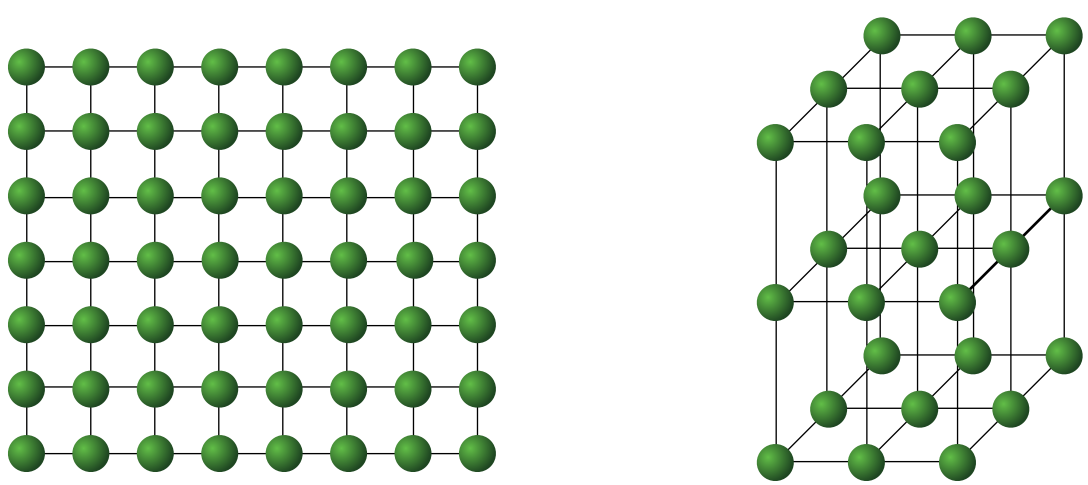
Reviews: U. Schollwöck, Ann. Phys. 326, 96 (2011)
R. Orús, Ann. Phys. 349, 117 (2014)

- **Problem:**



These methods only work efficiently in **1D**!

- Higher dimensions?



Important challenge!

Conceptually also higher dimensions are not problem:

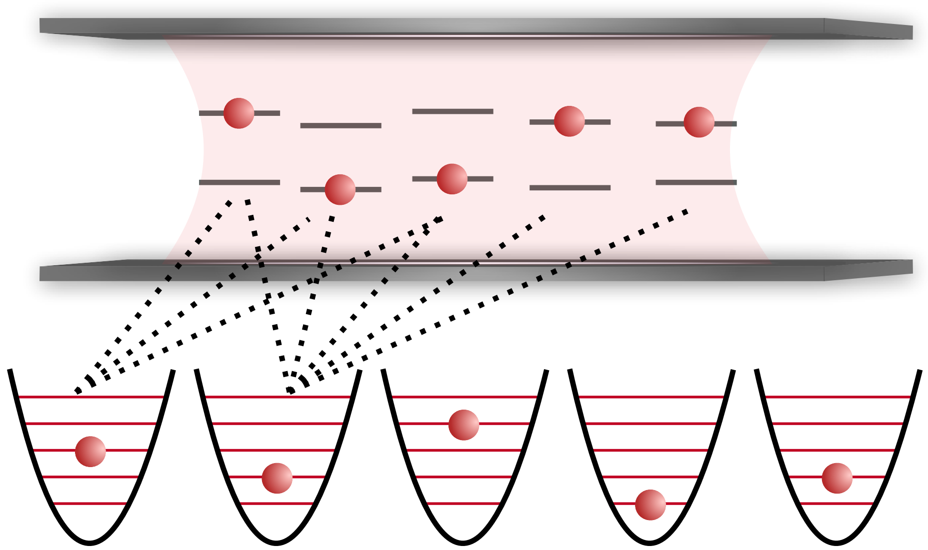
Projected entangled pair states (PEPS)

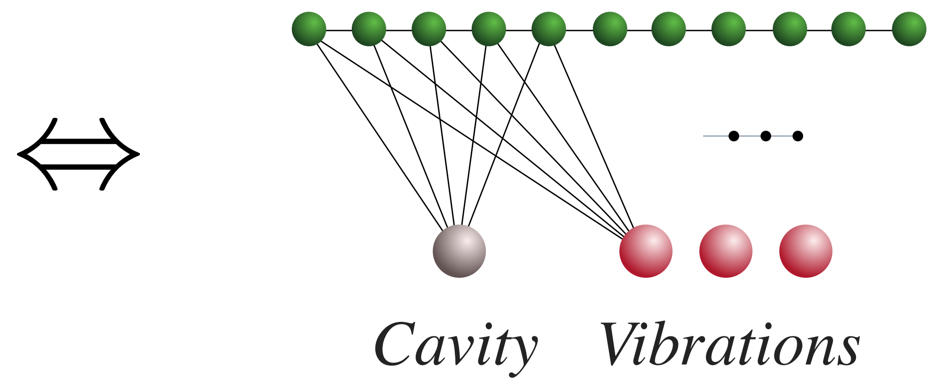
F. Verstraete, J. I. Cirac, arXiv:cond-mat/0407066 (2004)
F. Verstraete, J. I. Cirac, V. Murg, Adv. Phys. 57,143 (2008)

In practice: Not very efficient.

Spin-Boson models

- Tensor networks can be also useful for **cavity coupled molecular materials?**
  Important role of couplings to cavities and vibrations!

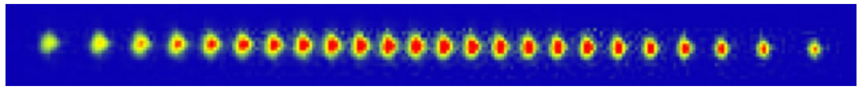




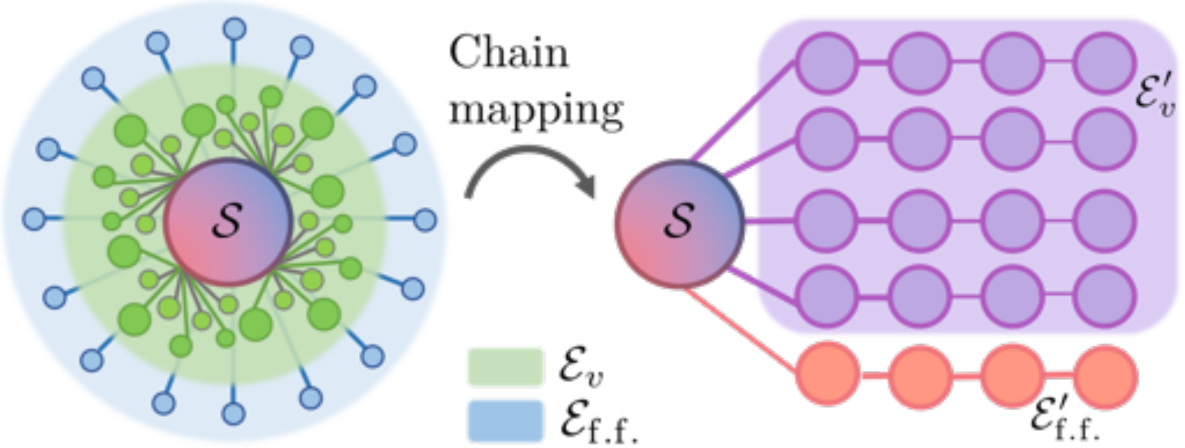
Similar to high-dimensional lattices

- MPS simulations of Spin-Boson models for **trapped ions:**

M. L. Wall, A. Safavi-Naini, A. M. Rey
Phys. Rev. A 94, 053637 (2016)



- For molecular polaritonics:

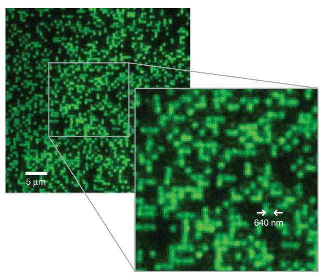
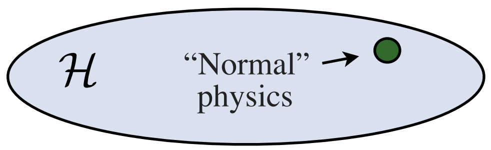


J. del Pino, F. A. Y. N. Schröder, A. W. Chin,
J. Feist, and F. J. Garcia-Vidal
Phys. Rev. Lett. 121, 227401 (2019),
Phys. Rev. B 98, 165416 (2018)

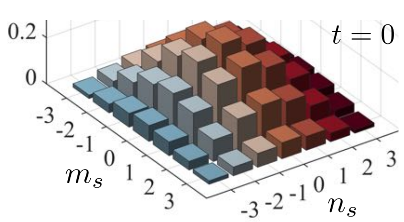
… systems (S) still have to be considered low-dimensional (few excitations or 1D)

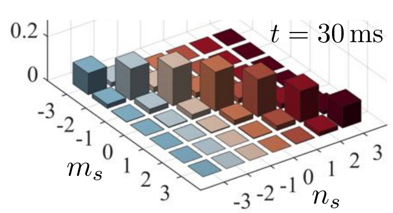
- **TEMPO:** A. Strathearn, P. Kirton, D. Kilda, J. Keeling, B. W. Lovett, *Nat. Comm. 9, 3322 (2018)*

Outline

Overview:
Ultra-cold atom physics and numerical simulations





Semi-classical phase-space method:
The generalized discrete truncated Wigner approximation

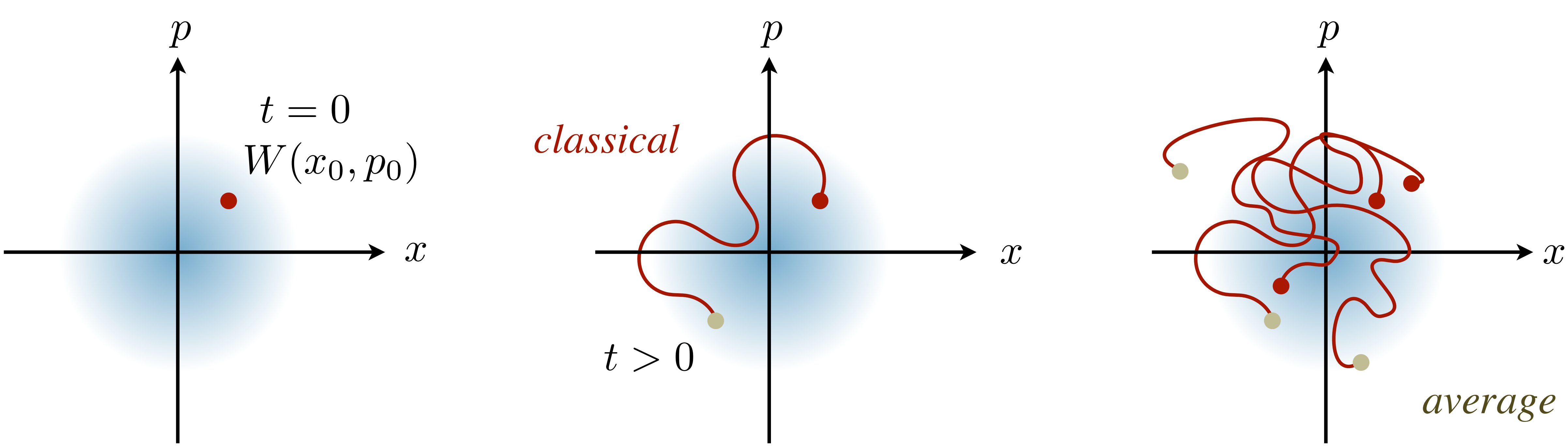
The truncated Wigner approximation (TWA)

- A semi-classical phase-space method:

Hilbert space	$\Leftrightarrow$	**Phase space**
Density matrix $\hat{\rho}$		*Wigner function* $W(x,p)$

- Exact dynamics in phase space is also complicated … but **TWA approximation:**

R. Graham, *Springer Tracts in Modern Physics*, **66**, (1973) A. Polkovnikov, *Ann. Phys.*, 325, 1790 (2010)
P. B. Blakie et al., *Adv. Phys.*, 57, 363 (2008)



- Classical dynamics, but quantum fluctuations of initial state are included.

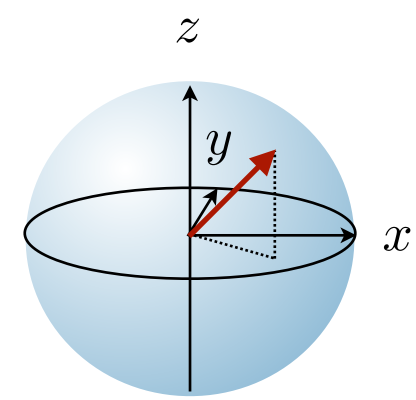
Phase-space of a two-level system?

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

- **Phase-space of a two-level system?**

$$\hat{\rho} = \frac{1}{2}\left(\mathbb{1} + \boldsymbol{r}\cdot\hat{\boldsymbol{\sigma}}\right) \Longleftrightarrow$$

Spin S = 1/2 Hilbert space

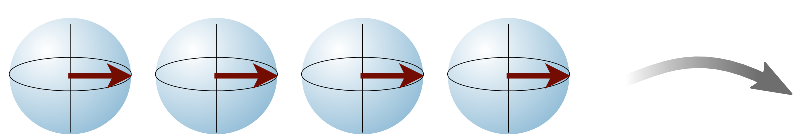


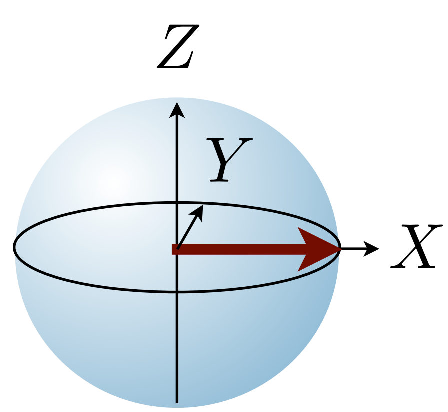
3D spin-components as phase space

$$\boldsymbol{r} = (x, y, z)$$

- **Wigner function?** *For S ≫ 1/2 the Wigner function can be approximated by a* ***Gaussian***

- Example:



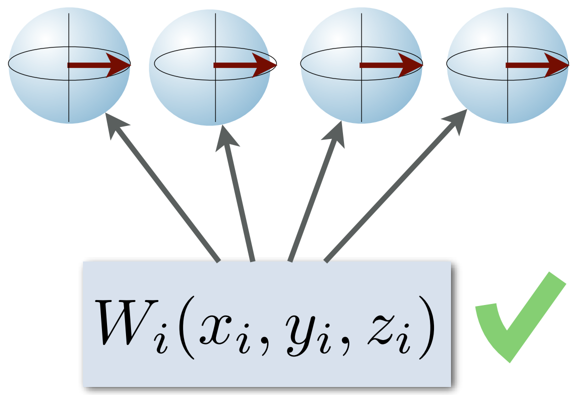


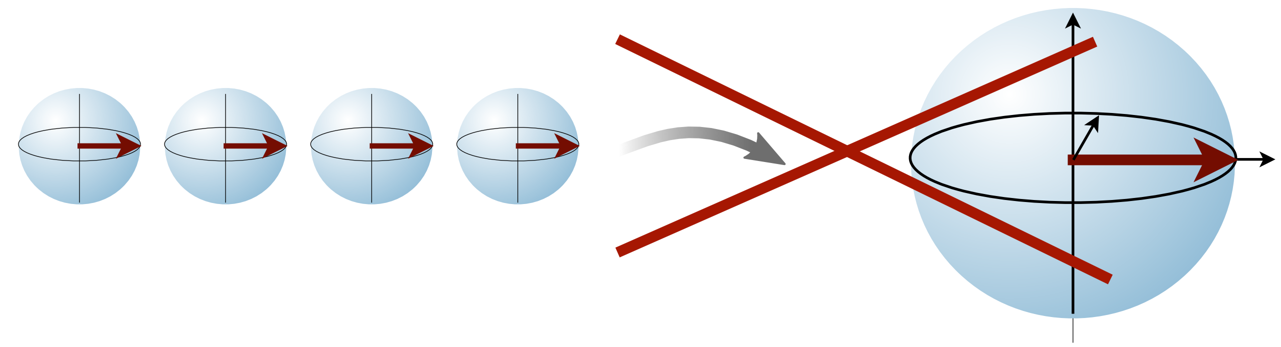
$$W(X,Y,Z) \propto \delta(X - S)e^{-(Y^2+Z^2)/S}$$

Collective state of many spin-1/2s pointing along "x"

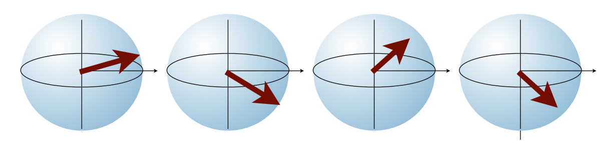
Review: A. Polkovnikov, *Ann. Phys.*, 325, 1790 (2010)

Sampling from a discrete distribution



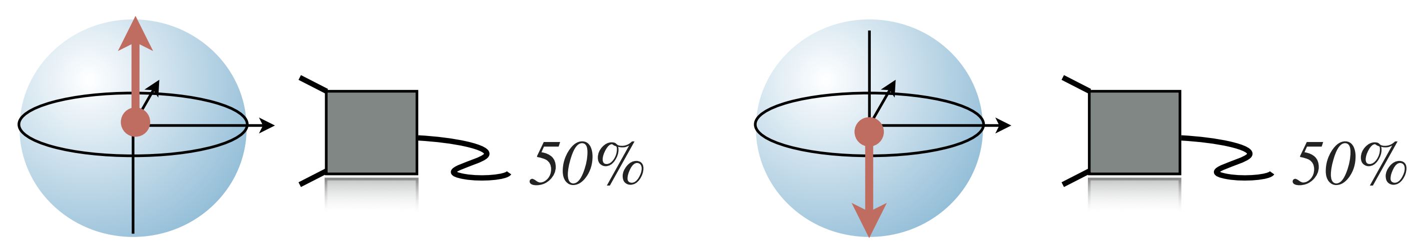


Sample quantum noise of each spin-1/2 individually!



- **Which Wigner function for a single spin?** (Gaussian not so good)

- The true quantum noise is discrete!



Uniform discrete sampling from $y_j, z_j \in \{-1, 1\}$ *reproduces exact quantum uncertainty*

- **Our proposal:** Do not use a Gaussian, but a discrete sampling!

Discrete truncated Wigner approximation (DTWA)

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

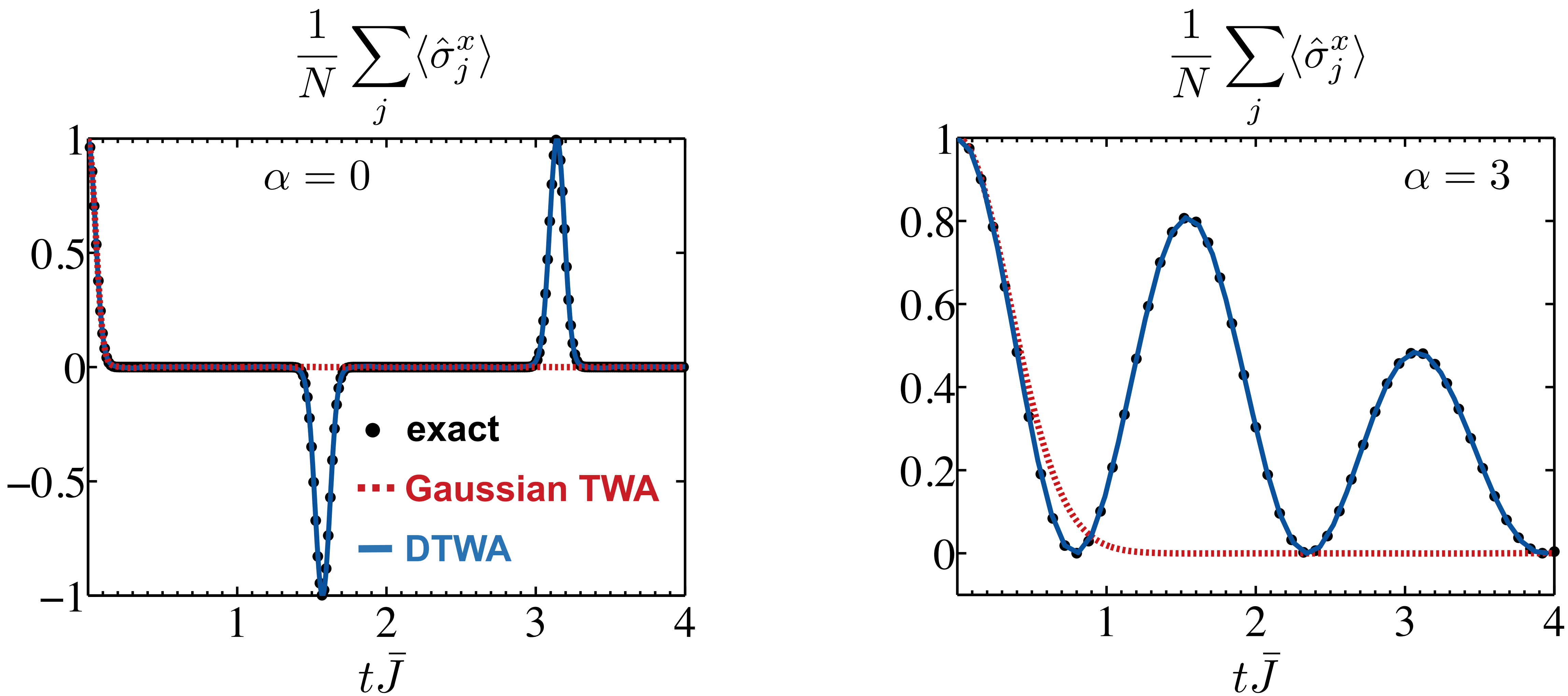
Benchmark: Ising couplings

- Initial state: $|\psi_0\rangle = \prod_j^N |\rightarrow\rangle_j$

Ising

$$\hat{H} = \sum_{i>j}^{N} \frac{J}{|i-j|^\alpha} \hat{\sigma}_j^z \hat{\sigma}_j^z$$

1D, N = 100



DTWA is *exact* for Ising couplings!

(… for this observable, analytical proof)

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

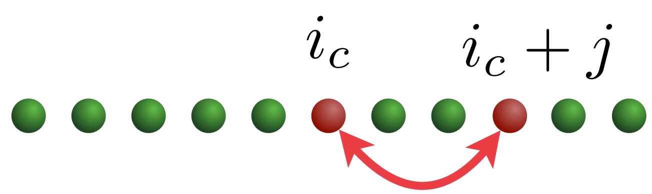
Benchmark: XY couplings

- **One dimension:**

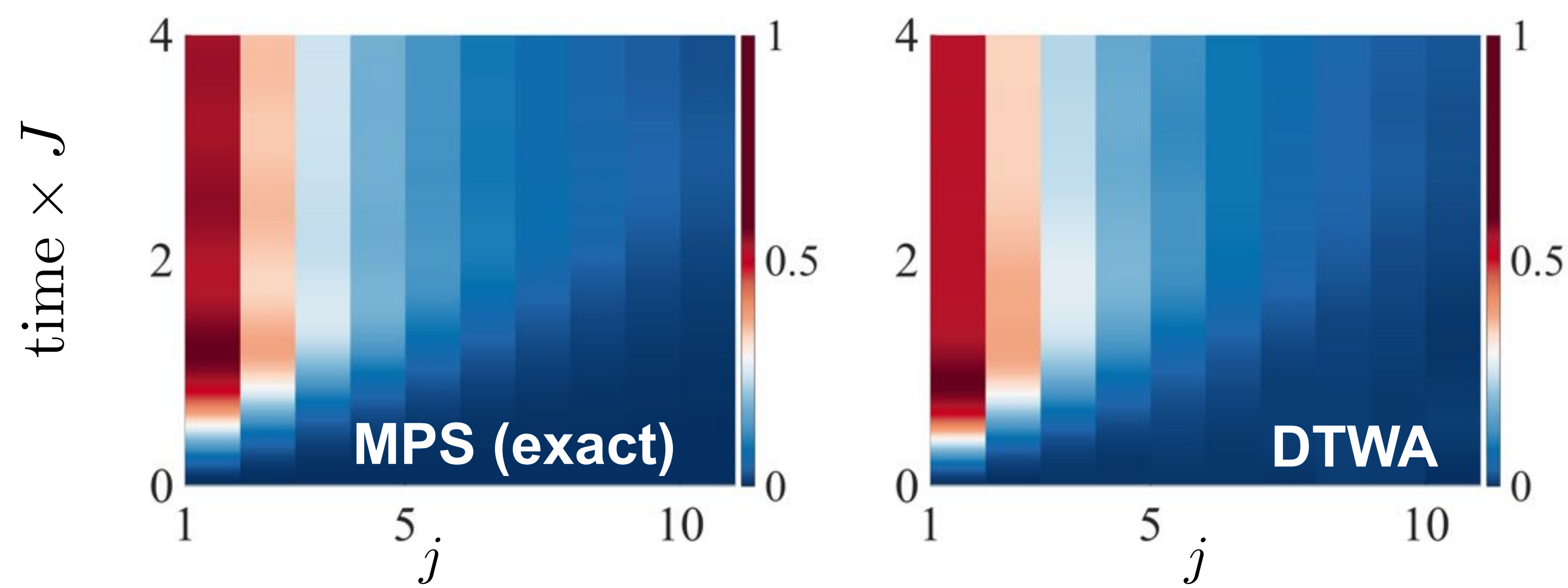
XY

$$\hat{H} = \frac{1}{2}\sum_{i\neq j}\frac{J}{|i-j|^3}(\hat{\sigma}_i^x\hat{\sigma}_j^x + \hat{\sigma}_i^y\hat{\sigma}_j^y)$$

1D, N = 100



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



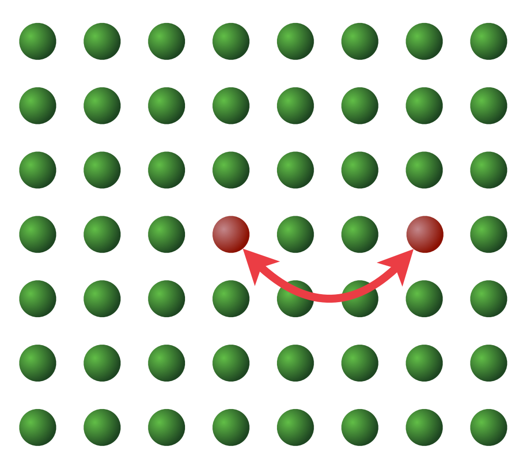
- Computationally, the DTWA is **cheap**:

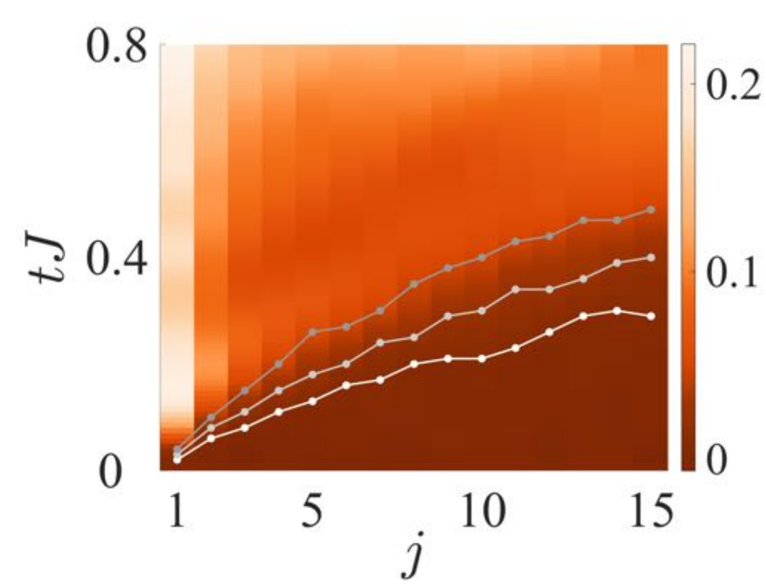
3N nonlinear equations

10 000 spins no problem!

- **Two dimensions:**

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



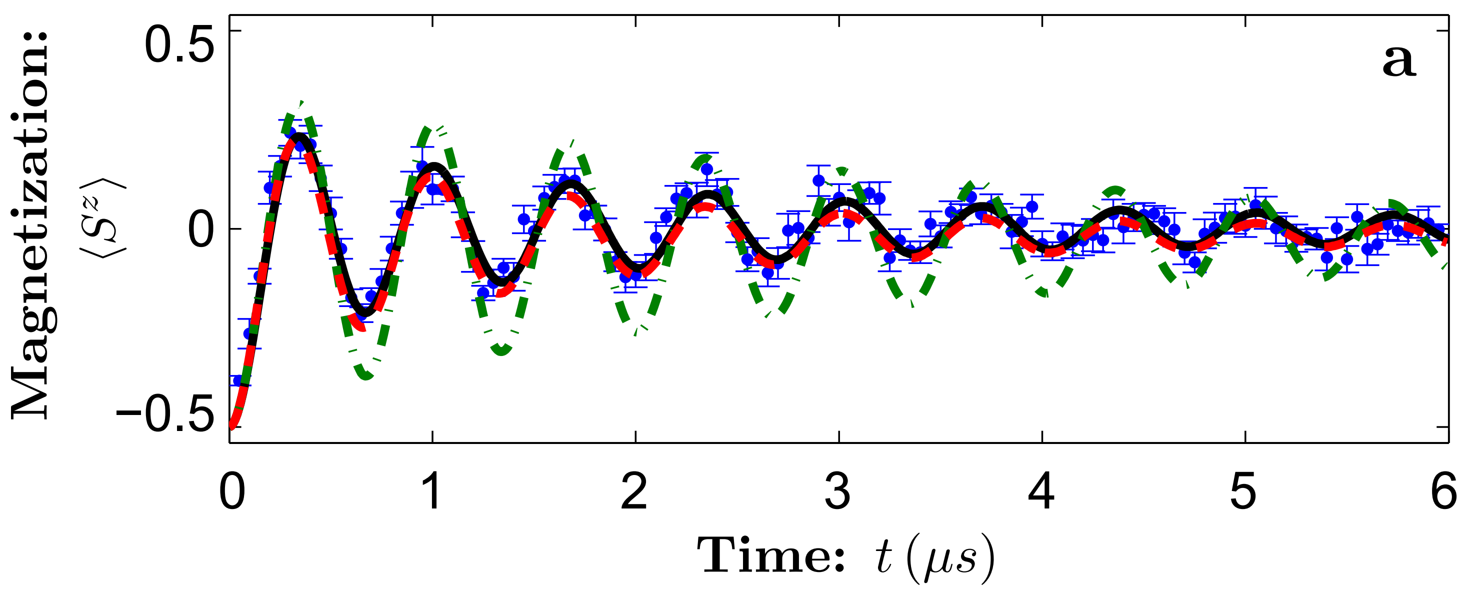


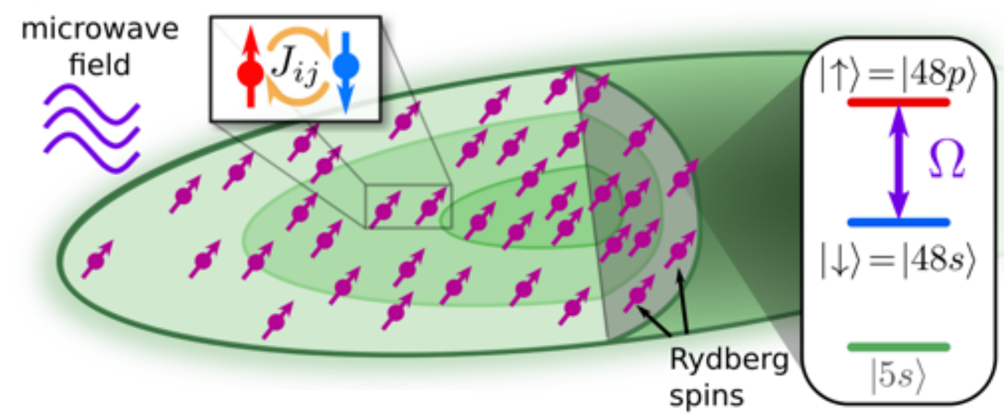
Successful applications of the DTWA (examples)

- DTWA modeling of Rydberg experiment in Heidelberg:

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

green: mean-field, red: DTWA





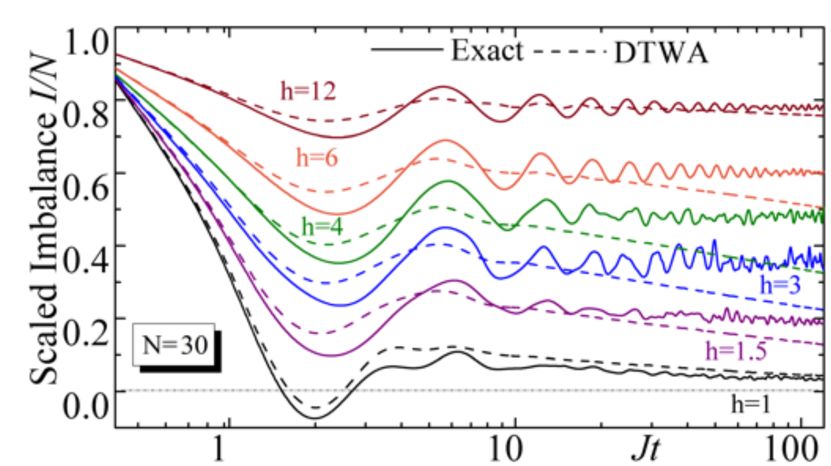
Weidemüller/Whitlock

- New theory insight into thermalization dynamics of spin-models with the DTWA:

S. Czischek, M. Gärttner, M. Oberthaler, M. Kastner, T. Gasenzer, Quantum Science and Technology 4, 014006 (2018)

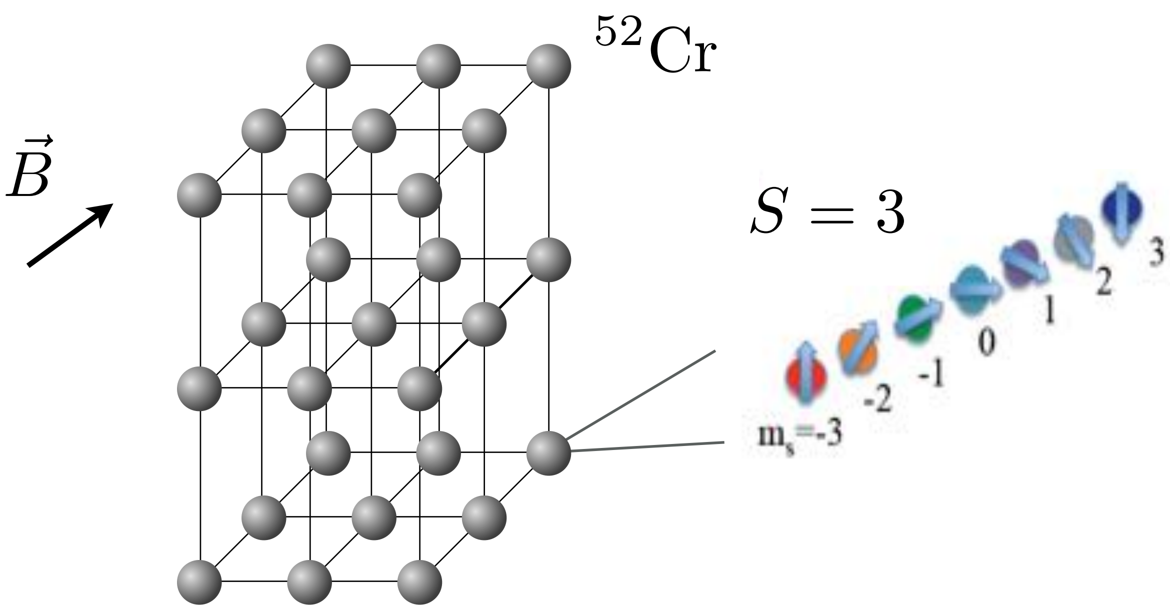
O. L. Acevedo, A. Safavi-Naini, JS, M. L. Wall, R. Nandkishore, and A. M. Rey, Phys. Rev. A 96, 033604 (2017)

L. Pucci, A. Roy, and Michael Kastner, Phys. Rev. B 93, 174302 (2016)



The Paris Chromium experiment — larger spins

- Chromium atoms trapped in (anisotropic) 3D optical lattice:



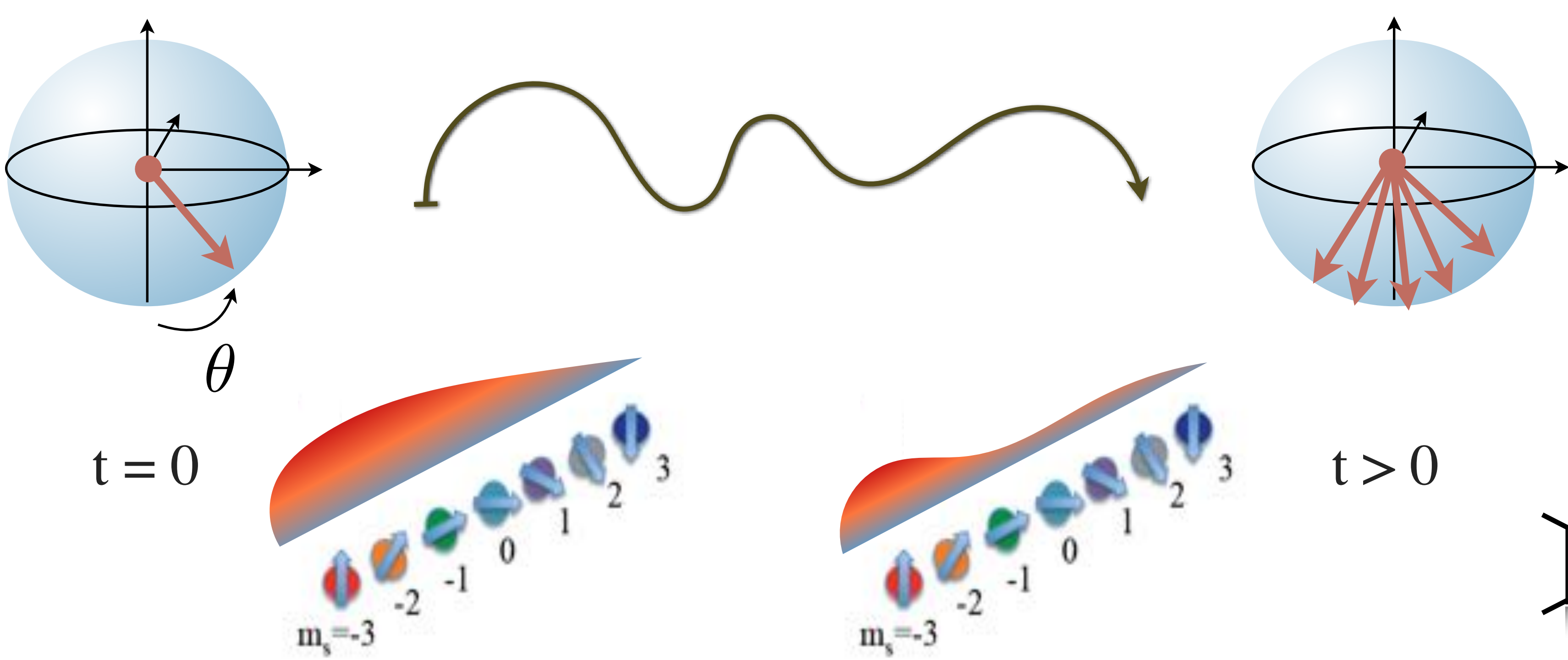
Magnetic dipole-dipole couplings

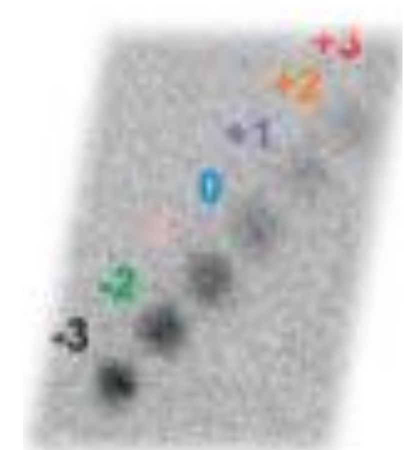
Spin S = 3 operators

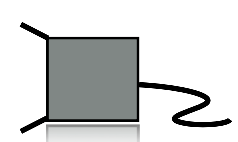
$$\hat{H} = \sum_{i>j} V_{ij} \left[\hat{S}_i^z \hat{S}_j^z - \frac{1}{2} \left(\hat{S}_i^x \hat{S}_j^x + \hat{S}_i^y \hat{S}_j^y \right) \right]$$

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

- Time evolution after initial tilt







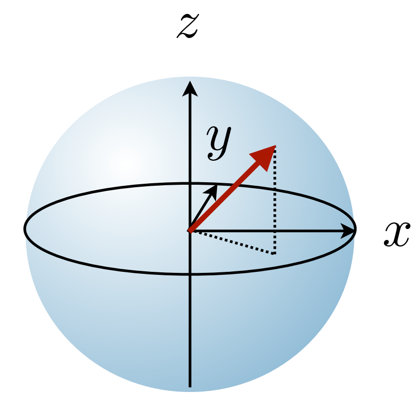
Measure Zeeman state populations

TWA for the Paris Chromium experiment?

$$\hat{\rho} = \frac{1}{2}\left(\mathbb{1} + \boldsymbol{r}\cdot\hat{\boldsymbol{\sigma}}\right)$$

Spin S = 1/2 Hilbert space

$\Leftrightarrow$



3D spin-components as phase space

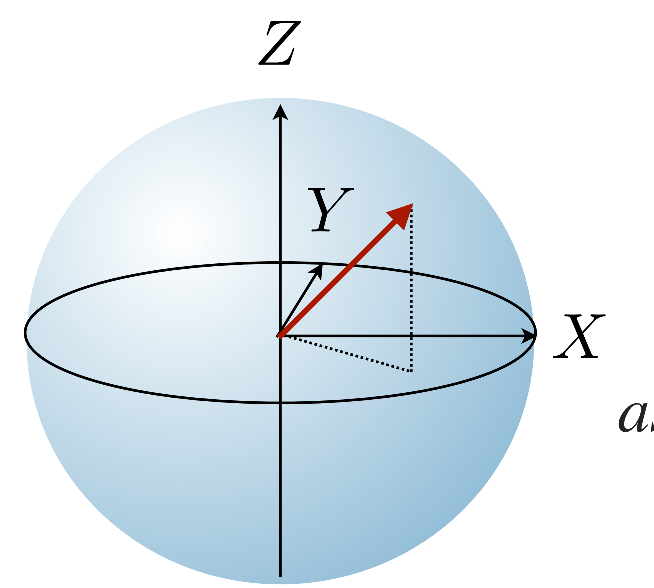
$$\boldsymbol{r} = (x, y, z)$$

- Now we have

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

Spin S = 3 operators

One could use: $\Leftrightarrow$



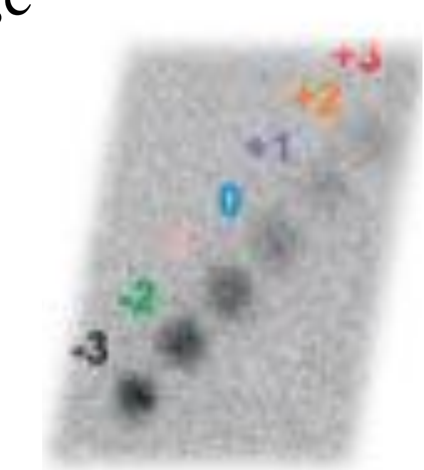
3D spin-3 components as phase space

- A Gaussian Wigner function can describe the initial state well since *S* is “large”

- **But:**

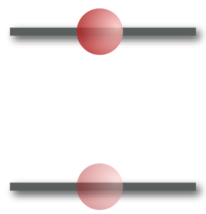
$$\hat{\rho} = \begin{pmatrix} \rho_{11} & \rho_{12} & \rho_{13} & \rho_{14} & \rho_{15} & \rho_{16} & \rho_{17} \\ \rho_{21} & \rho_{22} & \rho_{23} & \rho_{24} & \rho_{25} & \rho_{26} & \rho_{27} \\ \rho_{31} & \rho_{32} & \rho_{33} & \rho_{34} & \rho_{35} & \rho_{36} & \rho_{37} \\ \rho_{41} & \rho_{42} & \rho_{43} & \rho_{44} & \rho_{45} & \rho_{46} & \rho_{47} \\ \rho_{51} & \rho_{52} & \rho_{53} & \rho_{54} & \rho_{55} & \rho_{56} & \rho_{57} \\ \rho_{61} & \rho_{62} & \rho_{63} & \rho_{64} & \rho_{65} & \rho_{66} & \rho_{67} \\ \rho_{71} & \rho_{72} & \rho_{73} & \rho_{74} & \rho_{75} & \rho_{76} & \rho_{77} \end{pmatrix} \quad 7\times 7$$

…the experiments accesses the diagonals



…we need more than 3 spin variables.

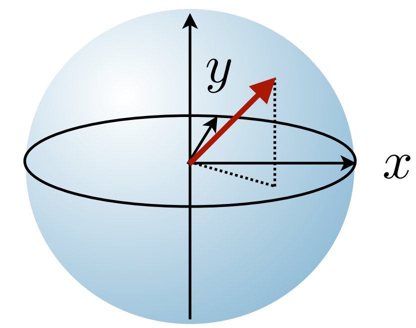
Phase-space for a D-level system



$$\hat{\rho} = \frac{1}{2}\left(\mathbb{1} + \boldsymbol{r}\cdot\hat{\boldsymbol{\sigma}}\right)$$

Spin S = 1/2 Hilbert space

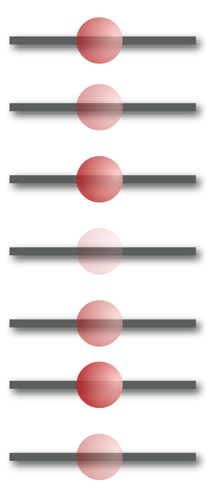
$\Leftrightarrow$



3D spin-components as phase space

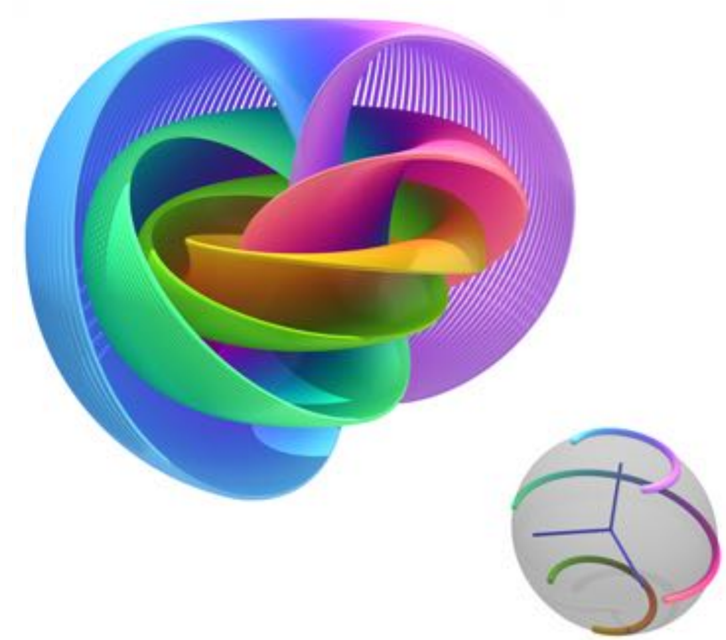
$$\boldsymbol{r} = (x, y, z)$$

- **Instead of a spin-phase space we use:**



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

$\Leftrightarrow$



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

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!

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

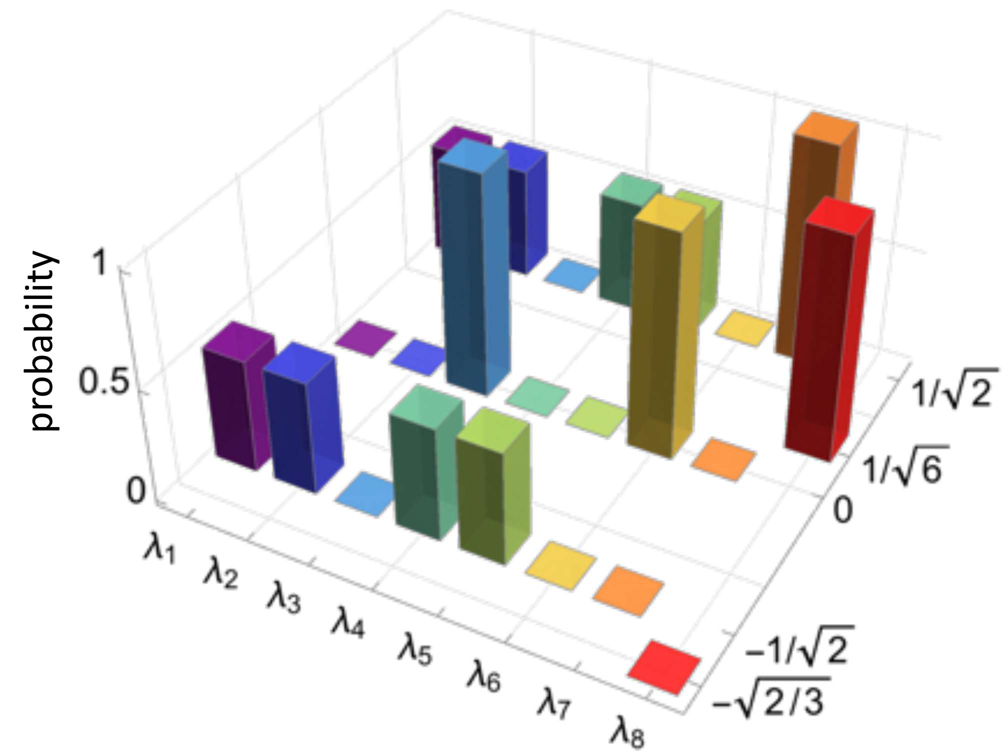
The generalized DTWA (GDTWA)

- For a D-level system:

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

- **1.** Sample a **discrete** probability distribution for the (D^2-1) GGM phase-space variables.

  (does work for most relevant states)



Example for 3-level system

- **2.** Evolve the samples with classical equations

…from a mean-field ansatz: $\hat{\rho}_N = \prod_j^N \hat{\rho}_j(t)$ → $\frac{d}{dt}\boldsymbol{\lambda}_j = \dots$ *48N nonlinear equations*

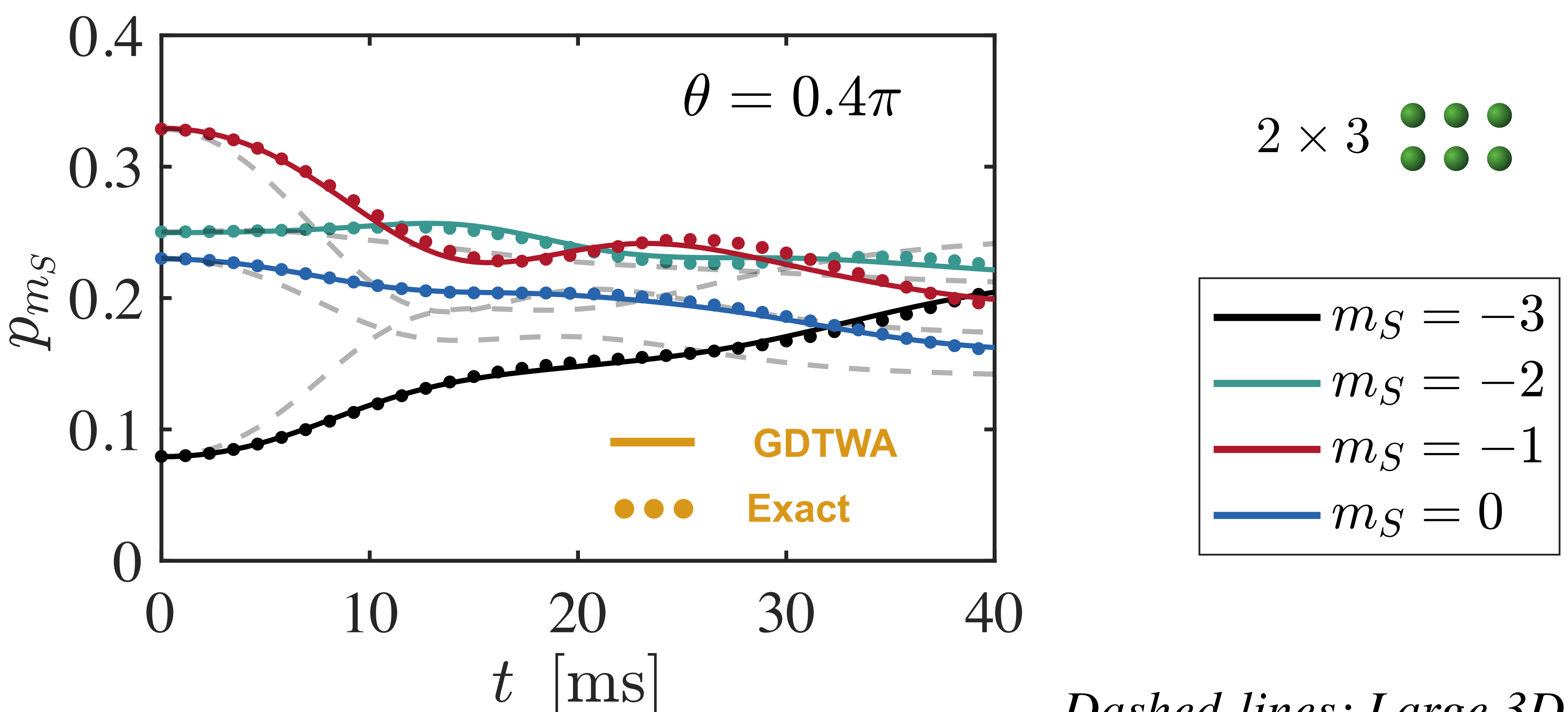
- **3.** Compute expectation values from statistical averages (expansion of the observable into GGMs)

Generalized DTWA (GDTWA)

B. Zhu, A. M. Rey, and J. Schachenmayer, *arXiv:1905:08782 (2019)*

Benchmark of GDTWA for experimental parameters

- Let's test dynamics for experimental parameters on a small plaquette:

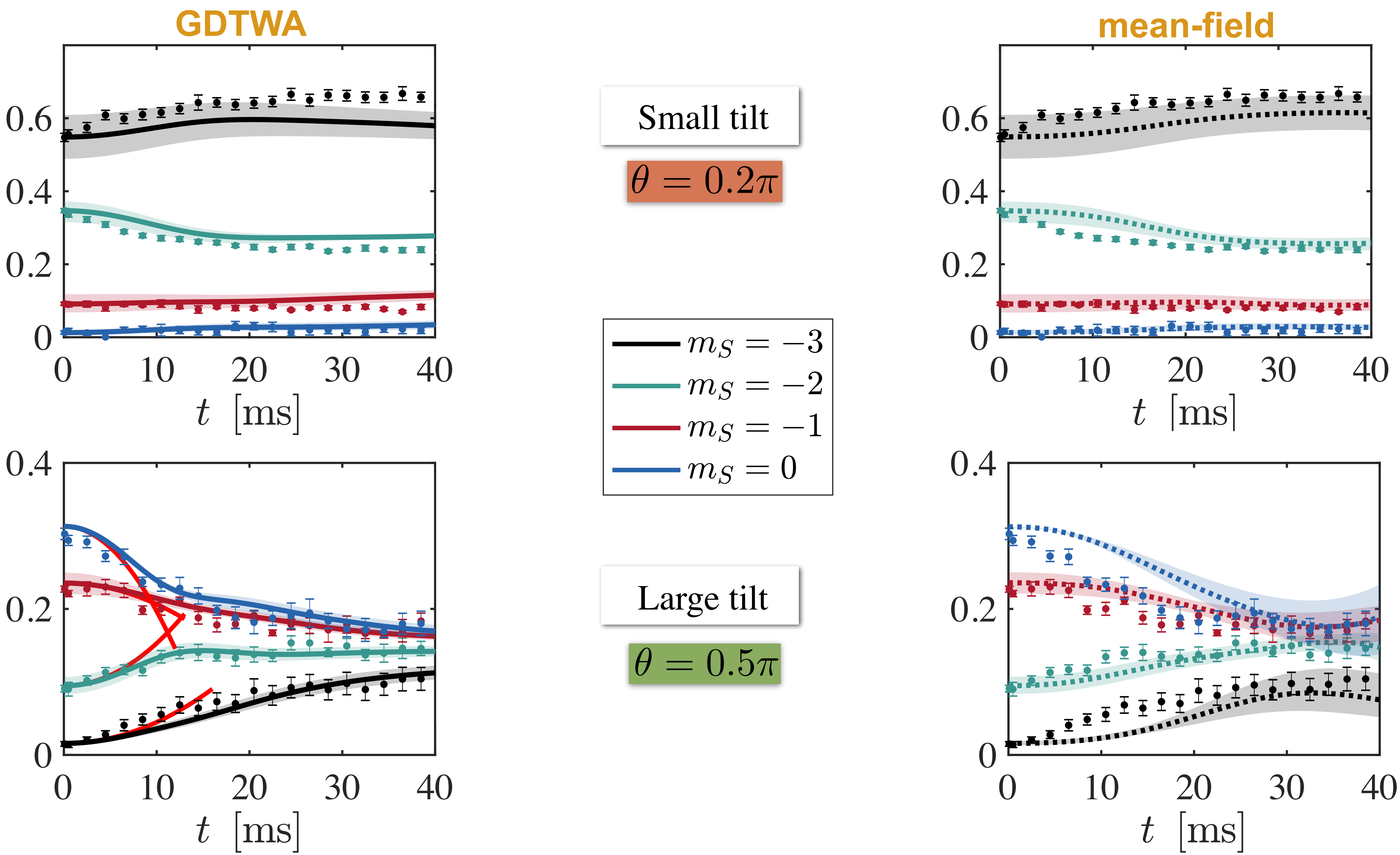


Dashed-lines: Large 3D system

- **1.** GDTWA works very well on the considered time-scale

- **2.** Small plaquette simulations are not enough to predict the experiment (dashed lines are "system-size converged")

Comparison to the experiment

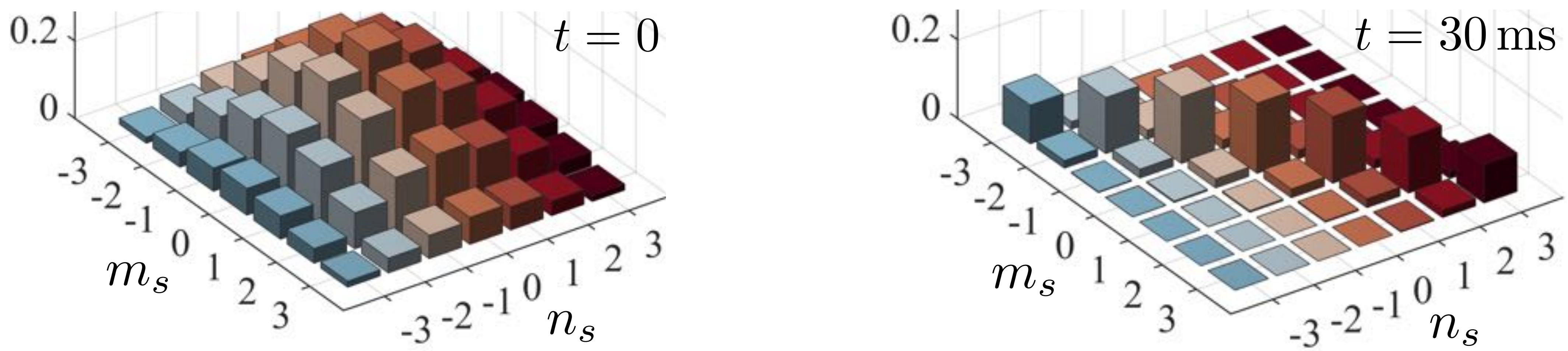


The larger the tilt, the better the GDTWA compared to mean-field!

Entanglement in the GDTWA

- … because, the **GDTWA** captures buildup of entanglement (and mean-field doesn't)

Evolution of S=3 reduced density matrix $|\rho_{m_S,n_S}|^2$



S. Lepoutre, J. Schachenmayer, L. Gabardos, B. Zhu, B. Naylor, E. Mar´echal, O. Gorceix,
A. M. Rey, L. Vernac, and B. Laburthe-Tolra,
Nature Communications 10,1714 (2019).

- **Other recent applications of the GDTWA:**

P. Fersterer, et al., arXiv:1905.06123 (2019) $\Leftrightarrow$ Chromium Experiment (Paris)

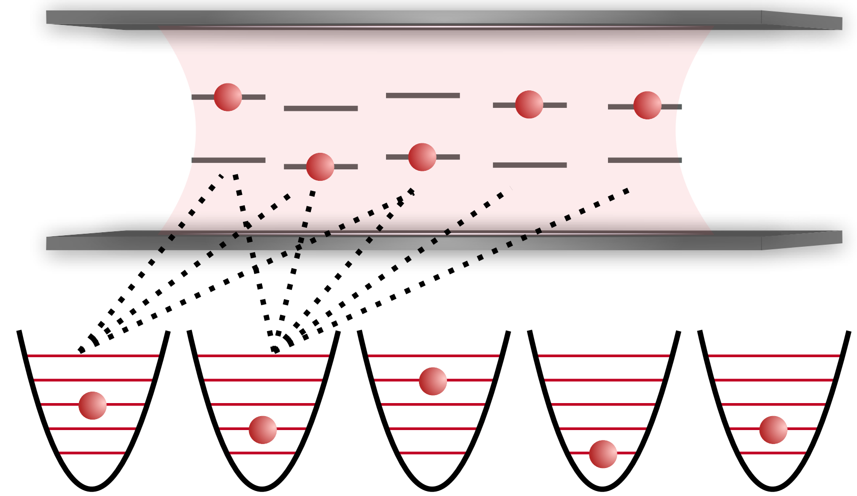
A. Patscheider, et al., arXiv:1904.08262 (2019) $\Leftrightarrow$ Erbium Experiment (Innsbruck, F. Ferlaino)

spin-19/2 system (20 levels on each site!)

Spin-Boson models

- Apply GDTWA to molecular polaritonics?

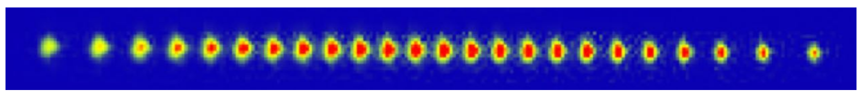
Cavity photon and vibrations:
Model as discrete levels with a cutoff



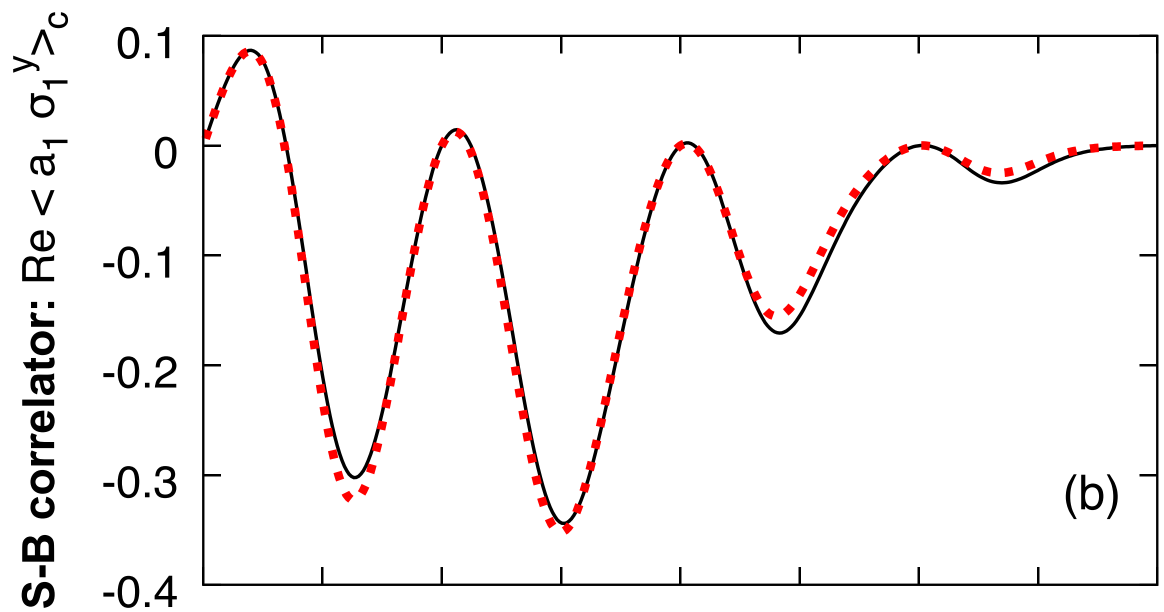
- Alternatively, one could use a **Hybrid method**

Cavity photon and vibrations	⇔	*Traditional TWA with a Gaussian Wigner function*
Electronic levels	⇔	*DTWA for two-level systems*

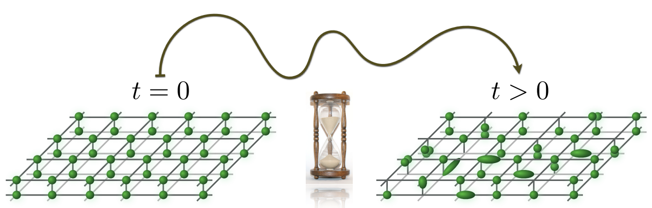
- This has also already been successful for spin-Boson models with trapped ions



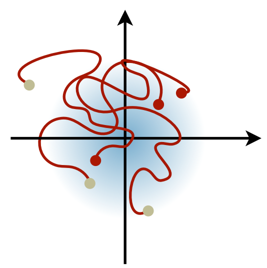
A. Piñeiro Orioli, A. Safavi-Naini, M. L. Wall, A. M. Rey, *Phys. Rev. A 96, 033607 (2017)*

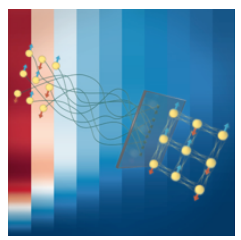


Conclusions



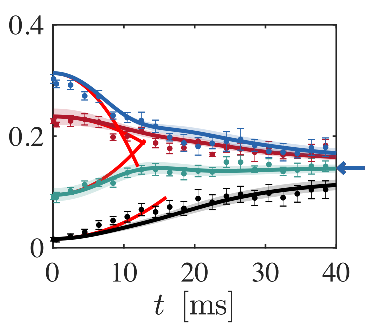
Non-equilibrium dynamics of many-body quantum models is fundamentally interesting. Experiments with atomic physics can study such dynamics. Can we do it numerically?

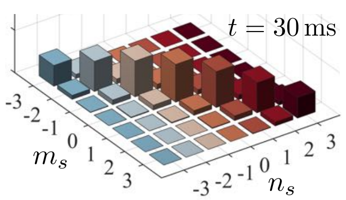




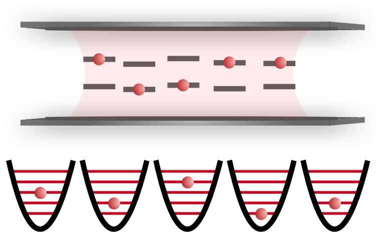
In 1D: Yes, MPS. **In 2D/3D:** We developed a numerical method based on the truncated Wigner approximation on *discrete* phase spaces:

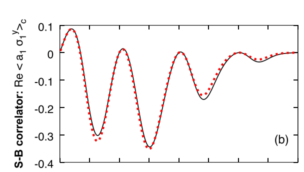
"The discrete truncated Wigner approximation (**DTWA**)*"*





The **DTWA** works surprisingly well. We extended it to arbitrary discrete lattice systems (GDTWA). The semi-classical GDTWA explains experimentally observed correlation build-up of a Chromium lattice experiment.





Both the 1D MPS and especially the **2D/3D GDTWA** methods can be very useful for **spin-boson models**, and could thus also be **useful for molecular polaritonics** (?)

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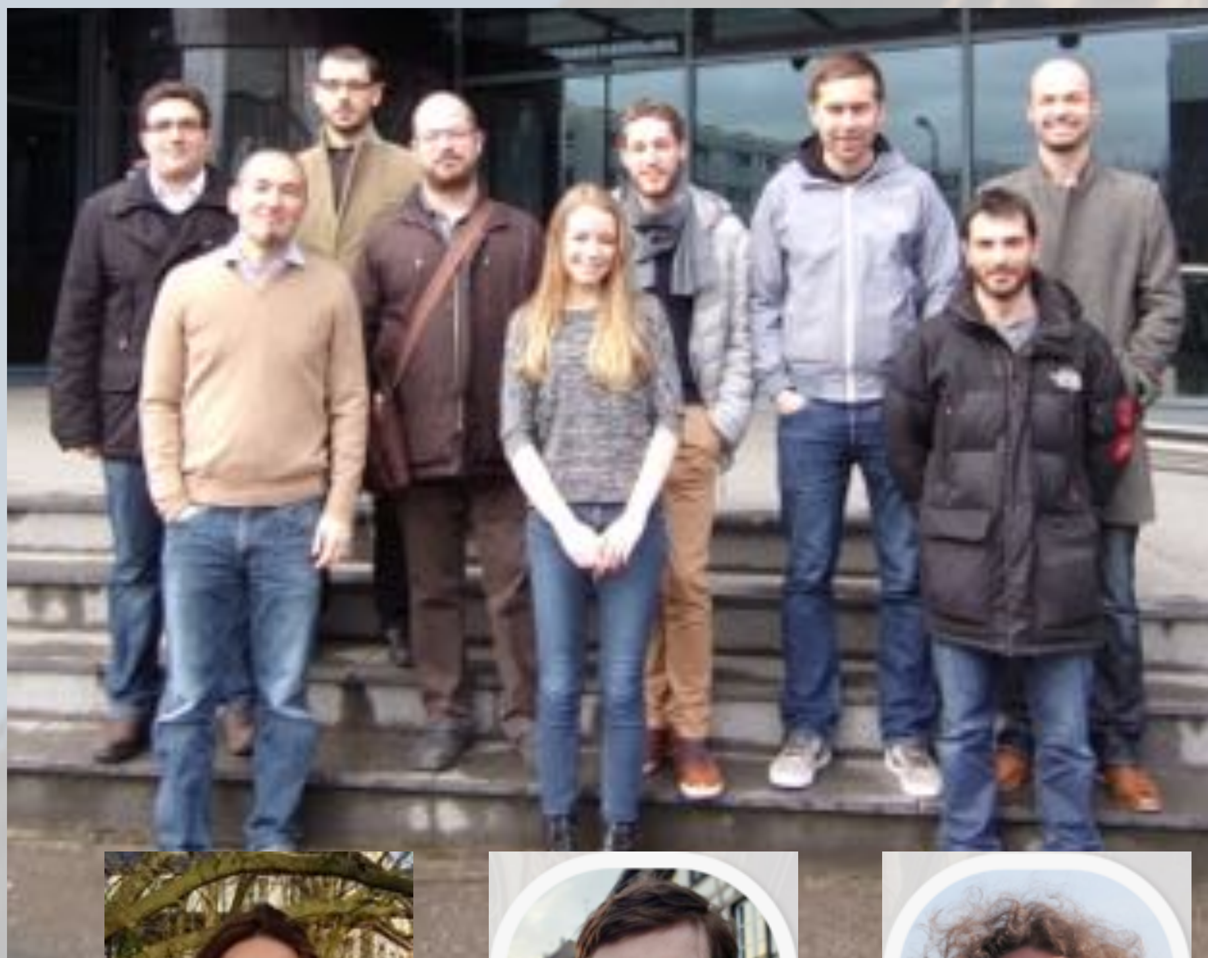
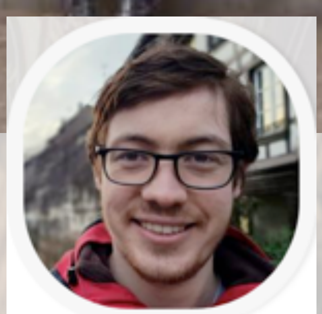
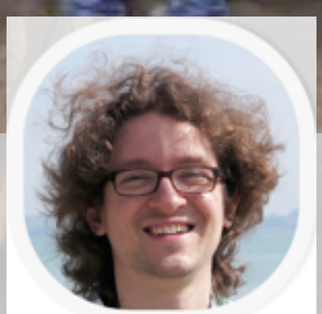
Strasbourg-Team (qmtheory.fr)



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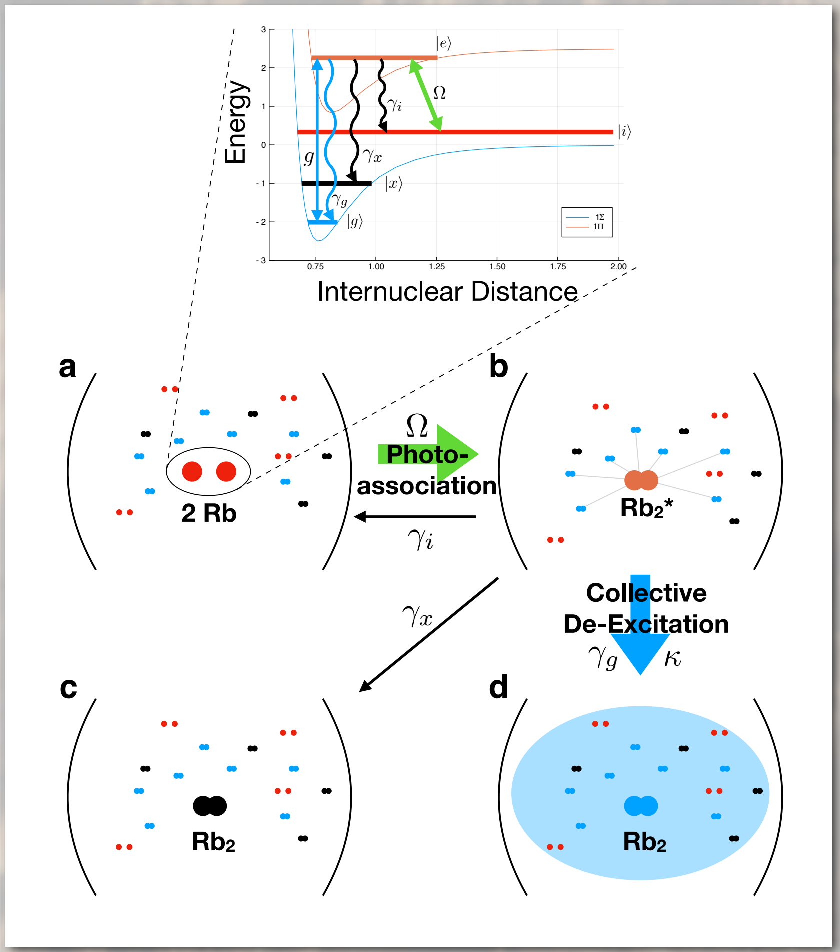
Poster

David Wellnitz

Controlling Ultra-Cold Molecules with Collective Dissipation



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