Sunny.jl Tutorial

HFM 2025, Toronto

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Installation

SunnyContributed / workshops / 2025_05_HFM

Su(n)ny


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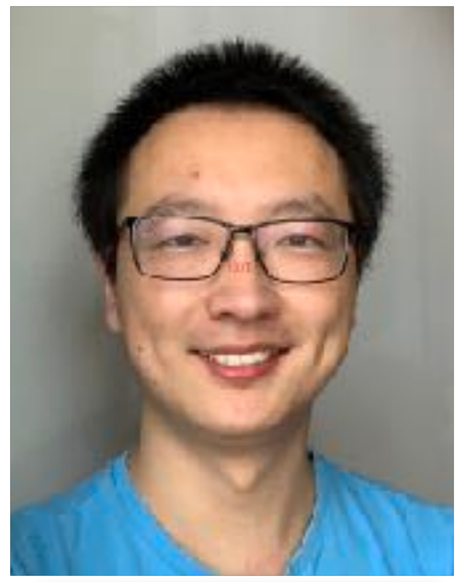
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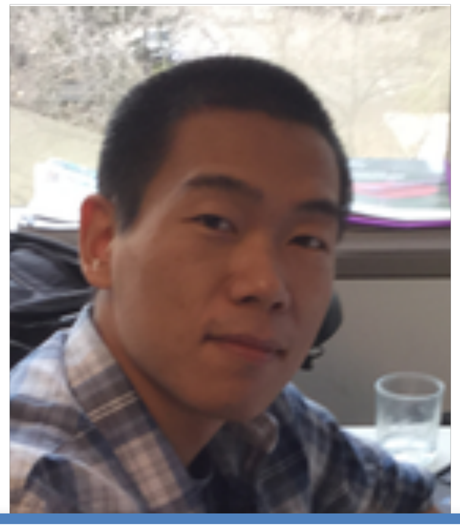
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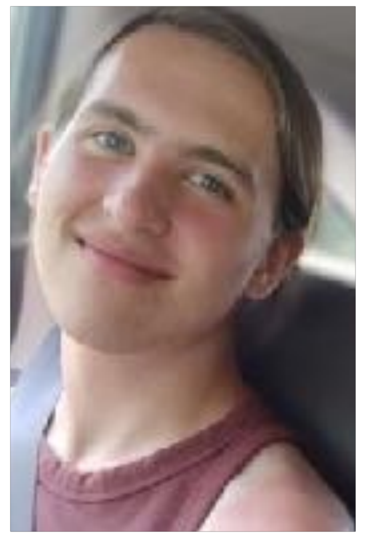
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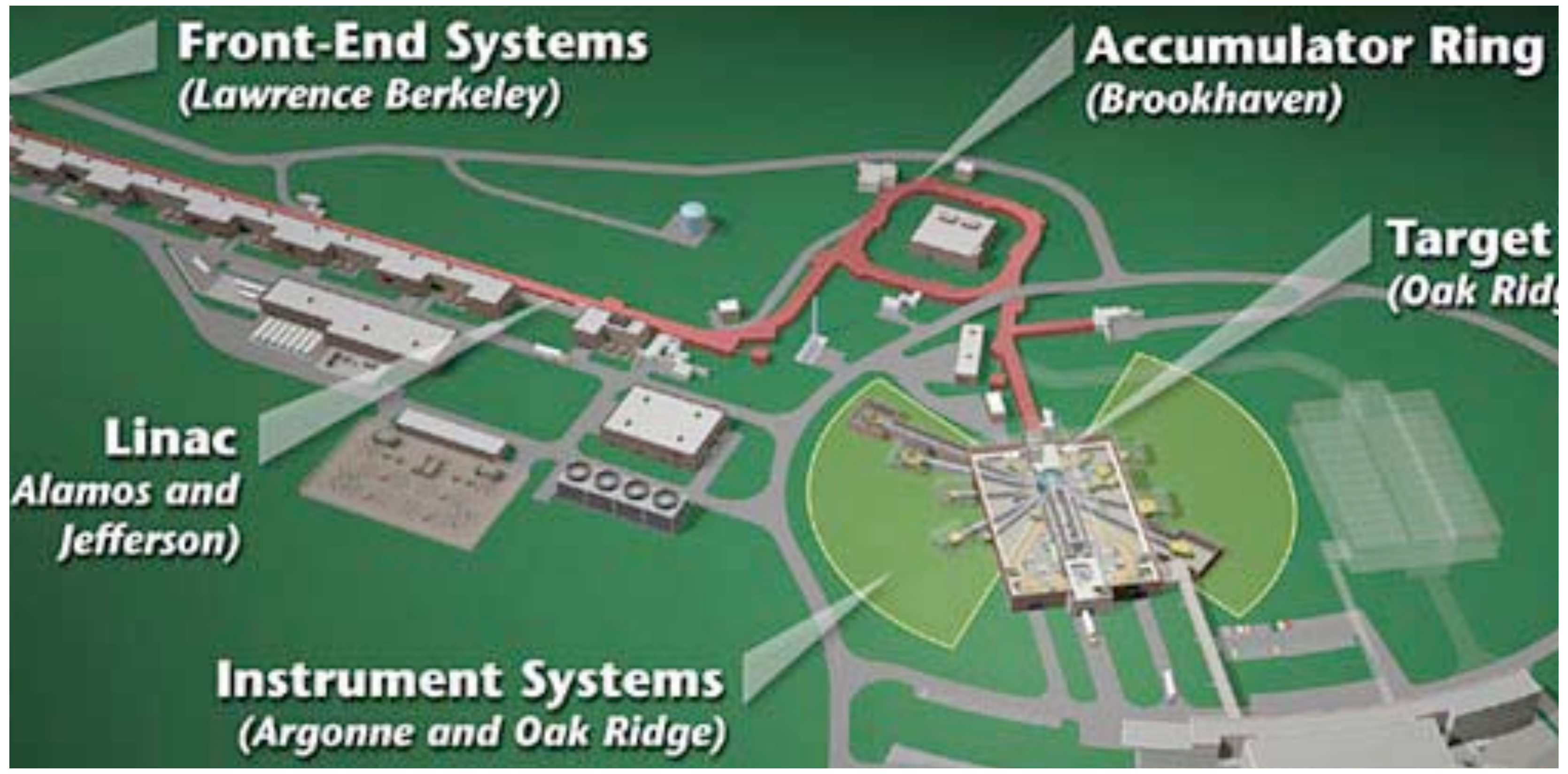
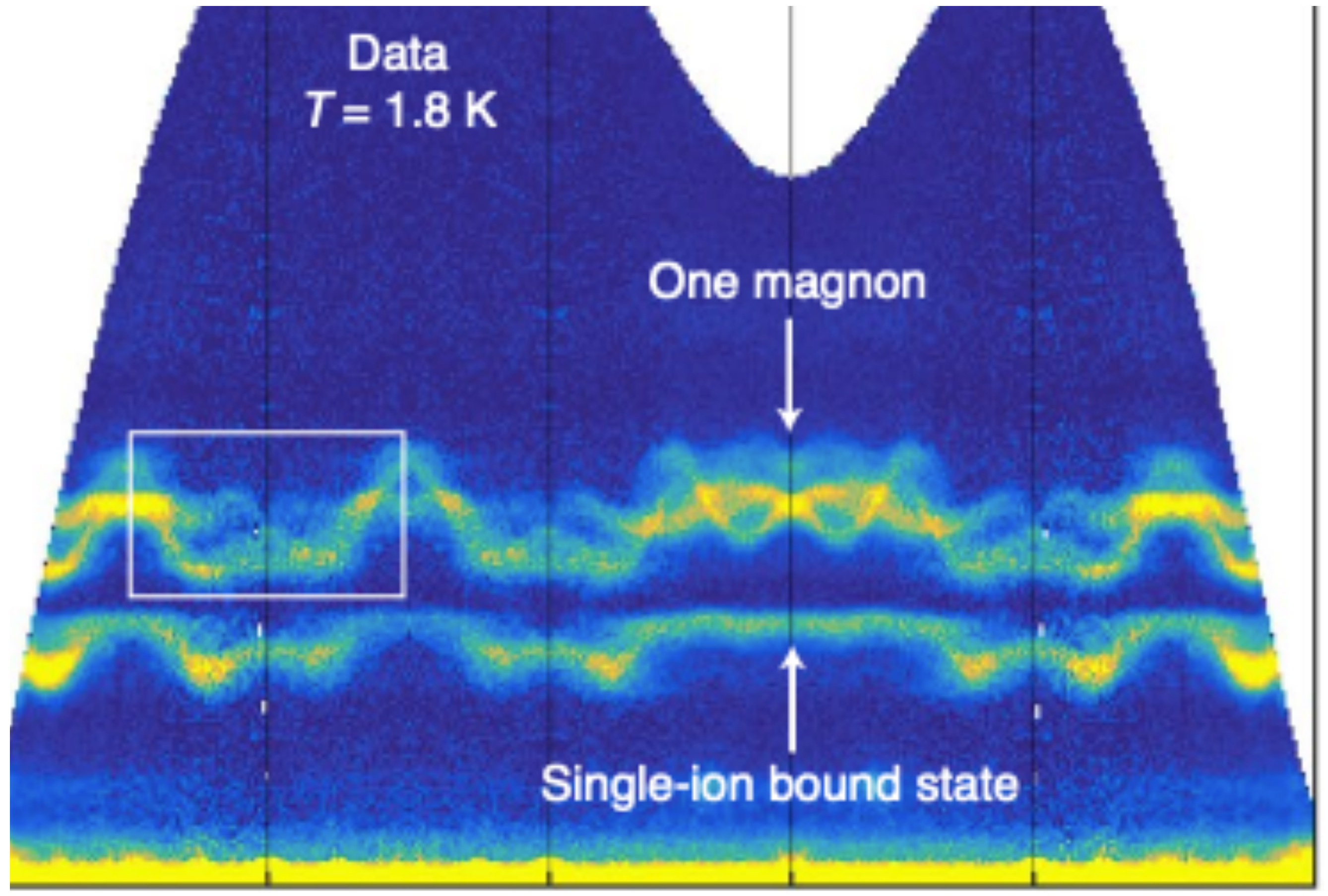
Experiment

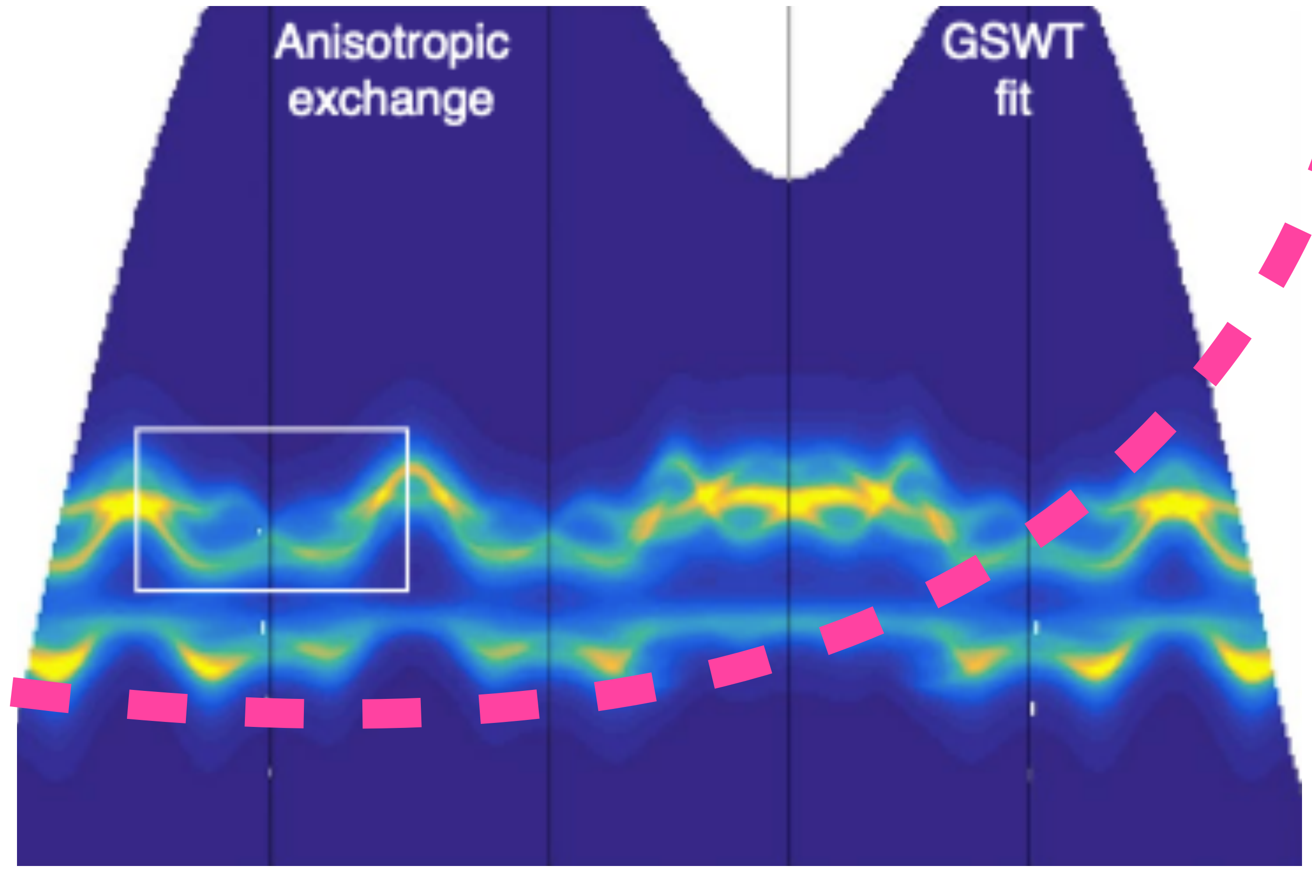




Theory

$$\hat{\mathcal{H}}$$

$$i\hbar\frac{d}{dt}\left|\Psi\right\rangle = \hat{\mathcal{H}}\left|\Psi\right\rangle$$



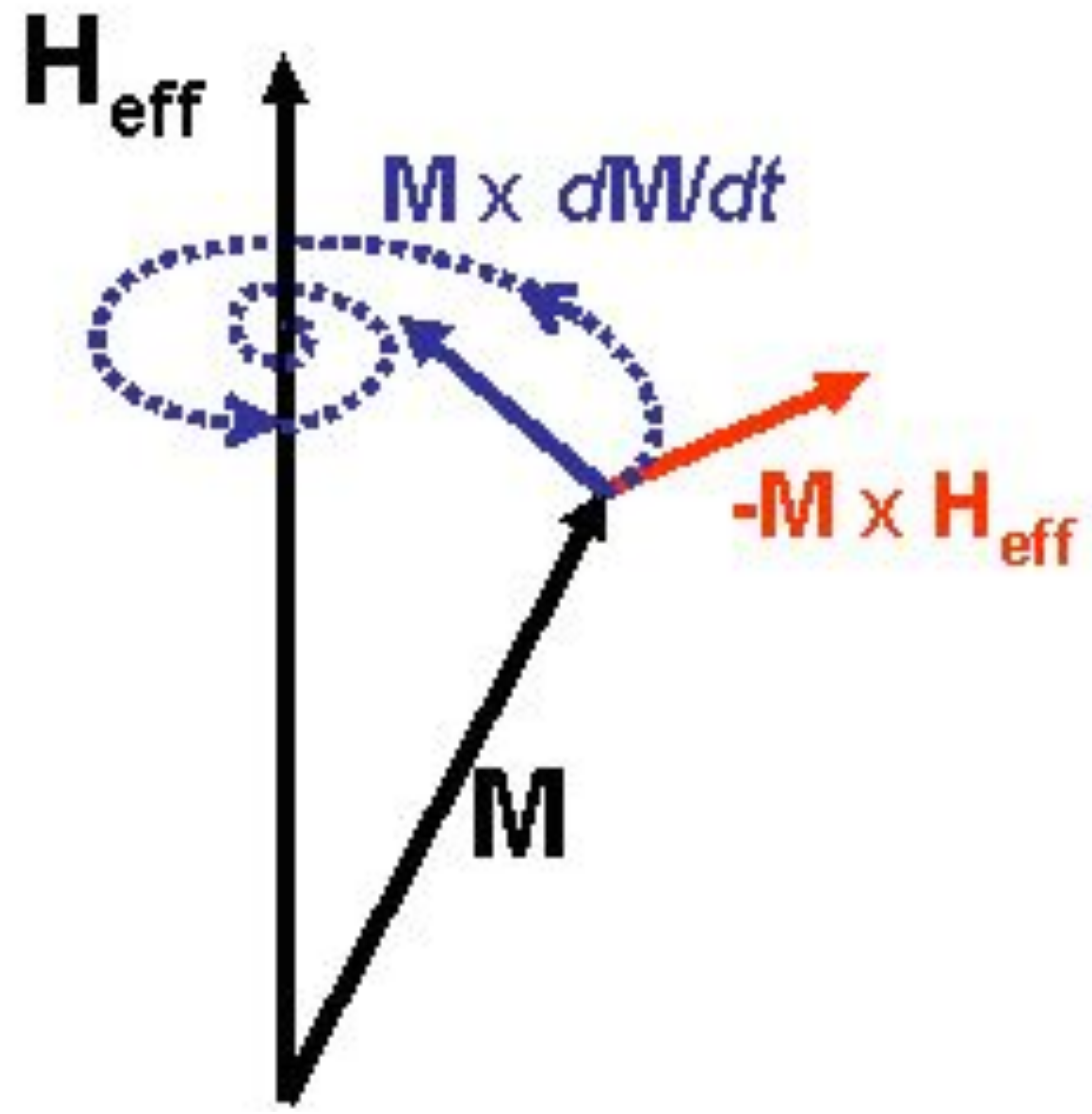
Bai et al. Nature Physics, 17, 467-472 (2021)

Landau-Lifshitz spin dynamics

$$\frac{d\mathbf{S}_j}{dt} = \mathbf{S}_j \times \frac{\partial H}{\partial \mathbf{S}_j}$$

Stochastic Landau-Lifshitz-Gilbert dynamics

$$\frac{d\mathbf{S}_j}{dt} = \mathbf{S}_j \times \mathbf{B}_j \quad -\lambda \mathbf{S}_j \times (\mathbf{S}_j \times \mathbf{B}_j) \quad +\mathbf{S}_j \times \boldsymbol{\xi}_j$$



Effective field $\quad \mathbf{B}_j = -\frac{\partial H}{\partial \mathbf{S}_j}$

Damping timescale $\quad \lambda$

White noise $\quad \langle \boldsymbol{\xi} \rangle = 0, \quad \langle \xi^{\alpha}(t) \xi^{\beta}(t)' \rangle = 2 k_B T \lambda \delta_{\alpha\beta}$

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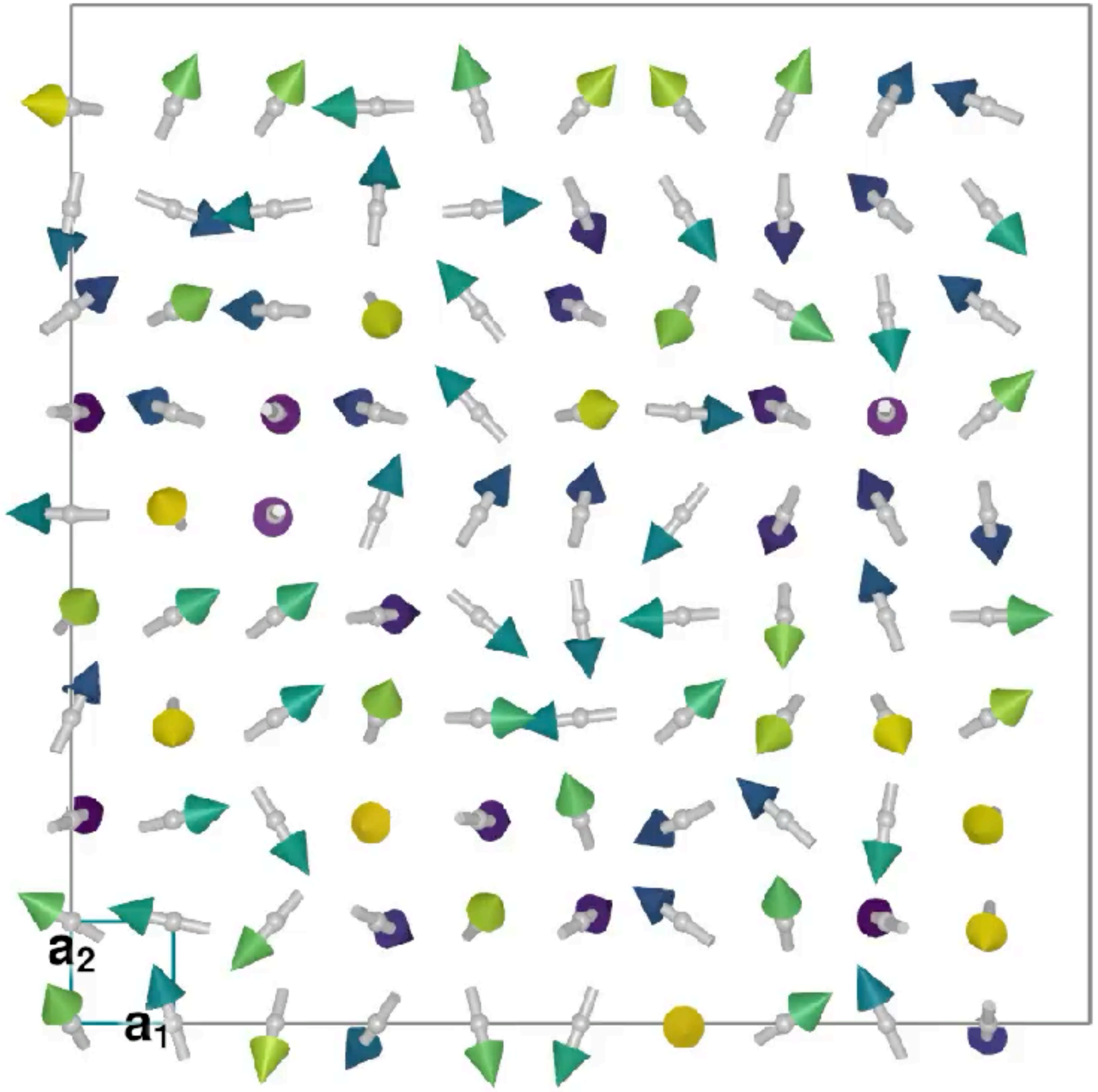
Sunny

```julia
using Sunny, GLMakie

# build crystal
latvecs = lattice_vectors(1, 1, 10, 90, 90, 90)
cryst = Crystal(latvecs, [[0,0,0]])

# build spin system
sys = System(cryst, (10,10,1), [SpinInfo(1, S=1, g=2)], :dipole; seed=1)
set_exchange!(sys, -1.0, Bond(1, 1, (1, 0, 0)))
randomize_spins!(sys)

# time integrate
fig = plot_spins(sys)
langevin = Langevin(0.1; kT=0, λ=0.05)
for _ in 1:500
    for _ in 1:5
        step!(sys, langevin)
    end
    notify(fig)
    sleep(1/60)
end
```



Thoughts on Julia for a "production" scientific code

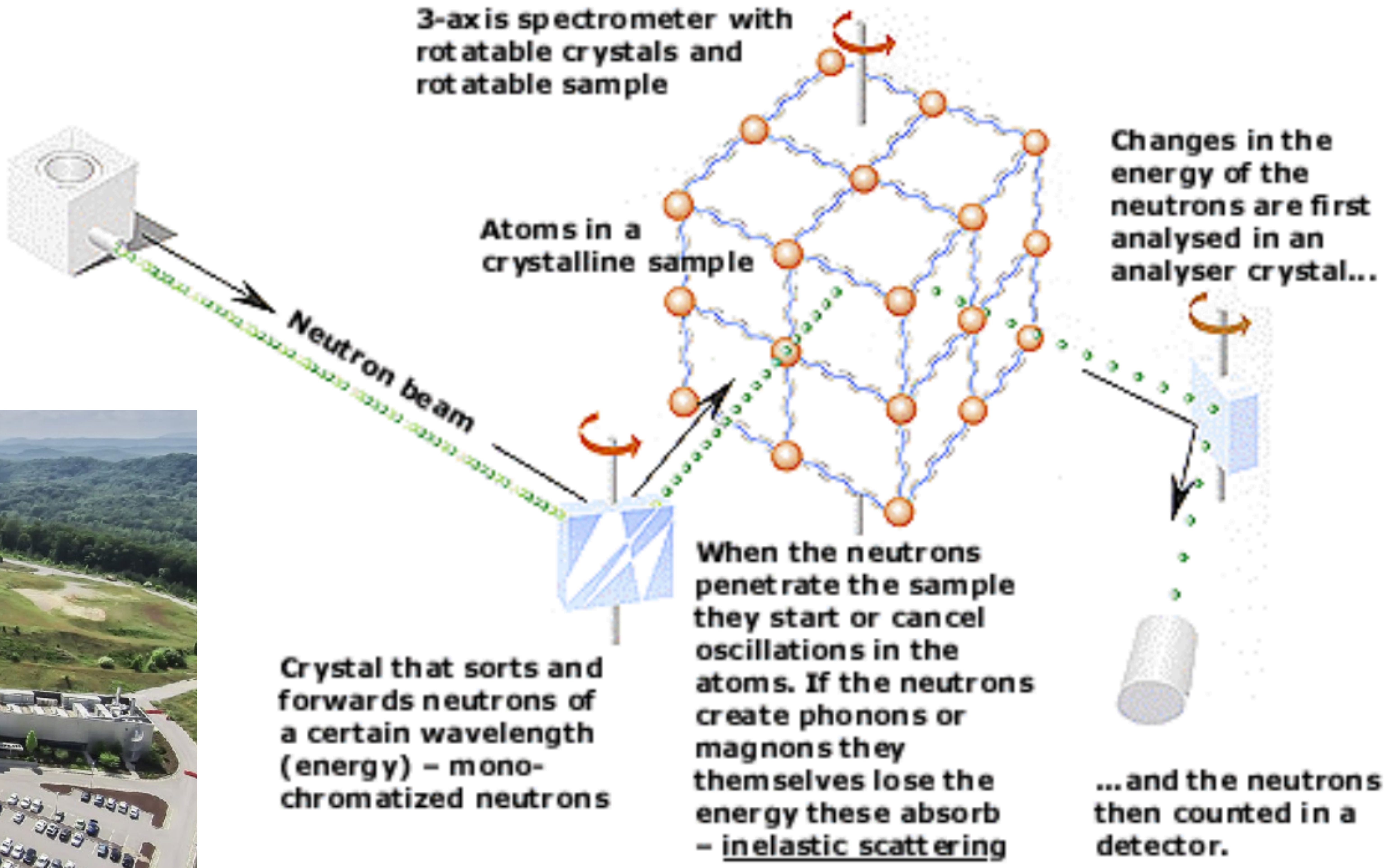
Superpower: Python flexibility and C++ performance

Pros:
- Express code like math (multi-method dispatch)
- Interactive development experience
- Built-in package manager
- Easily bind C++/Fortran/Python libraries
- "Drop down" to machine level (stack allocs / SIMD / JIT)
- Ecosystem of enthusiasts 👍👍

Cons:
- Performance learning curve
- JIT $\Longrightarrow$ Julia is a heavy dependency
- Small community $\Longrightarrow$ you'll find bugs

Neutrons an ideal probe for magnetism

https://neutrons.ornl.gov/sns



https://neutrons.ornl.gov/sites/default/files/intro_to_neutron_scattering.pdf

Spin order and dynamics in the diamond-lattice Heisenberg antiferromagnets $CuRh_2O_4$ and $CoRh_2O_4$

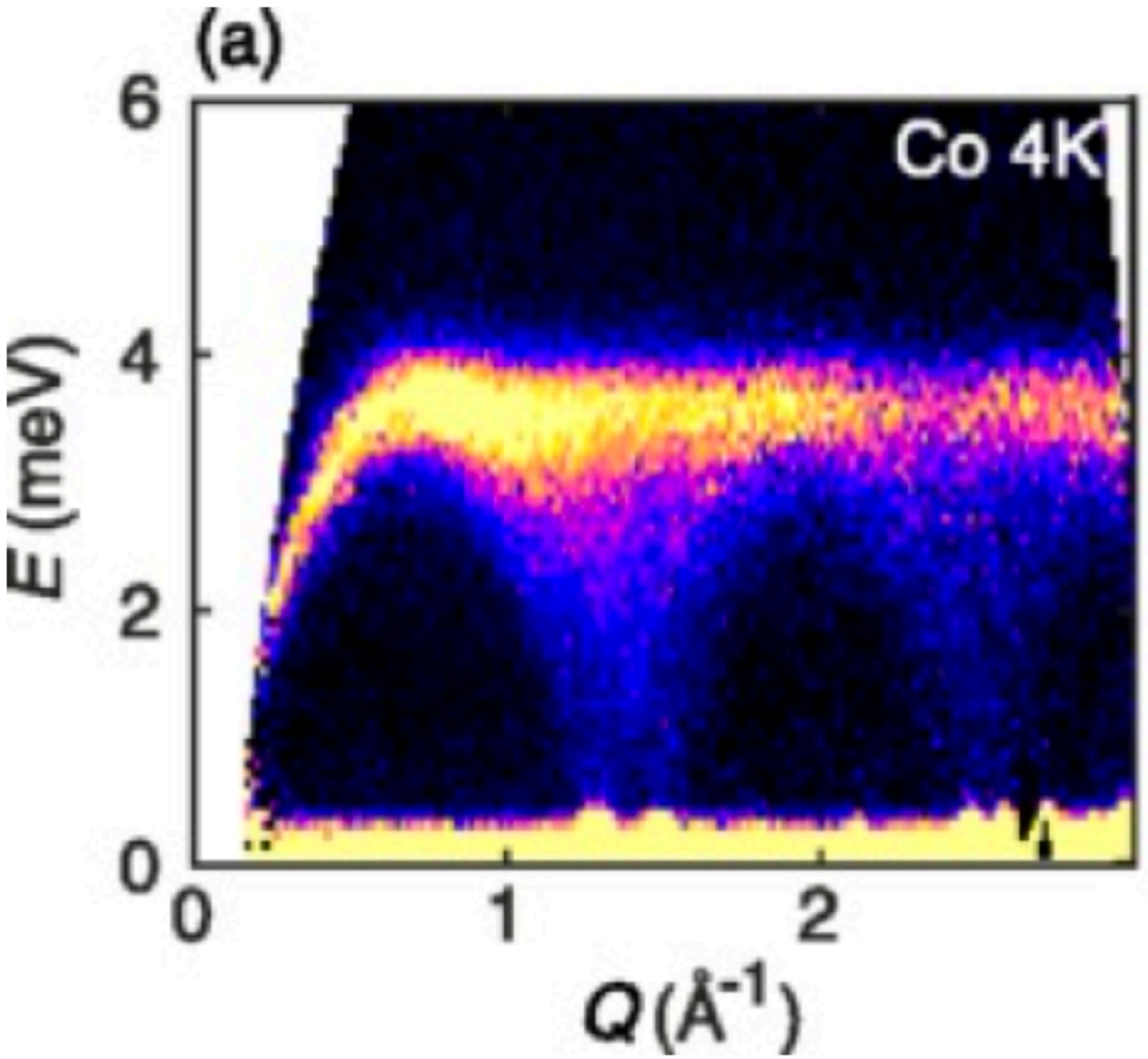
L. Ge[1], J. Flynn[2], J. A. M. Paddison[1,*], M. B. Stone[3], S. Calder[3], M. A. Subramanian[2], A. P. Ramirez[4], and M. Mourigal[1]

Phys. Rev. B **96**, 064413 – **Published 9 August, 2017**

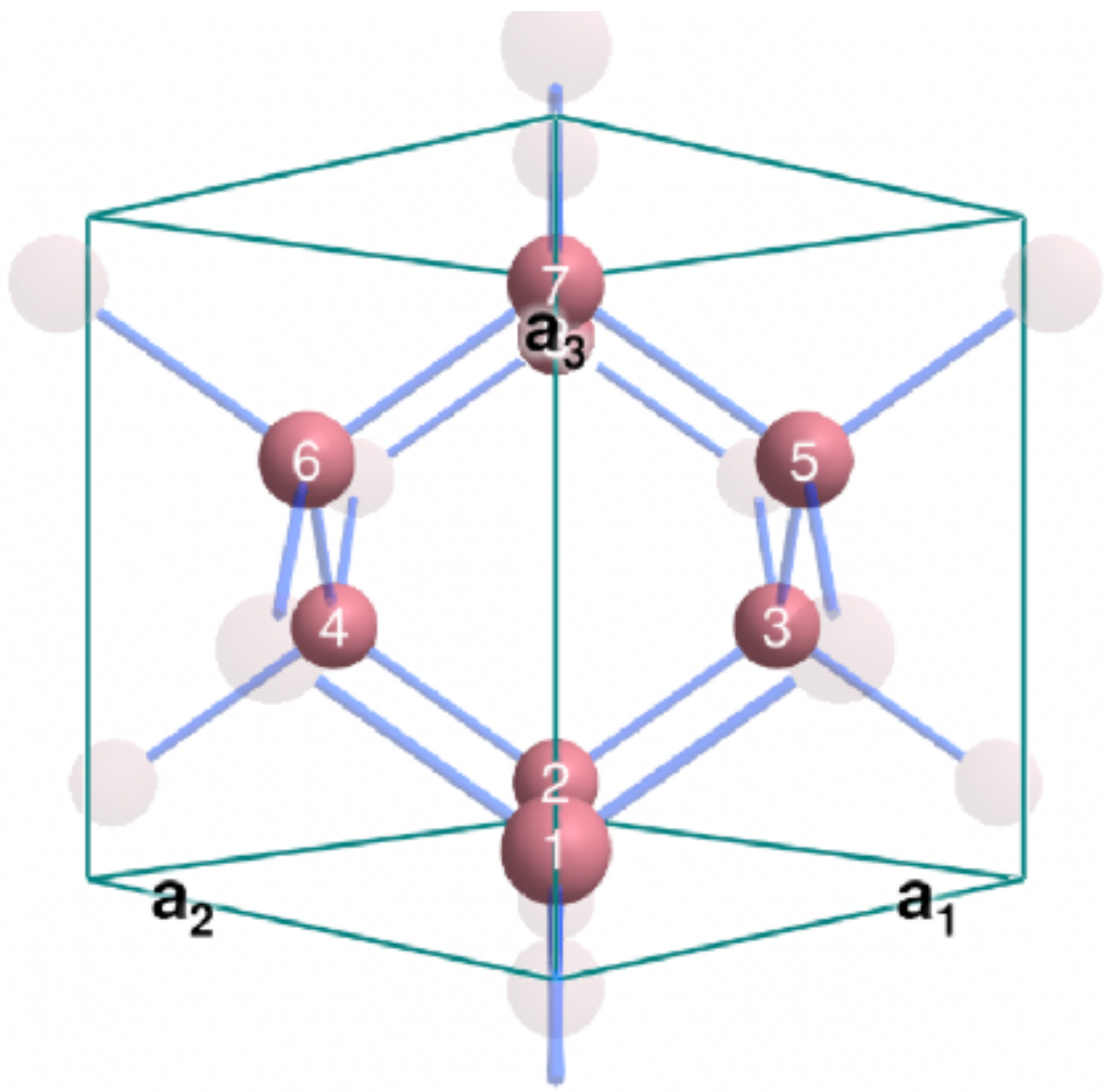
$$\langle \hat{\mathbf{S}}^{\alpha}(\mathbf{r}, t)\hat{\mathbf{S}}^{\beta}(\mathbf{0},0)\rangle$$

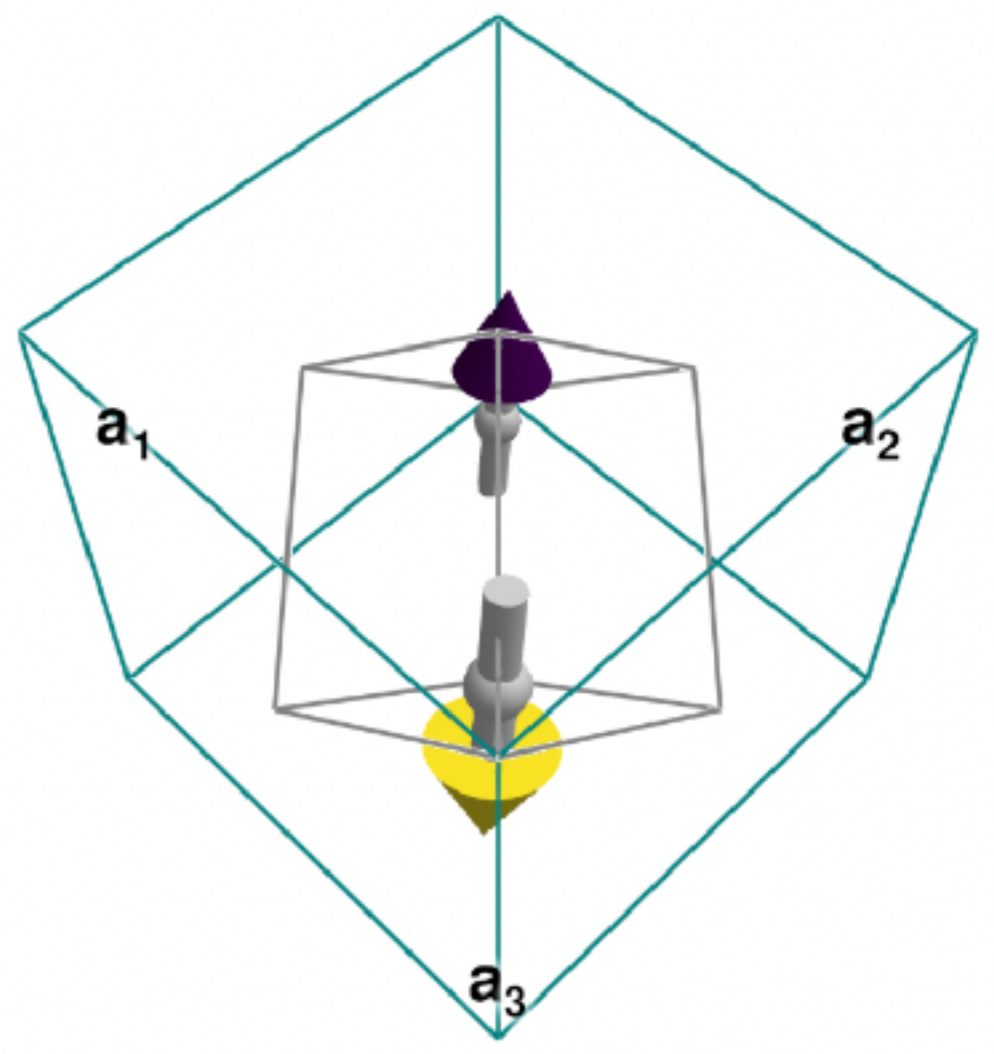
$$\mathcal{S}^{\alpha\beta}(\mathbf{k}, \omega) = \langle \hat{\mathbf{S}}^{\alpha}_{-\mathbf{k},-\omega}\hat{\mathbf{S}}^{\beta}_{\mathbf{k},\omega}\rangle$$

$$\frac{d\mathbf{S}_j}{dt} = \mathbf{S}_j \times \frac{\partial H}{\partial \mathbf{S}_j}$$

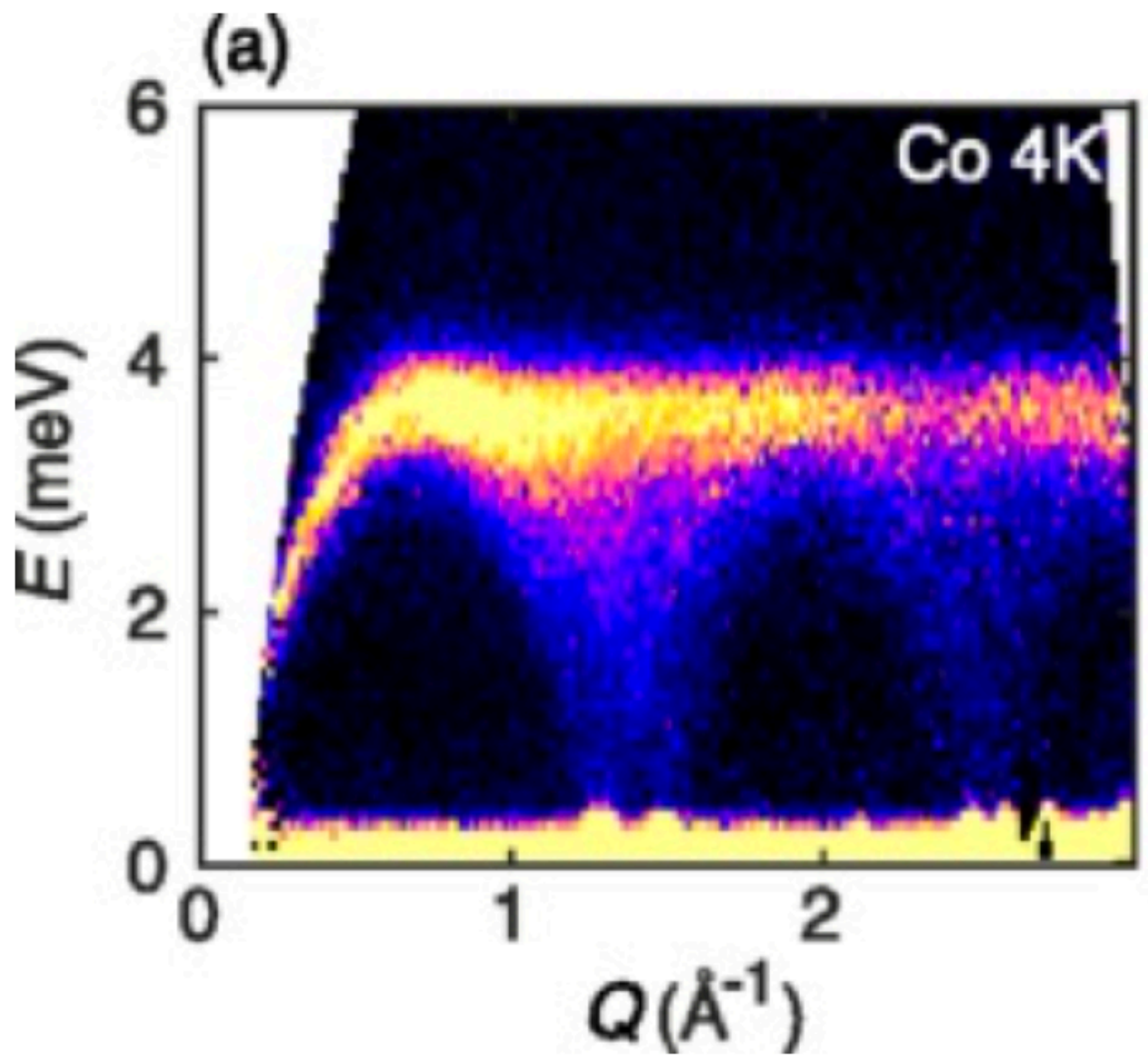


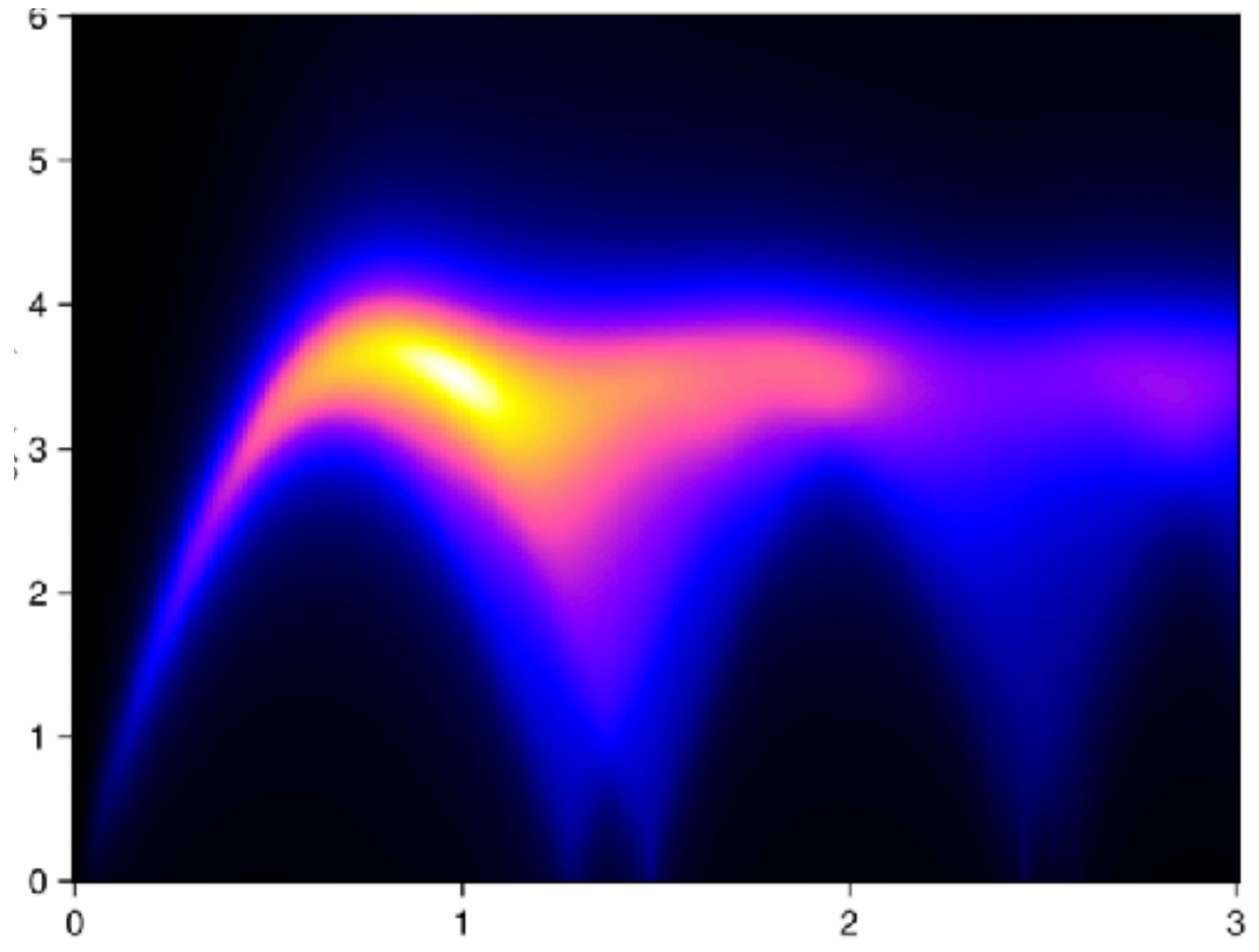
```julia
using Sunny, GLMakie
a = 8.5031 # (Å)
latvecs = lattice_vectors(a, a, a, 90, 90, 90)
positions = [[1/8, 1/8, 1/8]]
cryst = Crystal(latvecs, positions, 227; types=["Co"])
sys = System(cryst, [1 => Moment(s=3/2, g=2)], :dipole)
J = +0.63 # (meV)
set_exchange!(sys, J, Bond(2, 3, [0, 0, 0]))
randomize_spins!(sys)
minimize_energy!(sys)
sys_prim = reshape_supercell(sys, primitive_cell(cryst))
```






```julia
formfactors = [1 => FormFactor("Co2")]
measure = ssf_perp(sys_prim; formfactors)
swt = SpinWaveTheory(sys_prim; measure)
kernel = lorentzian(fwhm=0.8)
energies = range(0, 6, 300)
radii = range(0, 3, 200) # (1/Å)
res = powder_average(cryst, radii, 2000) do qs
    intensities(swt, qs; energies, kernel)
end
plot_intensities(res)
```





Quantum to classical (large-s)

$$\langle \hat{\mathbf{S}}_j \hat{\mathbf{S}}_k \rangle \longrightarrow \langle \hat{\mathbf{S}}_j \rangle \langle \hat{\mathbf{S}}_k \rangle = \mathbf{S}_j \mathbf{S}_k$$

$$\hat{\mathscr{H}} = -\sum_{jk} J_{jk} \hat{\mathbf{S}}_j \cdot \hat{\mathbf{S}}_k \longrightarrow H = -\sum_{jk} J_{jk} \mathbf{S}_j \cdot \mathbf{S}_k$$

$$\frac{d\hat{\mathbf{S}}_j}{dt} = \hat{\mathbf{S}}_j \times \frac{\partial \hat{\mathscr{H}}}{\partial \hat{\mathbf{S}}_j} \longrightarrow \boxed{\frac{d\mathbf{S}_j}{dt} = \mathbf{S}_j \times \frac{\partial H}{\partial \mathbf{S}_j}}$$

Landau-Lifshitz equation

Exact quantum spin Hamiltonian

$$\hat{\mathscr{H}} = -\sum_{jk} J_{jk} \hat{\mathbf{S}}_j \cdot \hat{\mathbf{S}}_k - D \sum_j (\hat{S}_j^z)^2$$

"Large-S" approximation

$$\langle \hat{\mathscr{H}} \rangle = -\sum_{jk} J_{jk} \boxed{\langle \hat{\mathbf{S}}_j \rangle \cdot \langle \hat{\mathbf{S}}_k \rangle} - D \sum_j \boxed{\langle \hat{S}_j^z \rangle^2}$$

Neglect entanglement

Neglect quantum spin structure!

SU(N) treatment

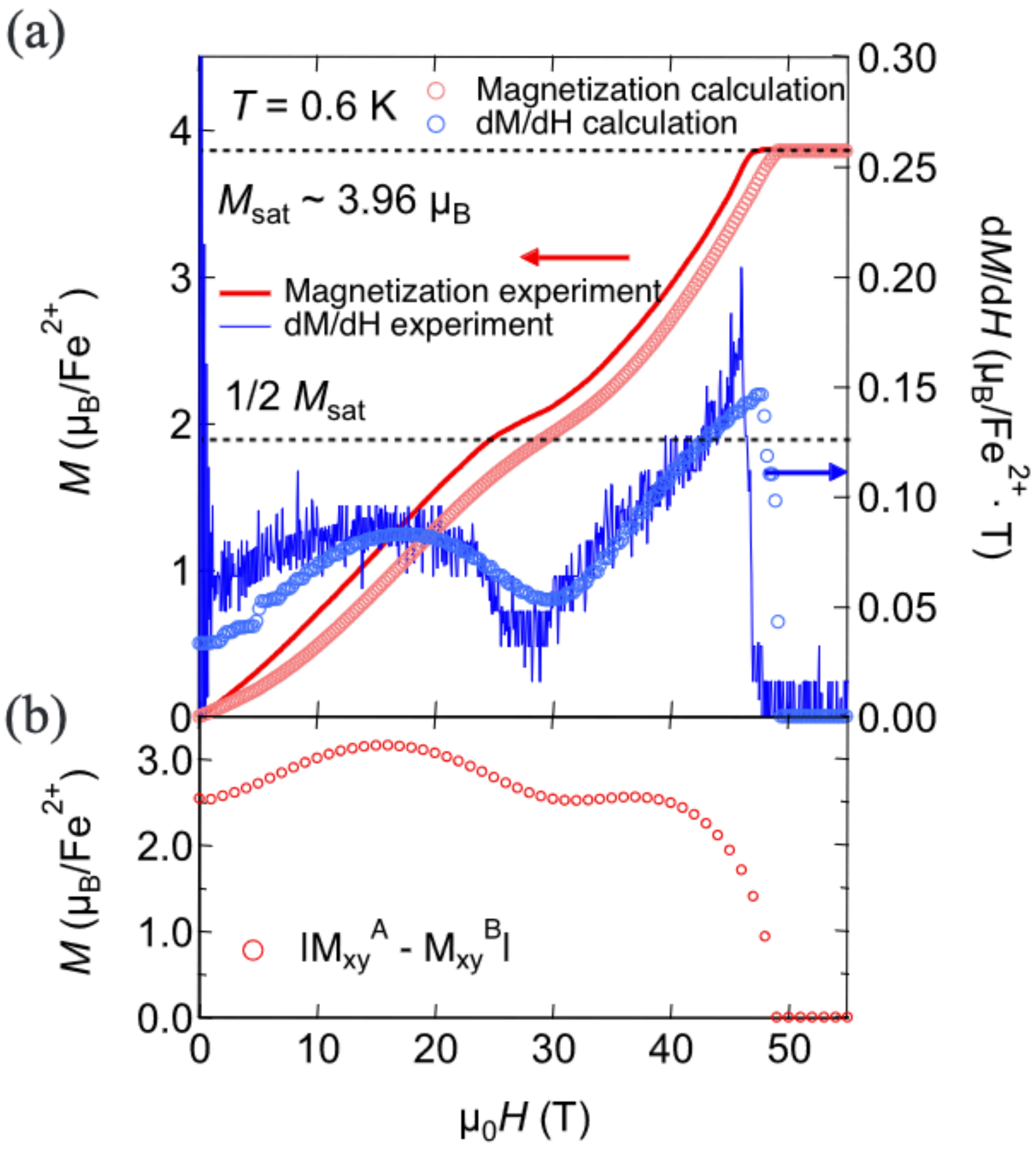
$$\hat{T}^\alpha = \{\hat{\mathbf{S}}^x, \hat{\mathbf{S}}^y, \hat{\mathbf{S}}^z,$$ Dipoles

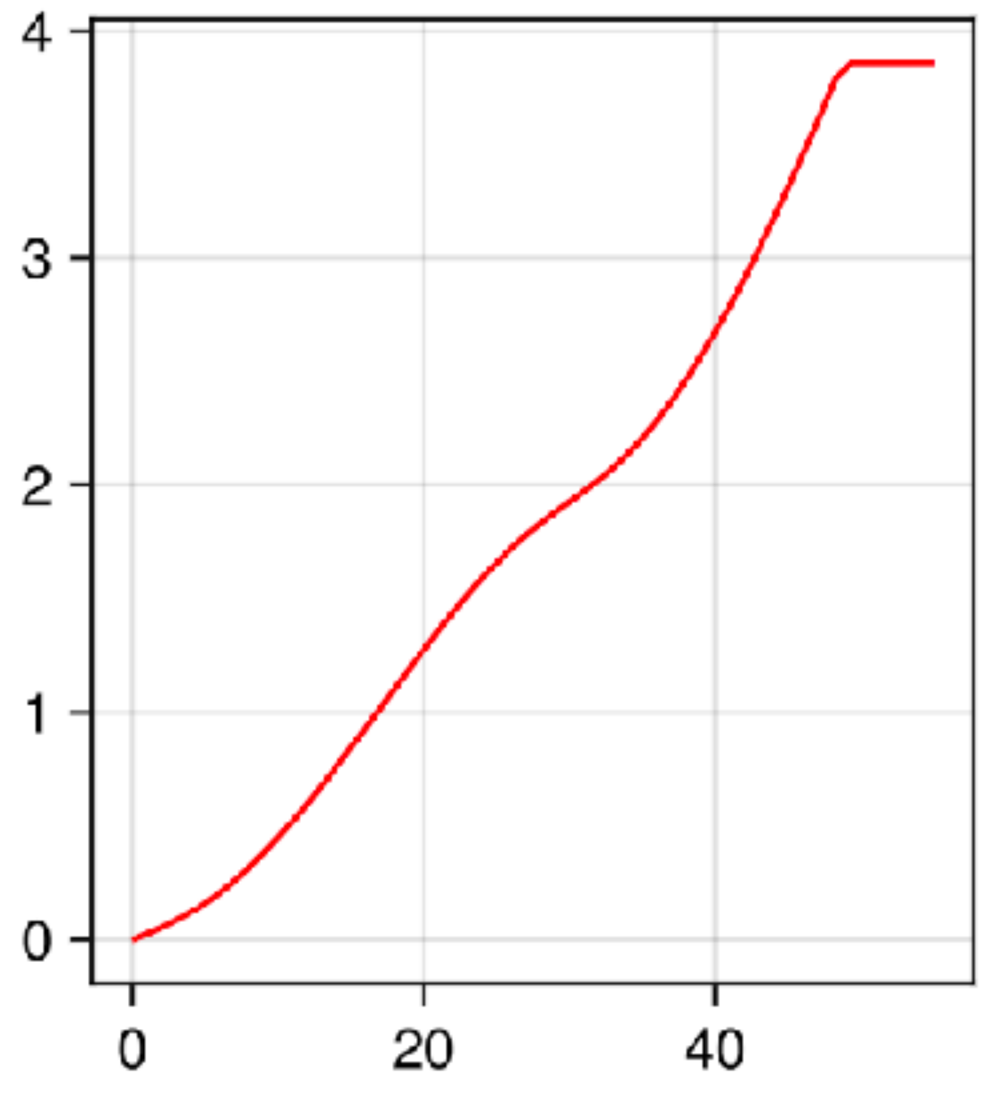
$$(\hat{\mathbf{S}}^x)^2 - (\hat{\mathbf{S}}^y)^2, \ldots\}$$ Quadrupoles

$$\frac{d\hat{T}_j^\alpha}{dt} = f^{\alpha\beta\gamma} \hat{T}_j^\beta \frac{\partial \hat{\mathscr{H}}}{\partial \hat{T}_j^\gamma}$$

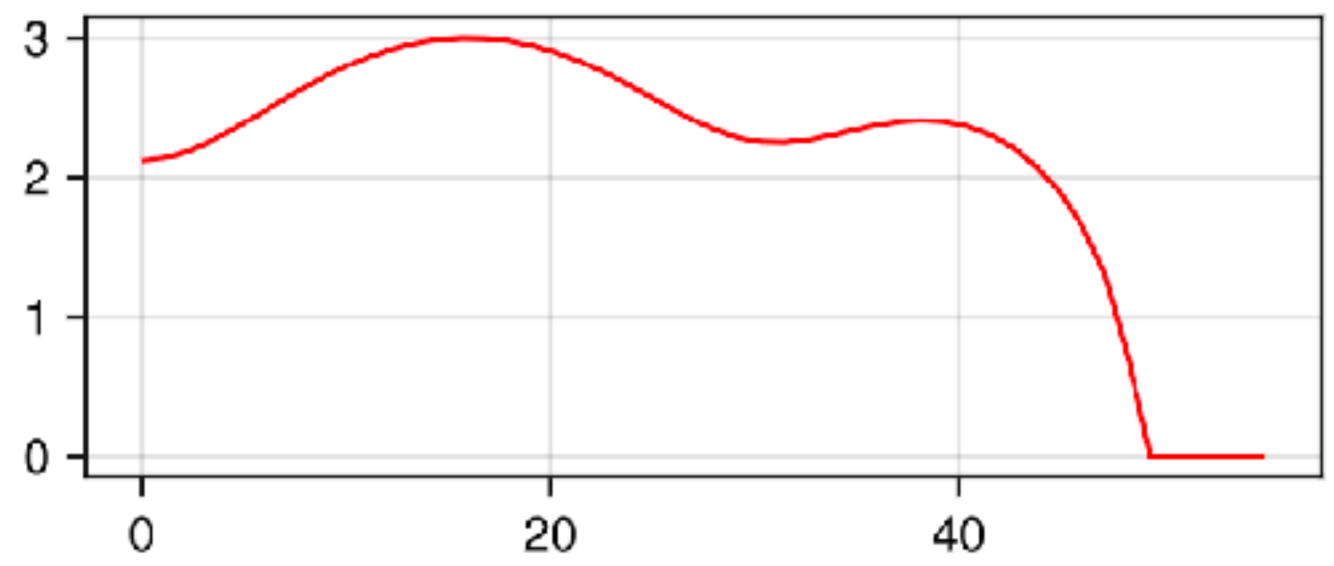
SU(5) Application: $Ba_2FeSi_2O_7$

Lee at al., PRB **107** 144427 (2023)





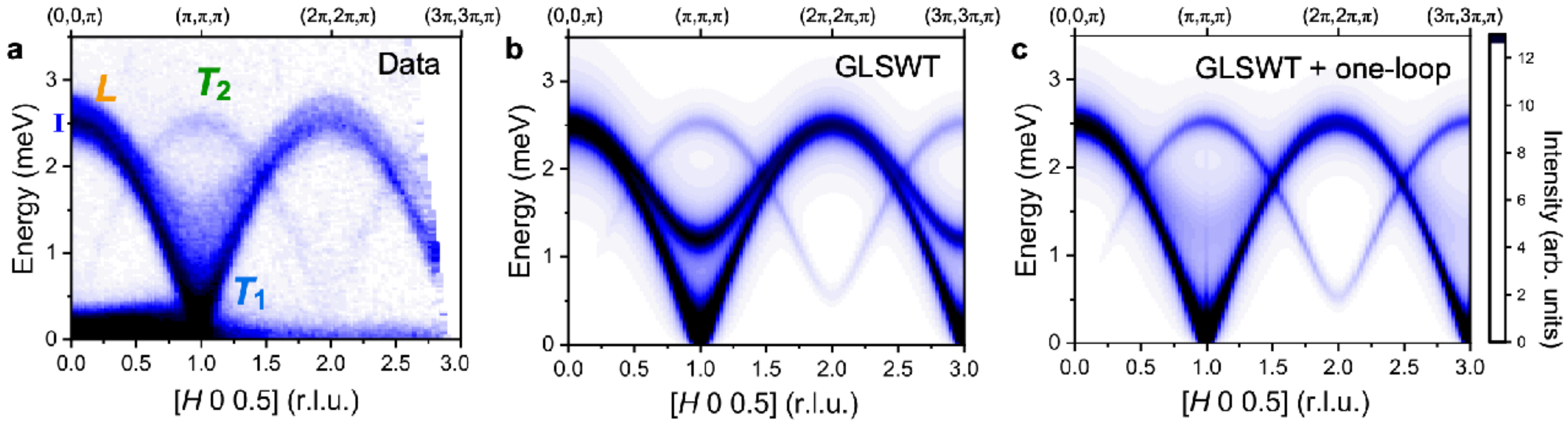
Net magnetization

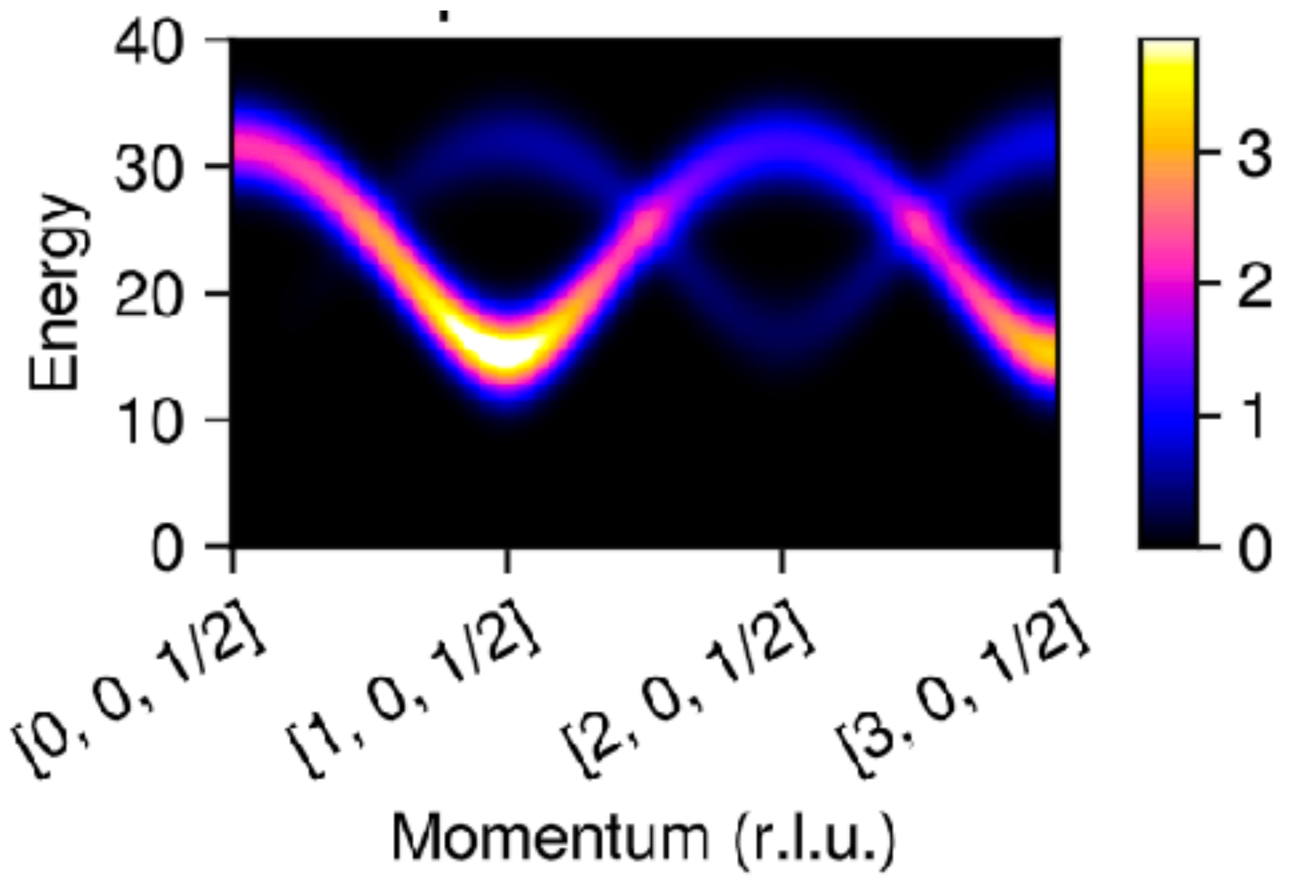


Staggered magnetization

SU(5) Application: $Ba_2FeSi_2O_7$

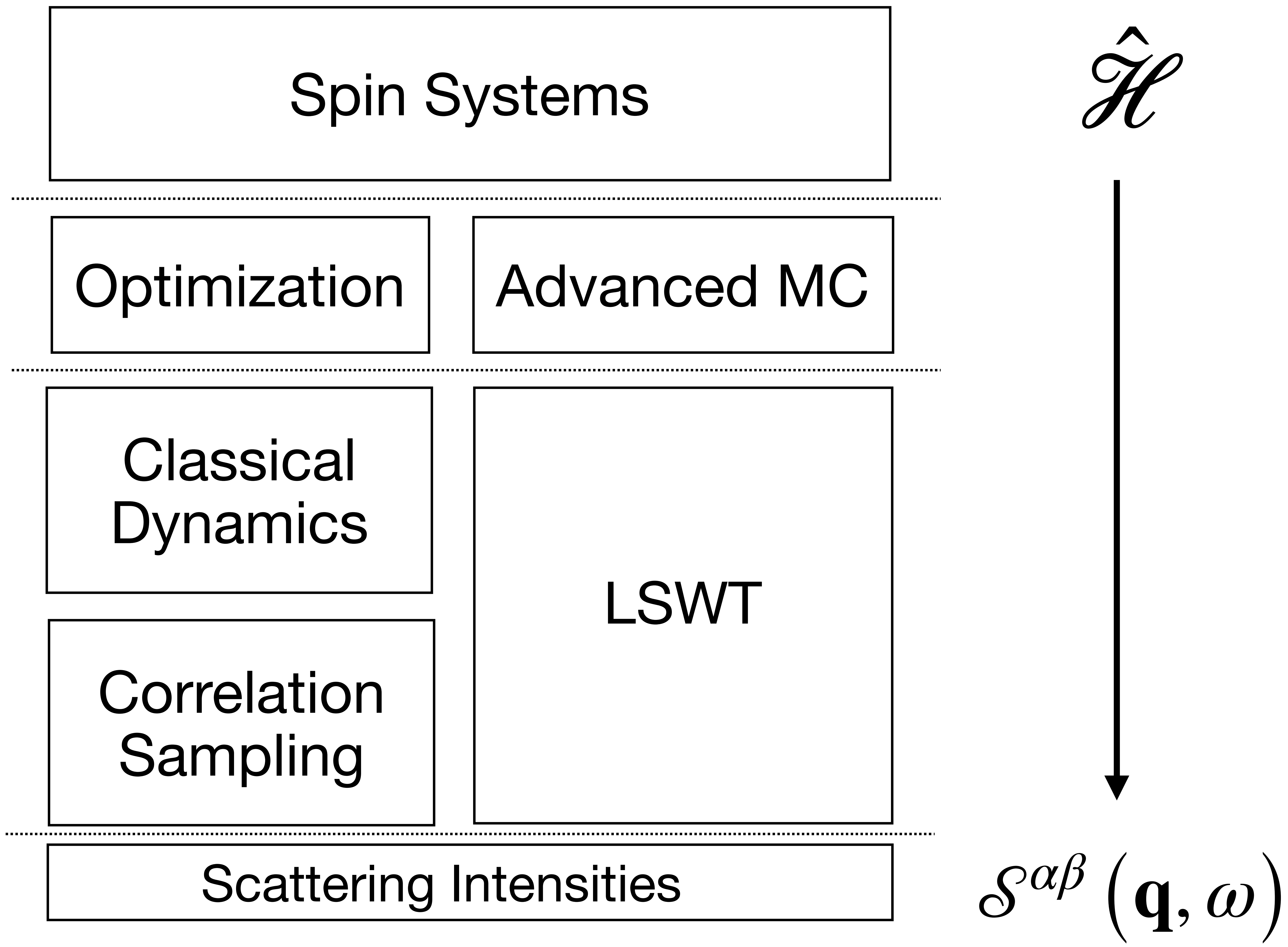
Do et al., Nature Communications 12:5331 (2021)

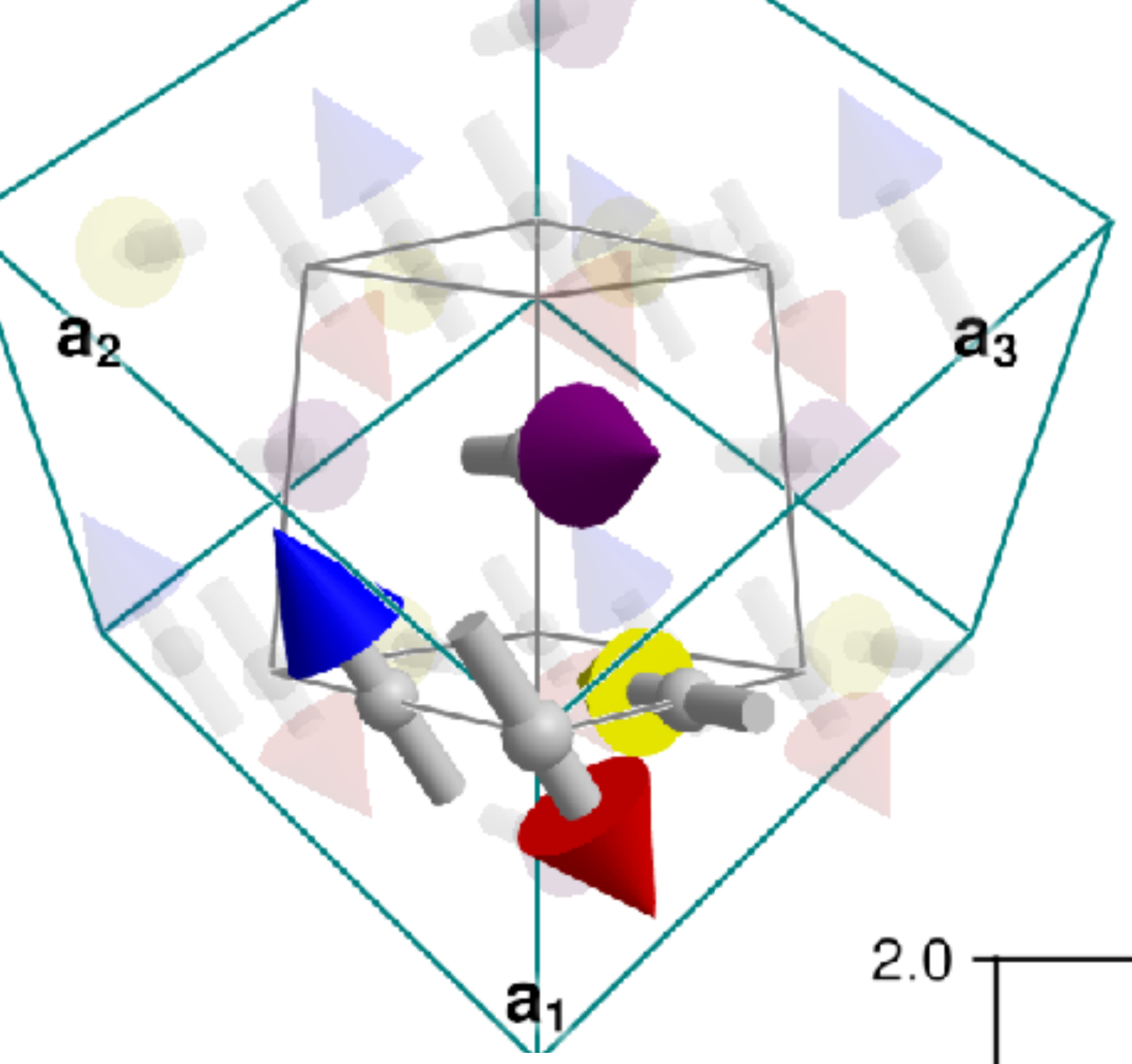




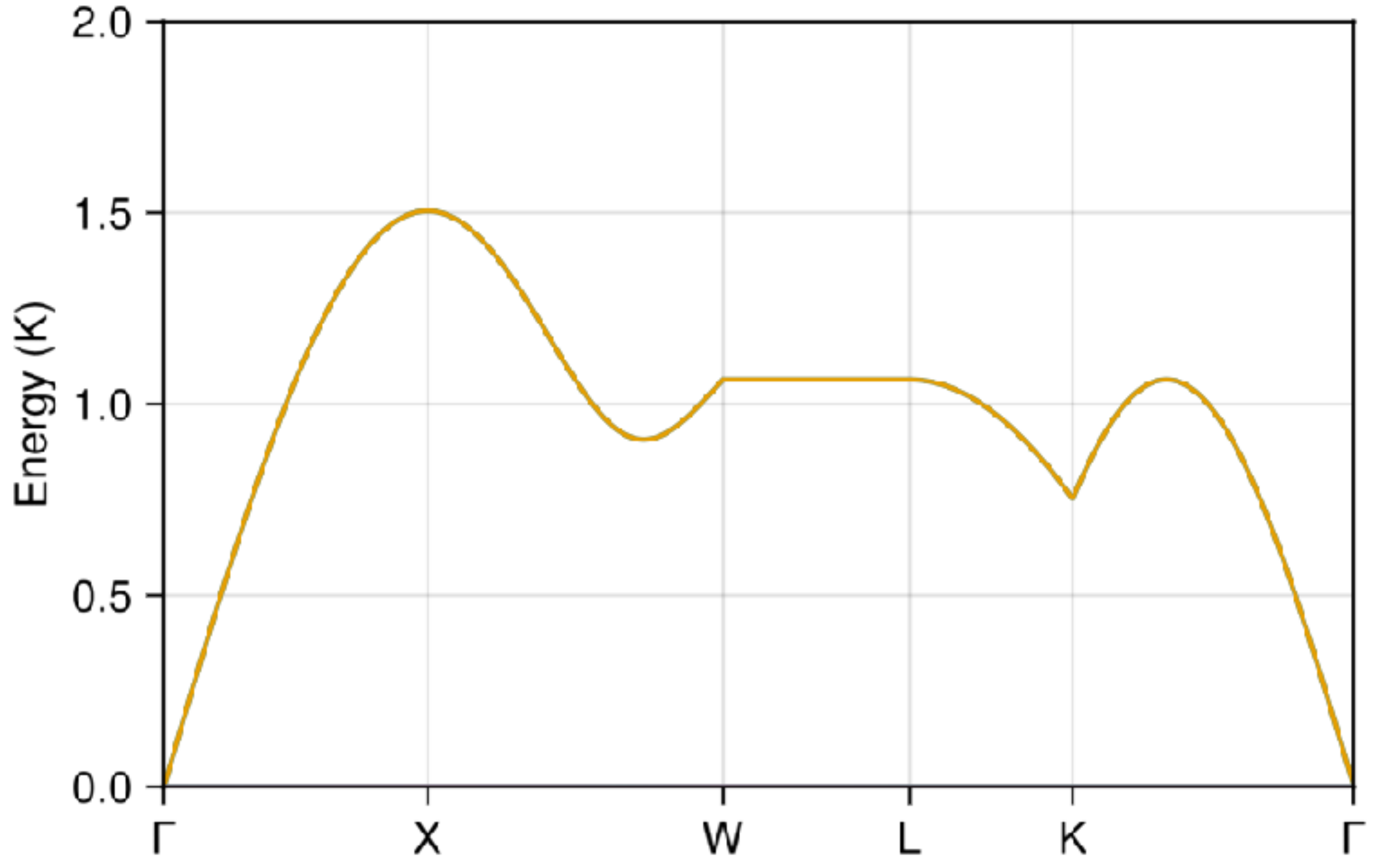
vs. traditional spin wave theory

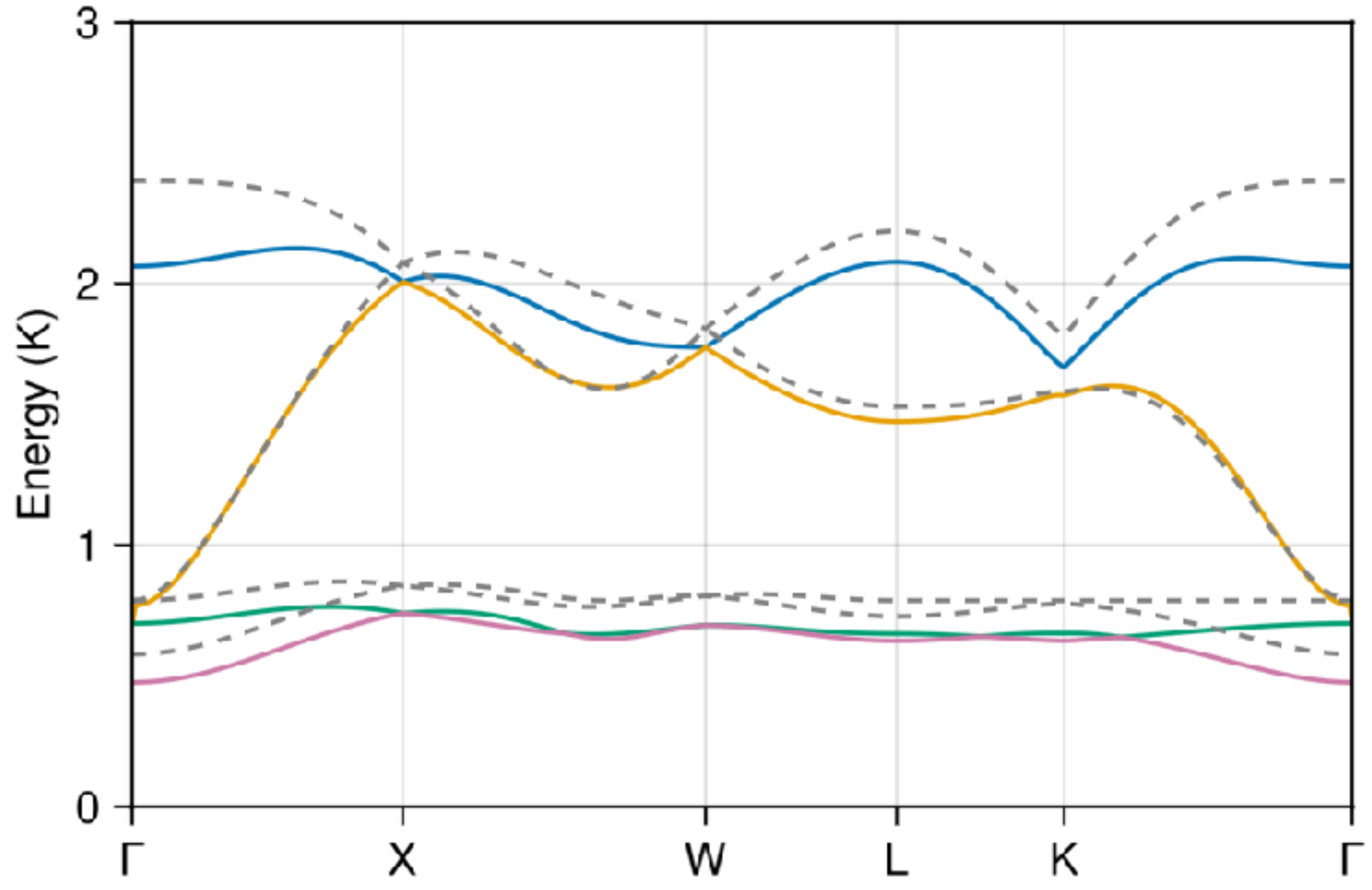
Sunny structure





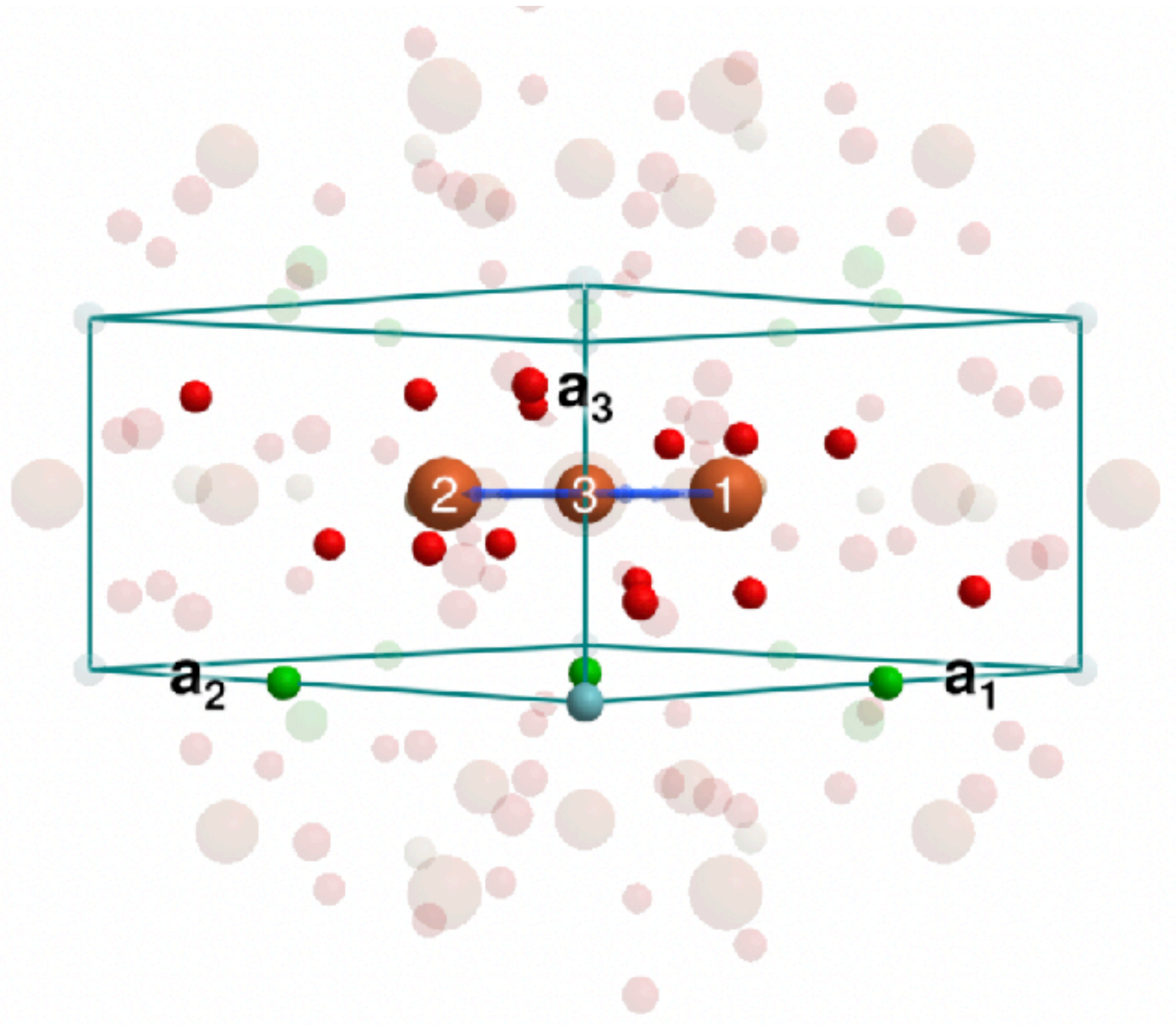
Long-range dipole-dipole

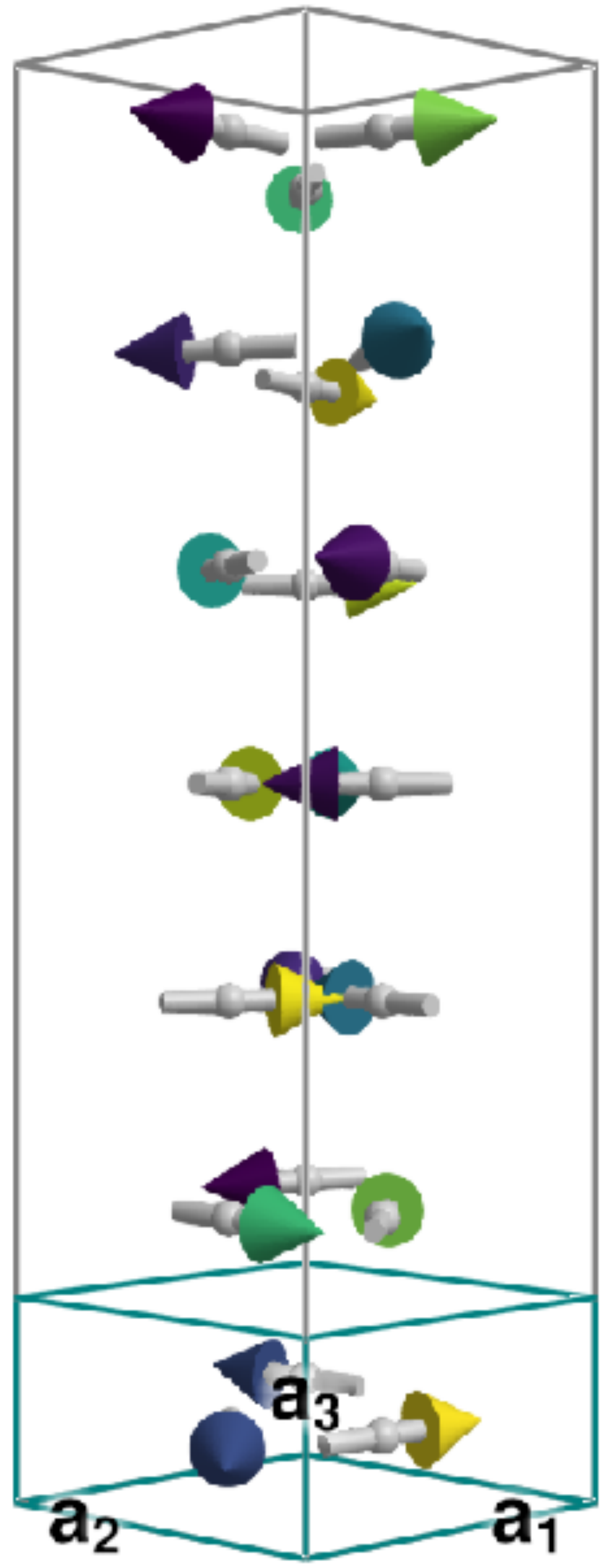




https://sunnysuite.github.io/Sunny.jl/stable/examples/07_Dipole_Dipole.html

Incommensurate spiral order





SpinW

Sunny

https://sunnysuite.github.io/Sunny.jl/stable/examples/spinw/SW15_Ba3NbFe3Si2O14.html

Classical dynamics beyond spin waves

Zhang et al, Nature Commun. **14**, 3626 (2023)

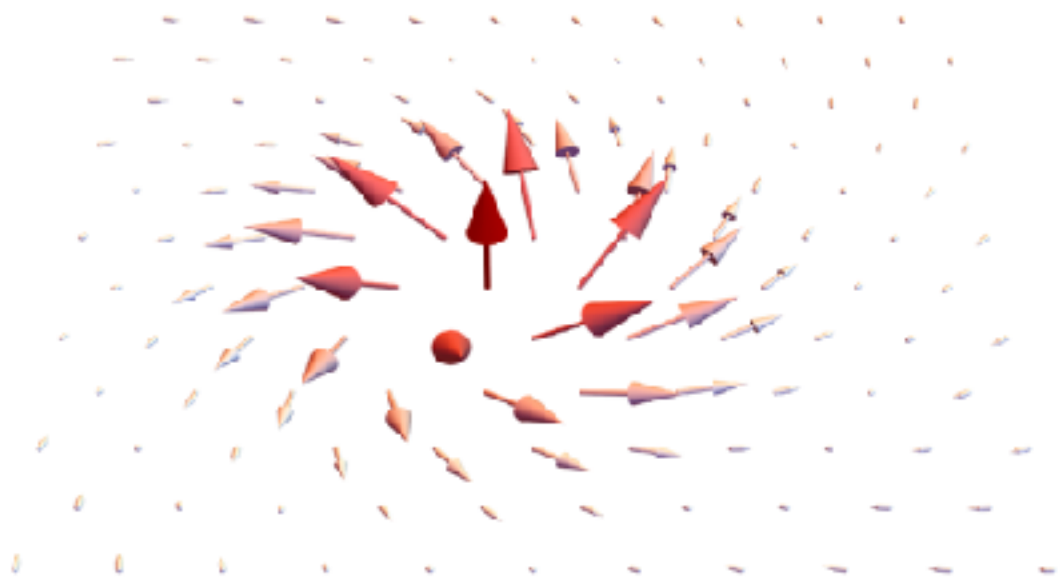
Baby skyrmions:

$$S^2 \mapsto S^2$$
$$\pi_2(S^2) \cong \mathbb{Z}$$

dipole + quadrupole ↔ 3 level state

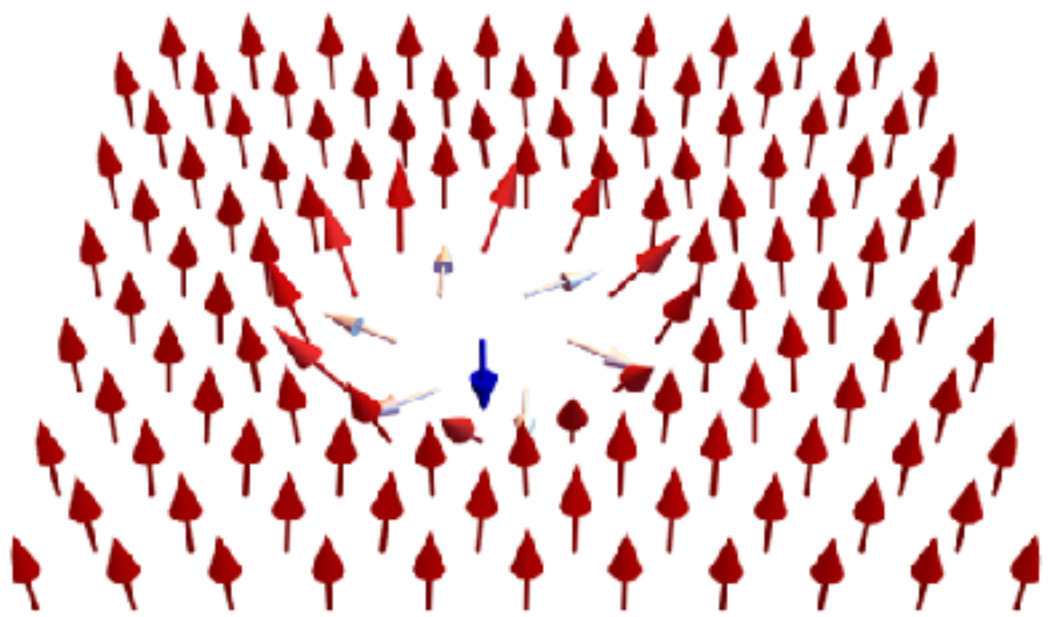
CP² skyrmions for spin-1:

$$S^2 \mapsto \mathrm{CP}^2$$
$$\pi_2(\mathrm{CP}^2) \cong \mathbb{Z}$$

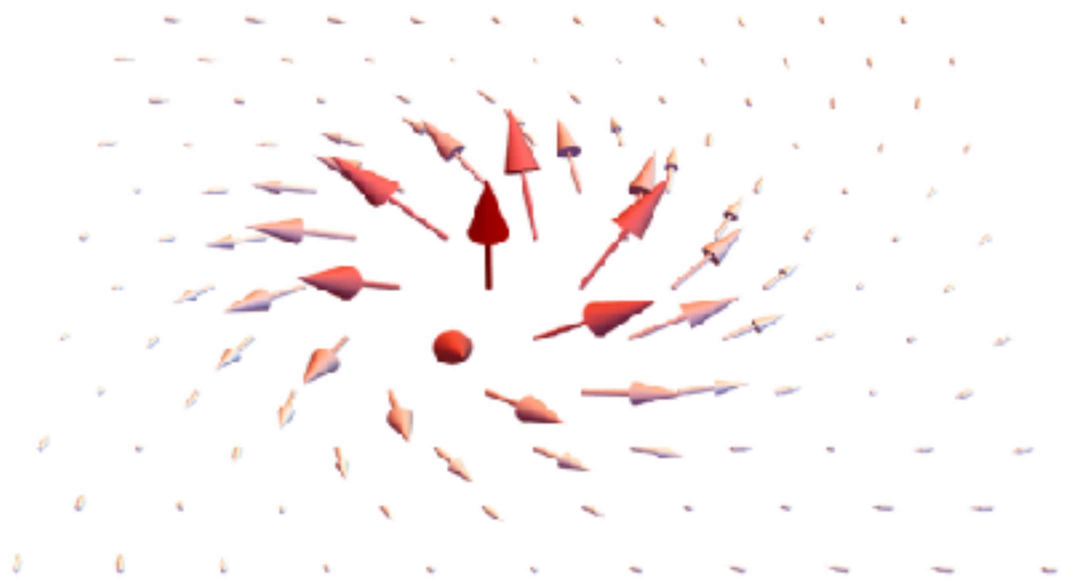


Topologically protected state on top of "boring" quantum paramagnet!

Examples

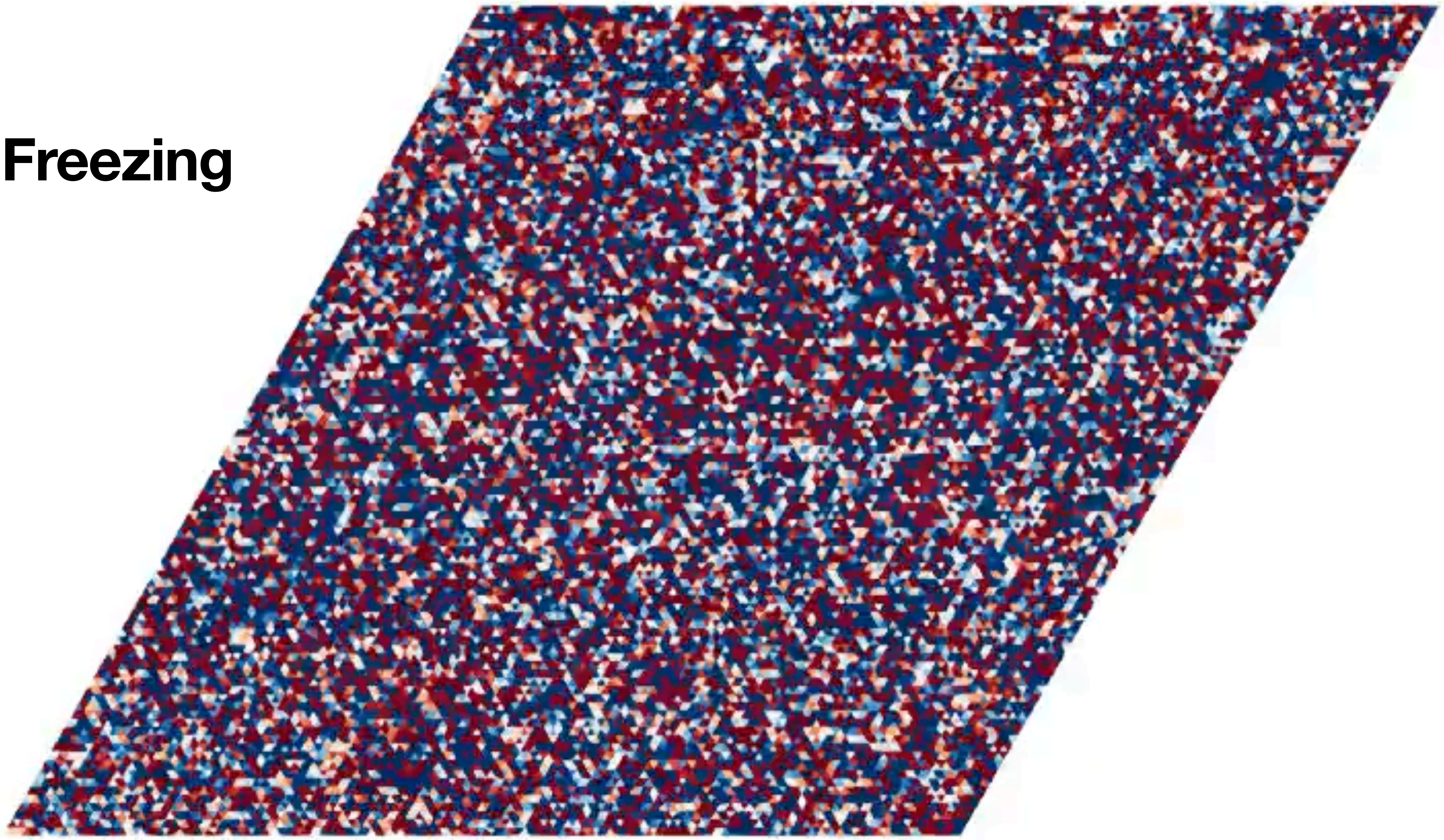


Traditional skyrmion

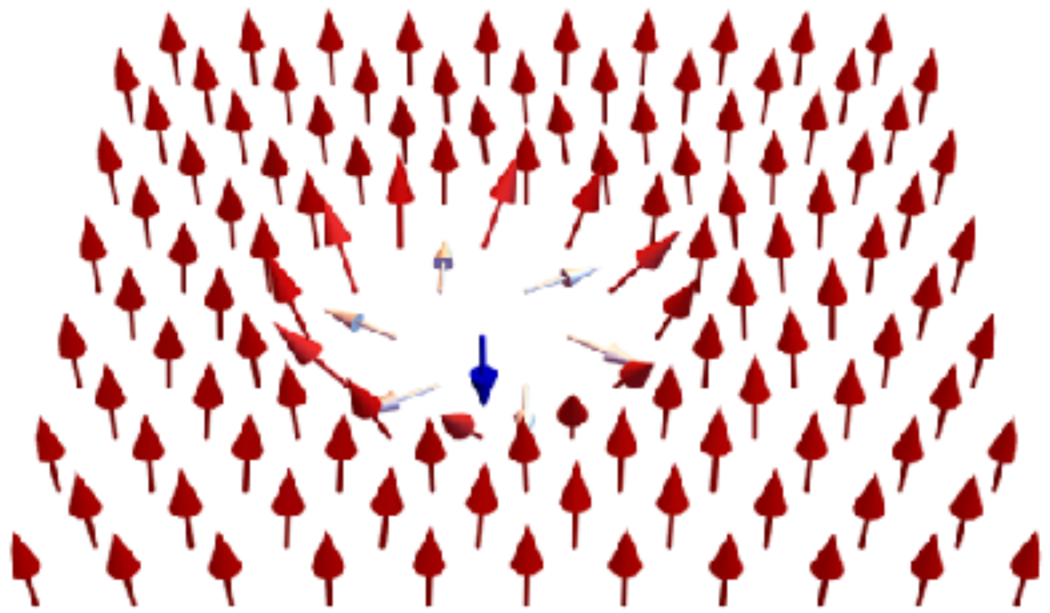


New CP^2 skyrmion

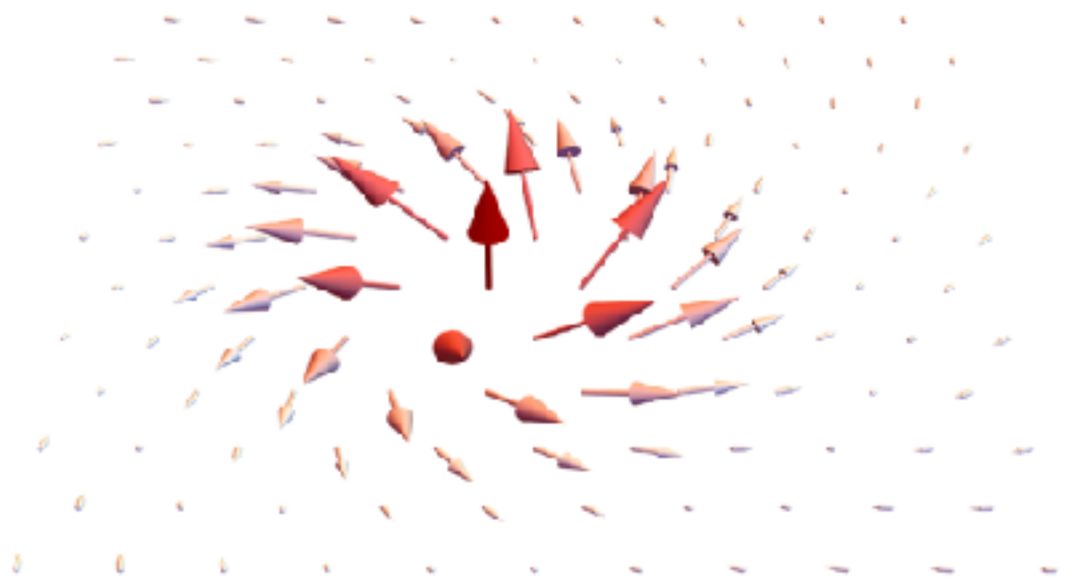
Freezing



Examples

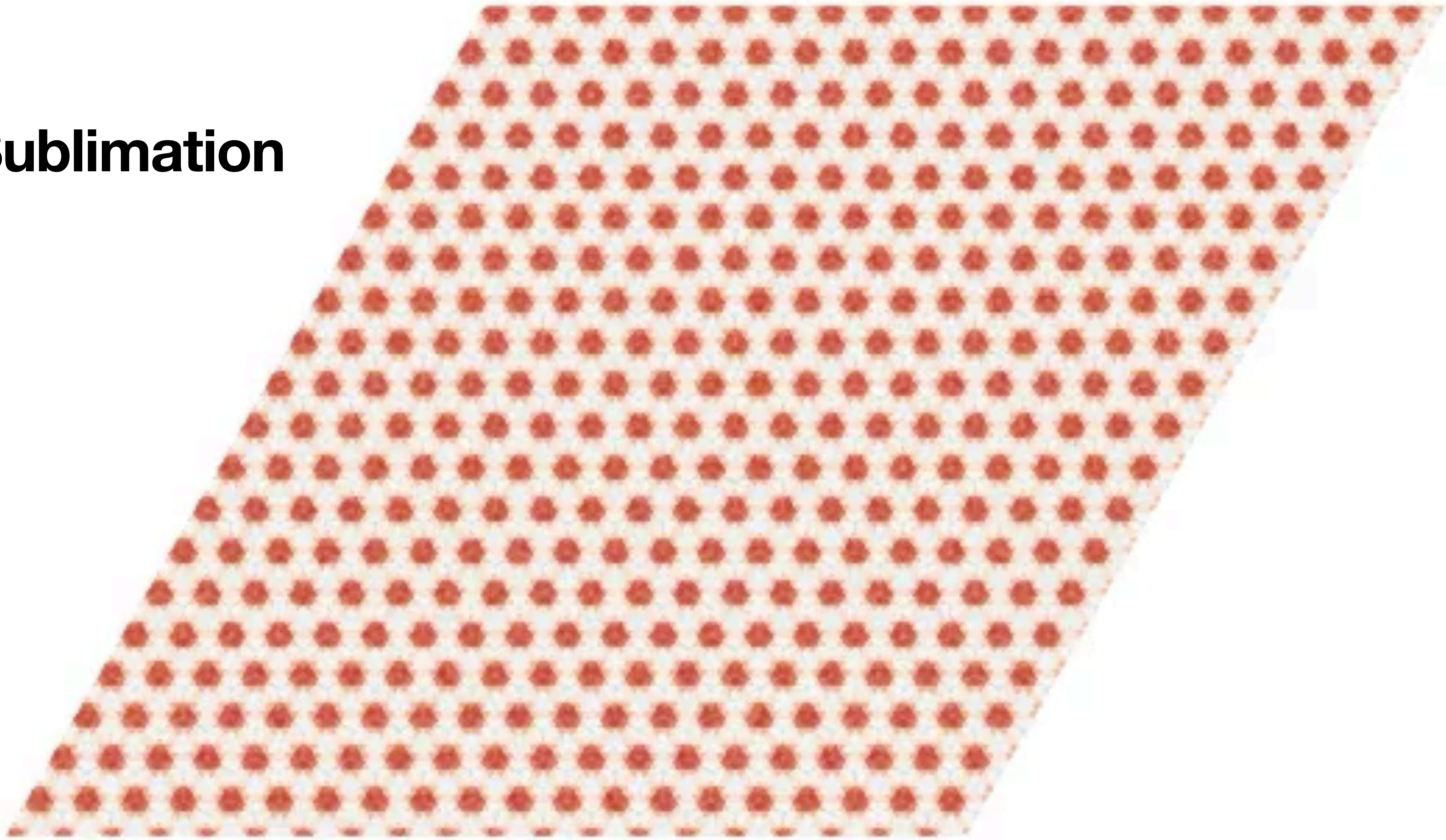


Traditional skyrmion



New CP^2 skyrmion

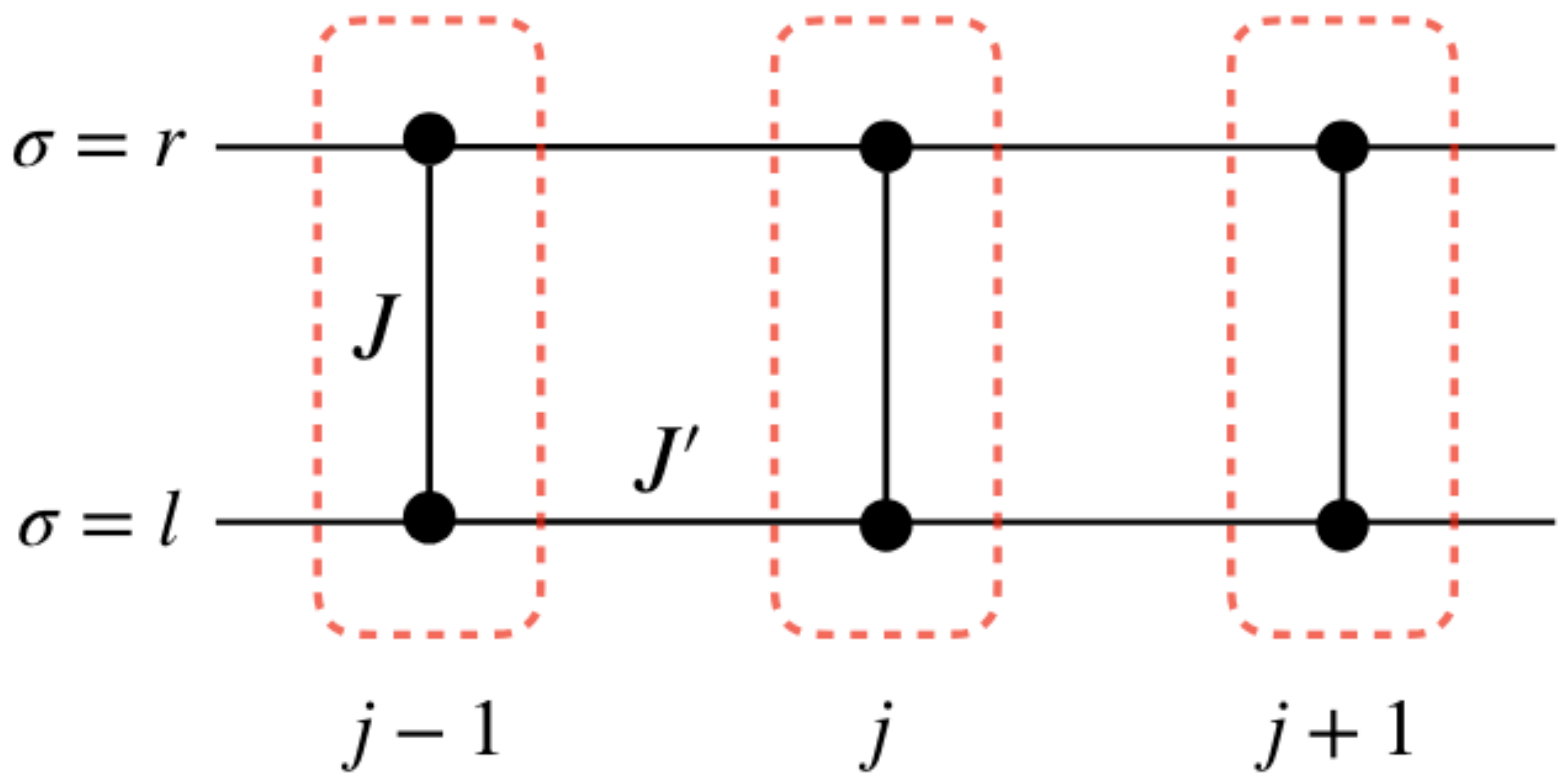
Sublimation



Feature preview: Entangled units

D. Dahlbom et al, Phys. Rev. B **110**, 104403 (2024)

Model as 1D chain, *N*=4
levels on each rung

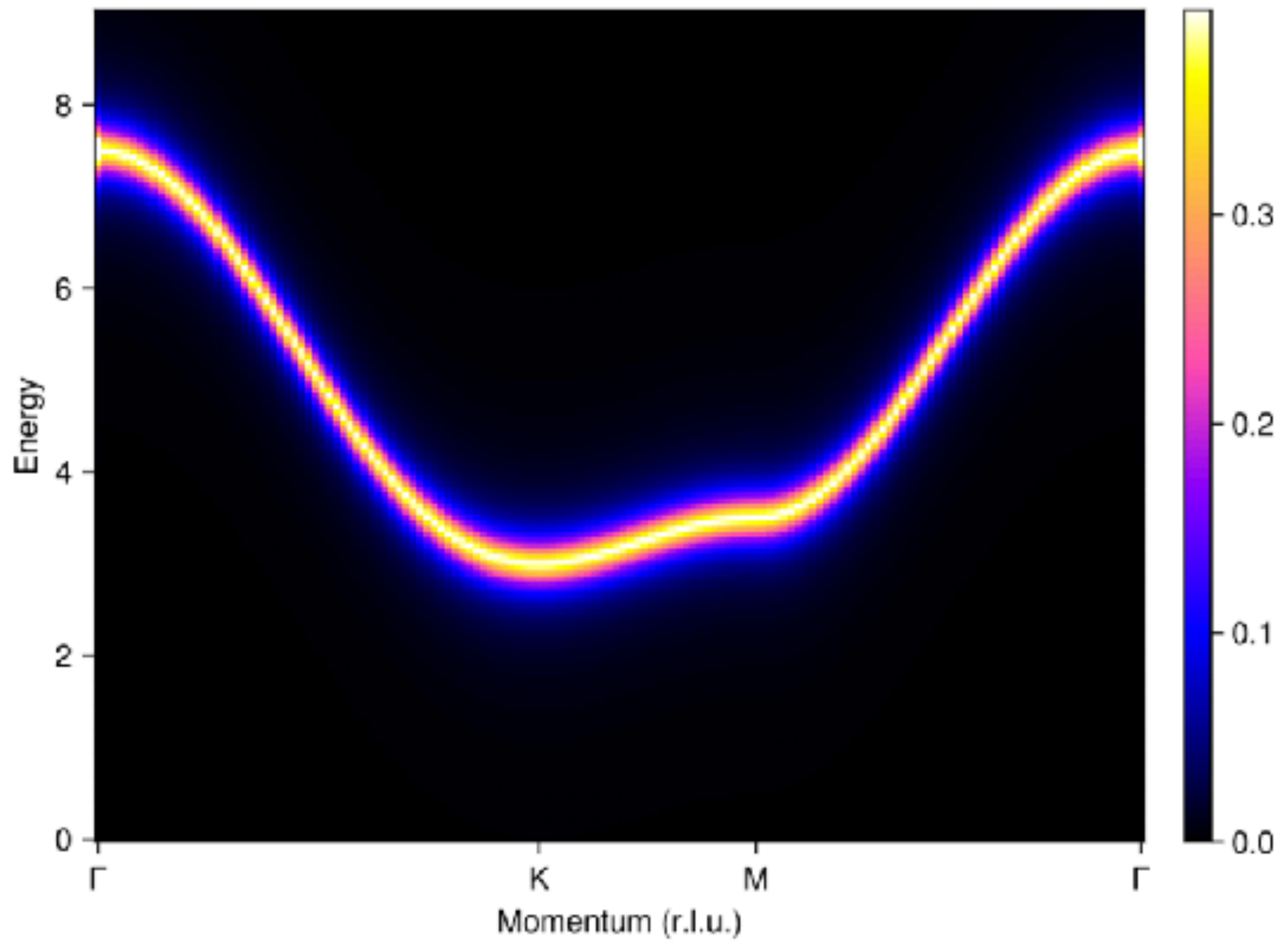


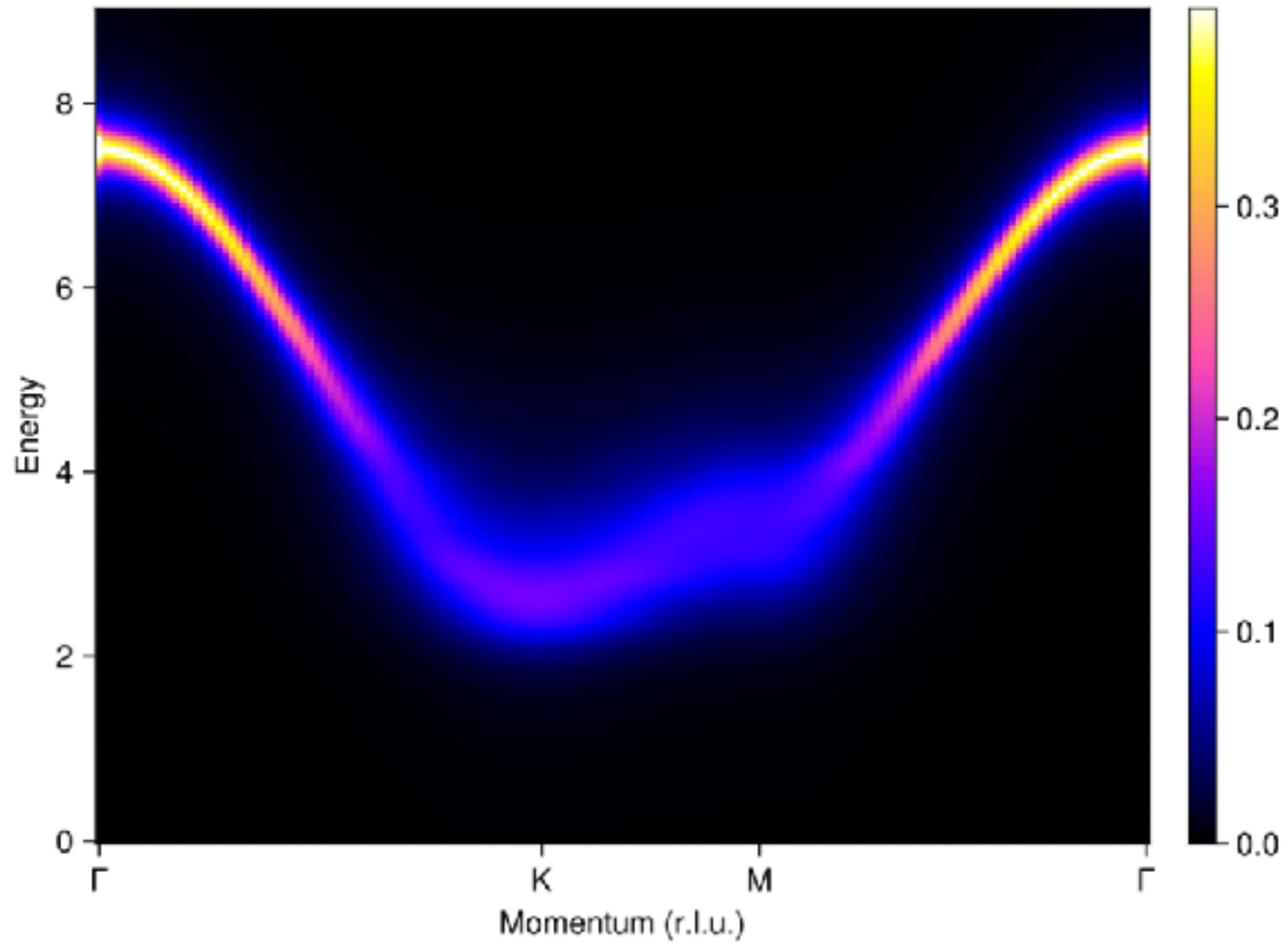
https://github.com/SunnySuite/SunnyContributed/blob/main/workshops/2024_09_ORNL/Thurs/EU-ladder.jl

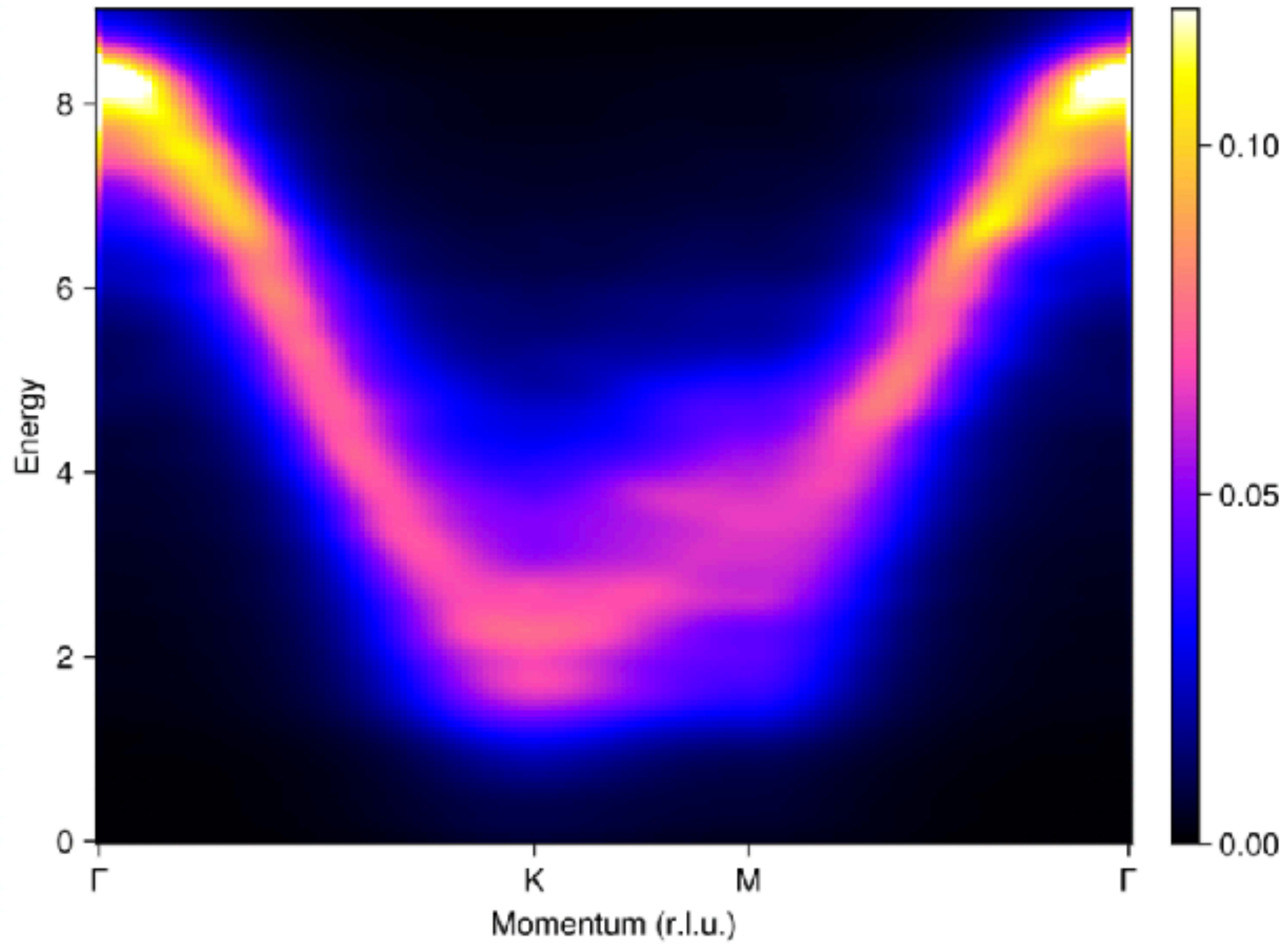
Disordered systems with KPM

H. Lane et al, SciPost Phys. **17**, 145 (2024)

H. Lane et al. [arXiv: 2501.03980]



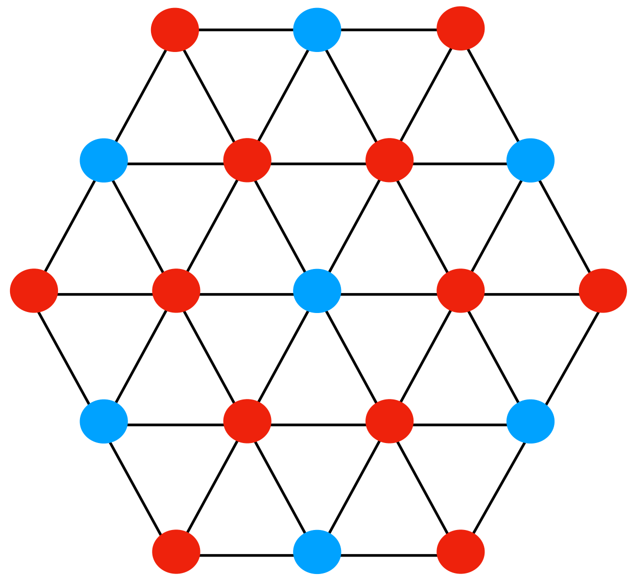




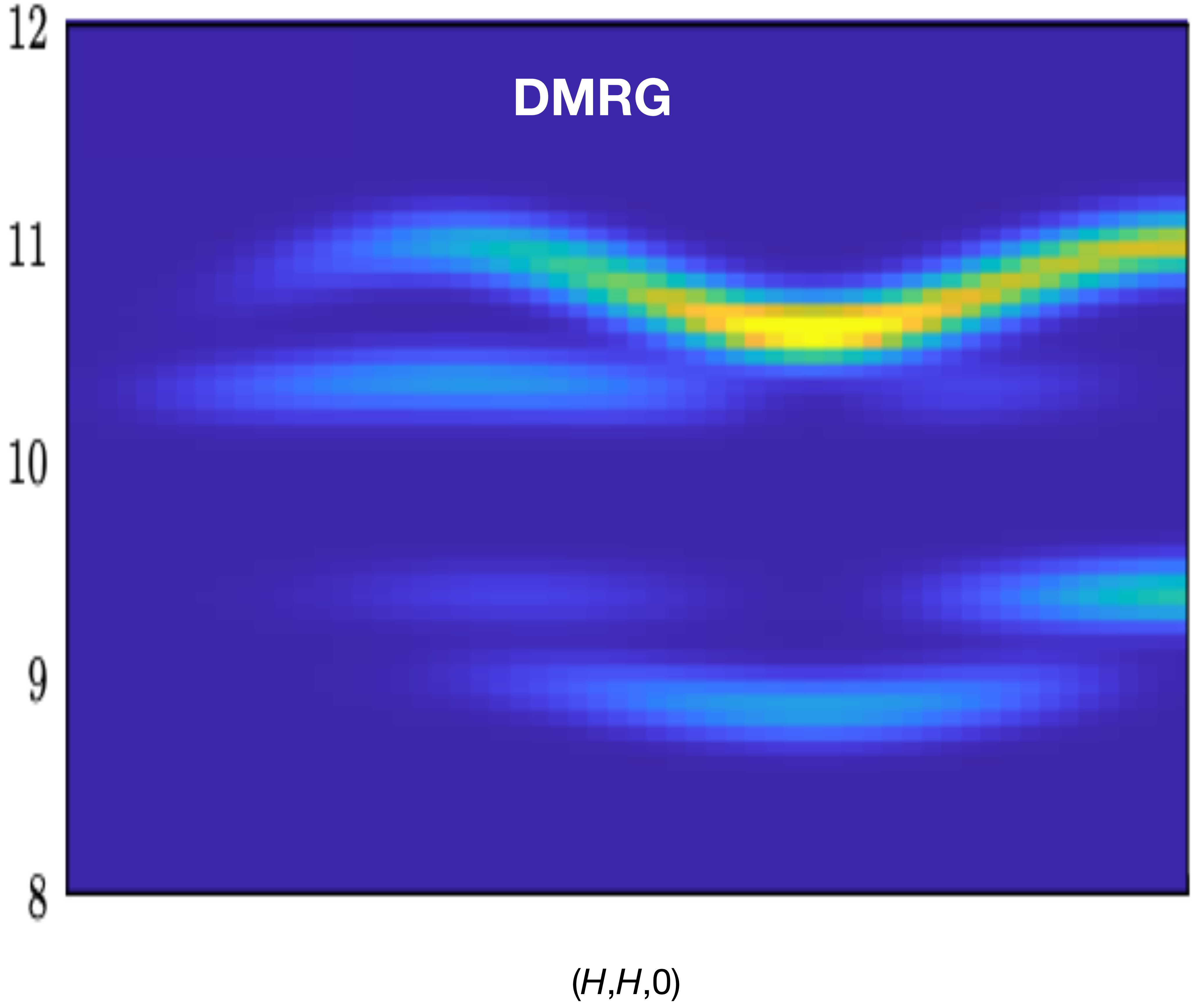
https://sunnysuite.github.io/Sunny.jl/stable/examples/09_Disorder_KPM.html

Feature preview: Corrections to Spin Wave Theory

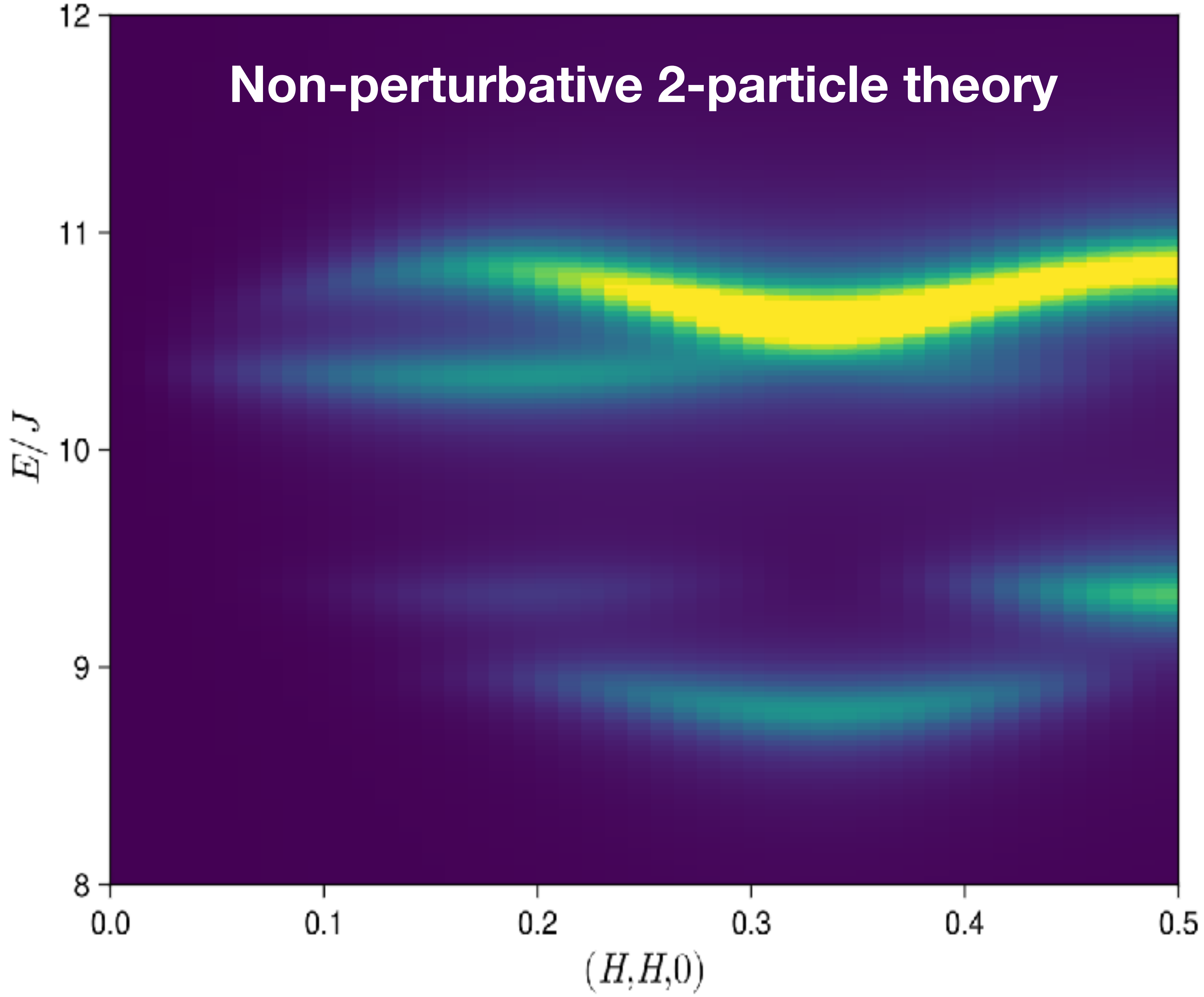
Spin bound states, Hao Zhang



$$\mathscr{H} = J\sum_{\langle i,j\rangle}\left[S_i^xS_j^x + S_i^yS_j^y + \Delta S_i^zS_j^z\right] - H\sum_i S_i^z$$



T. Xie, et al. *npj Quantum Materials* 8.1 (2023): 48.



In preparation

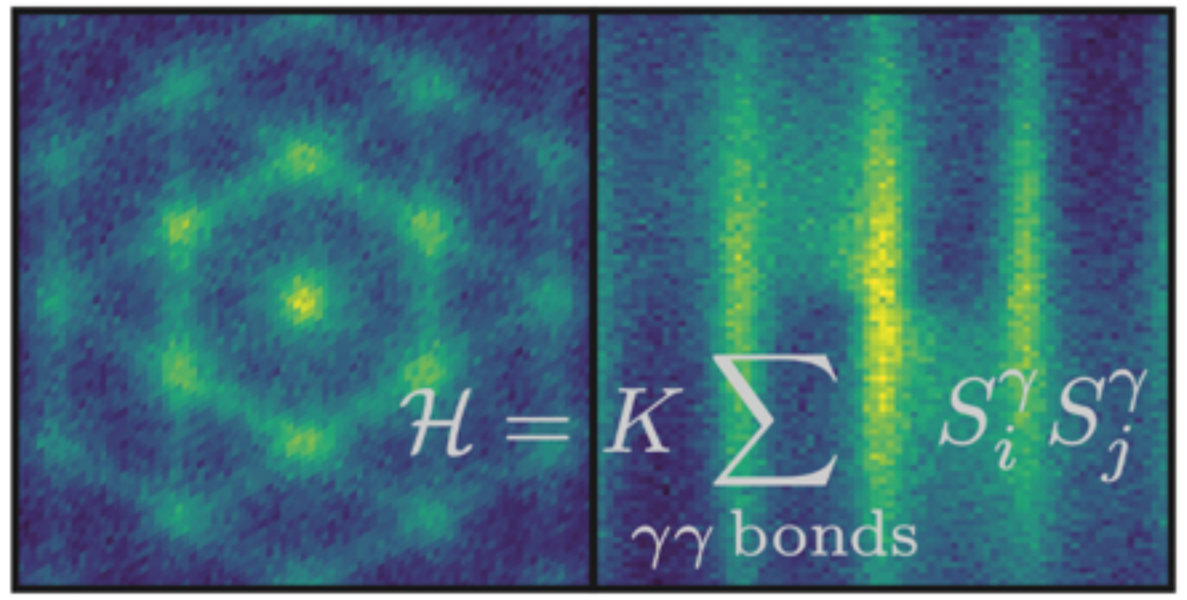
Feature preview: Self-consistent Gaussian approximation

(Harry Lane)

$$P[S] \sim \exp[-\beta S_{-\mathbf{q}}(J_{\mathbf{q}} + \lambda)S_{\mathbf{q}}]$$

$$\int \langle S_{-\mathbf{q}} S_{\mathbf{q}} \rangle d^3\mathbf{q} = \text{const.}$$

Sunny



Spinteract

https://github.com/SunnySuite/Sunny.jl/pull/355

Thanks!

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- D. Dahlbom, H. Zhang, C. Miles, S. Quinn, A. Niraula, B. Thipe, M. Wilson, S. Matin, H. Mankad, S. Hahn, D. Pajerowski, S. Johnston, Z. Wang, H. Lane, Y. W. Li, X. Bai, M. Mourigal, C. D. Batista, K. Barros, *Sunny.jl: A Julia Package for Spin Dynamics* [arXiv:2501.13095].

- H. Zhang, C. D. Batista, *Classical spin dynamics based on SU(N) coherent states*, Phys. Rev. B **104**, 104409 (2021) [arXiv:2106.14125].
- D. Dahlbom, H. Zhang, C. Miles, X. Bai, C. D. Batista, K. Barros, *Geometric integration of classical spin dynamics via a mean-field Schrödinger equation*, Phys. Rev. B **106**, 054423 (2022) [arXiv:2204.07563].
- D. Dahlbom, C. Miles, H. Zhang, C. D. Batista, K. Barros, *Langevin dynamics of generalized spins as SU(N) coherent states*, Phys. Rev. B **106**, 235154 (2022) [arXiv:2209.01265].
- D. Dahlbom, H. Zhang, Z. Laraib, D. M. Pajerowski, K. Barros, C. D. Batista, *Renormalized Classical Theory of Quantum Magnets*, Submitted, [arXiv:2304.03874].
- D. Dahlbom, D. Brooks, M. S. Wilson, S. Chi, A. I. Kolesnikov, M. B. Stone, H. Cao, Y.-W. Li, K. Barros, M. Mourigal, C.D. Batista, X. Bai, *Quantum to classical crossover in generalized spin systems -- the temperature-dependent spin dynamics of FeI2*, Phys. Rev. B **109**, 014427 [arXiv:2310.19905].
- H. Lane, H. Zhang, D. Dahlbom, S. Quinn, R. D. Somma, M. Martin, C. D. Batista, K. Barros, *Kernel Polynomial Method for Linear Spin Wave Theory*, SciPost Phys. **17**, 145 (2024) [arXiv:2312.08349].