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Sunny.jl: A Julia Package for Spin Dynamics*

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Summary

Sunny is a Julia package designed to serve the needs of the quantum magnetism community. It supports the specification of a very broad class of spin models and a diverse suite of numerical solvers. These include powerful methods for simulating spin dynamics both in and out of equilibrium. Uniquely, it features a broad generalization of classical and semiclassical approaches to SU(N) coherent states, which is useful for studying systems exhibiting strong spin-orbit coupling or local entanglement effects. Sunny also offers a well-developed framework for calculating the dynamical spin structure factor, enabling direct comparison with scattering experiments. Ease of use is a priority, with tools for symmetry-guided modeling and interactive visualization.

Statement of need

Progress in quantum magnetism depends on the development of accurate models of magnetic materials. Scattering techniques, such inelastic neutron scattering (INS) and resonant inelastic X-ray scattering (RIXS), are among the most informative methods available for probing the dynamics of quantum magnets, yielding the dynamical spin structure factor $\mathcal{S}(\mathbf{q},\omega)$ as experimental output. To evaluate the validity of a hypothetical model, it is necessary to calculate $\mathcal{S}(\mathbf{q},\omega)$ theoretically. This is generally an intractable problem that must be treated numerically or with various approximation schemes. The difficulty of this step represents a bottleneck in the development of accurate models and impedes the advancement of our understanding of quantum materials.

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The Sunny project is a collaborative effort among theorists, experimentalists and computational scientists aimed at developing theoretical and numerical methodologies for modeling realistic quantum magnets. The central product of this effort is the Sunny software package, which makes recent theoretical advances available in a form readily accessible to students and researchers. Distinguishing features of Sunny include:

- Symmetry analysis tools that facilitate model specification, visualization and data retrieval.
- A suite of optimizers, Monte Carlo samplers, and spin dynamics solvers that can all be applied to the same system specification.
- Implementation of the SU(N) coherent state formalism for classical and semiclassical calculations.
- An interface tailored toward the needs of scattering scientists, with tools for integrating scattering intensities over regions of reciprocal space.
- Code written entirely in Julia, a language that can achieve speeds comparable to C++ or Fortran while offering an interactive workflow that will be familiar to users of Python and Matlab.
- A well documented codebase, an extensive collection of correctness tests, a website featuring many tutorials, and an active Slack channel where users can ask questions.

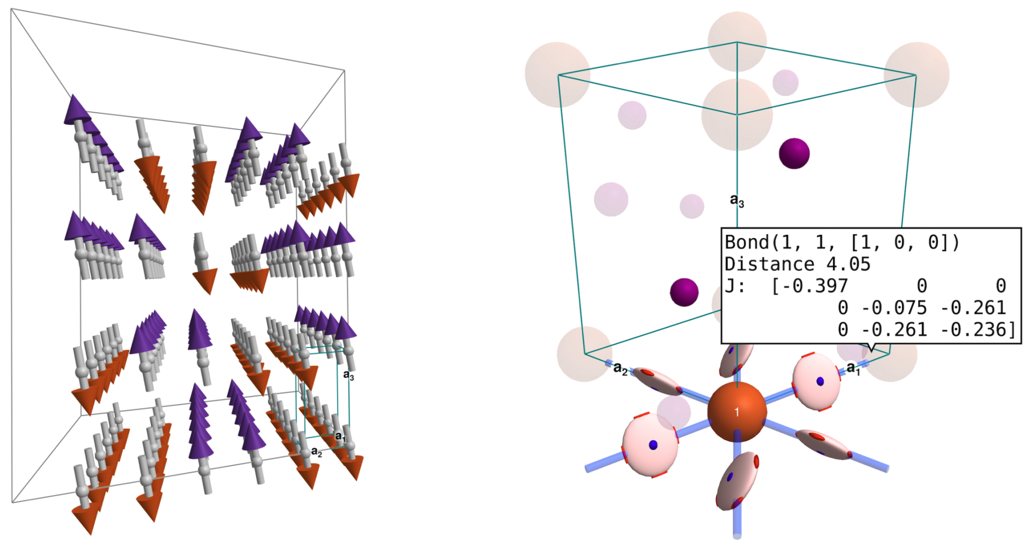
There are a number of existing codes that can calculate $\mathcal{S}(\mathbf{q},\omega)$ using linear spin wave theory (LSWT), some of which have served as inspiration to the Sunny project [Rotter (2004); (2024a); Petit & Damay (2016); weber:2016; (2024b)]. The symmetry analysis tools of SpinW in particular have served as a model (Toth & Lake, 2015). There are also codes that perform classical spin simulations using Landau-Lifshitz (LL) dynamics (2024c; Evans et al., 2014; Müller et al., 2019). Sunny is unique in offering both approaches and generalizing them through a formalism based on SU(N) coherent states (Muniz et al., 2014; H. Zhang & Batista, 2021). Sunny additionally permits completely general single-ion anisotropies and coupling of multipolar moments; provides an efficient implementation of long-range dipole-dipole interactions; automates the application of a number of quantum renormalizations (Dahlbom et al., 2023); and offers iterative solvers for efficient LSWT on large magnetic cells (Lane et al., 2024).

The value of collecting all these tools together in a modern, easy-to-use package is evidenced by the large number of publications that have already made use of Sunny, a partial list of which is maintained on the GitHub wiki (2024d). We note a number of experimental studies that have relied on Sunny for analysis (Bai et al., 2021, 2023; Do et al., 2023; Kim et al., 2023; Lee et al., 2023; Na et al., 2024; Nagl et al., 2024; Paddison et al., 2024; Park et al., 2023; Park, Sala, et al., 2024; Park, Ghioldi, et al., 2024; Park, Cho, et al., 2024; Scheie et al., 2023); as well as theoretical and methodological works (Dahlbom, Brooks, et al., 2024; Dahlbom, Thomas, et al., 2024; H. Zhang et al., 2023; Hao Zhang & Lin, 2024). Additional papers documenting the theoretical and algorithmic advances that have enabled the development of Sunny are discussed below.

Feature Overview

Symmetry analysis

By unifying and extending existing open source frameworks for the symmetry analysis of crystals – including Spglib (Togo et al., 2024), Brillouin.jl (2024e), and CrystalInfoFramework.jl (2024f) – Sunny facilitates the process of determining the complete set of interactions allowed by spacegroup symmetries. Similarly, any interaction specified on a site or bond will be automatically propagated to all symmetry-equivalent sites and bonds, as required by the spacegroup symmetries. Models may also be specified according to symmetry properties and subsequently made "inhomogenous," allowing the arbitrary modification of pair interactions and site properties without regard to symmetry constraints. This greatly facilitates the modeling of systems exhibiting chemical disorder. Finally, the symmetry information enables convenient specification of paths and slices through reciprocal space, aiding visualization and comparison to experimental data. All these tools can be applied just as easily to a user-specified crystal or to a crystal loaded from an industry-standard CIF file (Hall et al., 1991).



a) b)

Figure 1: a) Ground state of $\mathrm{FeI_2}$, found using Sunny's `minimize_energy!` function and visualized with `plot_spins`. b) The crystal of $\mathrm{FeI_2}$ visualized with the `view_crystal` function. Hovering the cursor over a bond reveals the exchange interaction, if already assigned, or a general expression for all symmetry-allowed interactions.

Visualization

Both the symmetry analysis and data retrieval features of Sunny include 3D visualization tools built on the Makie package (Danisch & Krumbiegel, 2021). These can be used to plot spin configurations, investigate the symmetries of a crystal Figure 1, generate animations of dynamic behavior, and plot the predicted results of scattering experiments Figure 2.

SU(*N*) Formalism and System Modes

Traditional classical and semiclassical approaches to spin dynamics are based on the assignment of a classical dipole to each lattice site. Recent theoretical work has generalized this picture, replacing dipoles with richer objects, namely SU(*N*) coherent states. Such states capture the full structure of an *N*-level quantum system. Setting $N = 2s + 1$ enables the faithful representation of a quantum spin-s and of the crystal field levels of a single-ion. The formalism can also be adapted to model local entanglement effects, where this entanglement may be between the spin and orbital degrees of freedom on a single site or within a cluster of spins on different sites.

The SU(*N*) formalism applies equally to LSWT calculations (Muniz et al., 2014) and classical spin dynamics (H. Zhang & Batista, 2021). Users can access this framework simply by setting the "mode" of a spin system to `:SUN`. Sunny also offers a `:dipole` mode, which is similar to the traditional classical approach but includes quantum renormalizations of biquadratic and single-ion anisotropy terms (Dahlbom et al., 2023). Finally, there is a mode that implements the traditional approach without any additional corrections, `:dipole_uncorrected`. Most Sunny features are supported in all modes.

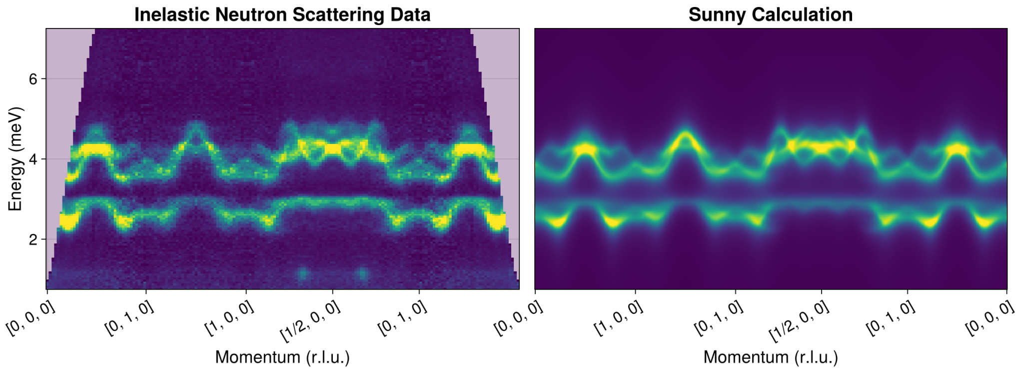


Figure 2: *Left*: Scattering intensities of $\mathrm{FeI_2}$ as measured on the SEQUOIA instrument at the Spallation Neutron Source, Oak Ridge National Laboratory (Bai et al., 2021). *Right*: Predicted scattering intensities calculated with Sunny's SU(N) linear spin wave solver. The figure was generated with Sunny's data retrieval and plotting functions.

Optimization and Monte Carlo Tools

Identifying a classical ground state is often the first step when calculating the scattering response of a magnet. Sunny provides several tools for finding such states, including gradient optimizers built on the Optim.jl package (Mogensen & Riseth, 2018). These optimizers work on supercells as well as spiral orderings. Sophisticated Monte Carlo tools are also provided, which can be used both to anneal into ground states and to estimate finite temperature statistics. In particular, the classical dynamics can be run with Langevin coupling to a thermal bath (Dahlbom, Miles, et al., 2022), and samplers are provided that implement the Wang-Landau (Wang & Landau, 2001) and parallel tempering algorithms (Swendsen & Wang, 1986).

Linear Spin Wave Theory (LSWT)

Sunny has extensive support for LSWT calculations, including for systems with arbitrarily complex single-ion anisotropies, general bilinear and biquadratic interactions, and long-range dipole-dipole interactions. Like SpinW, Sunny provides efficient LSWT calculations for systems that exhibit incommensurate spiral orderings (Toth & Lake, 2015). Additionally, Sunny provides tools to efficiently calculate $\mathcal{S}(\mathbf{q},\omega)$ on very large magnetic cells using iterative matrix-vector multiplications (Lane et al., 2024). The simulation of large supercells is essential to study systems with chemical disorder or complex magnetic orderings.

Classical Dynamics

The efficiency of LSWT calculations makes it the preferred tool when studying magnets near zero temperature. At elevated temperatures or in out-of-equilibrium conditions, however, classical dynamics becomes a valuable technique. Sunny supports both traditional Landau-Lifshitz dynamics and its generalization to SU(N) coherent states (H. Zhang & Batista, 2021). Dissipationless trajectories are calculated using a symplectic integration scheme (Dahlbom, Zhang, et al., 2022), and a generalization of the stochastic Landau-Lifshitz-Gilbert equations to SU(N) coherent states (Dahlbom, Miles, et al., 2022) enables the simulation of dynamics coupled to a thermal bath. This is particularly valuable for simulating, e.g., thermal transport, pump-probe experiments, and spin-glass relaxation.

Sunny as a Platform for Future Developments

To make these existing features more widely available, work at ORNL is underway to integrate Sunny into the Calvera platform for neutron data analysis (Watson et al., 2022). Sunny itself can serve as a platform for new solvers and analysis techniques, building on its mature model specification and data retrieval features. Current efforts are directed at supporting: the self-consistent Gaussian approximation for diffuse scattering, enabling functionality inspired by (Paddison, 2023); the modeling of local entanglement effects generated by spin-orbit coupling or strongly coupled clusters of spins; non-perturbative corrections to LSWT for the modeling of continua and bound states, which can be probed in INS and terahertz spectroscopy experiments (Bai et al., 2023; Legros et al., 2021); and observables relevant to RIXS experiments.

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