Sunny.jl: Overview and SU(N) Capabilities

ACNS Tutorial, 2024

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Su(n)ny

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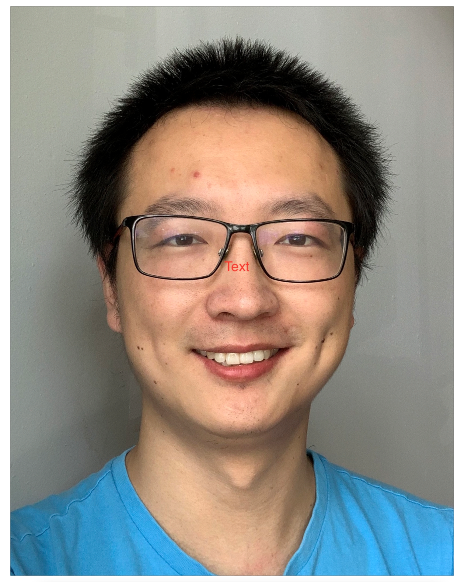

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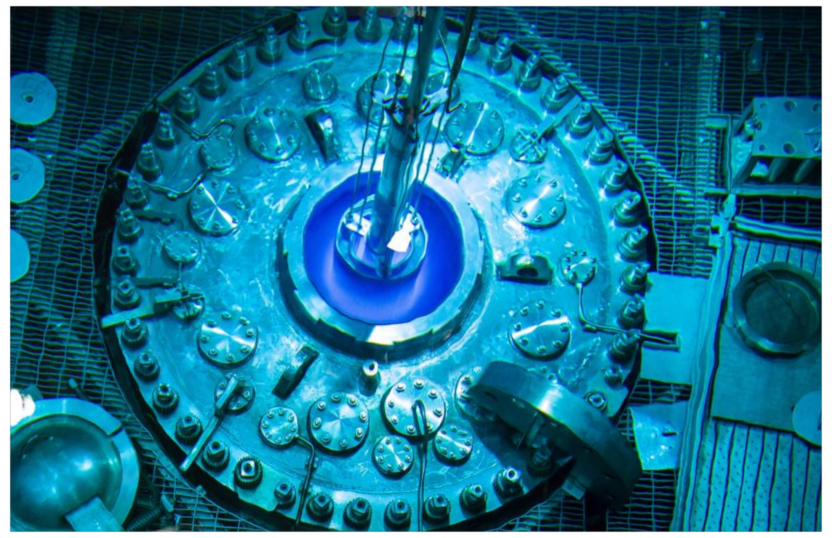

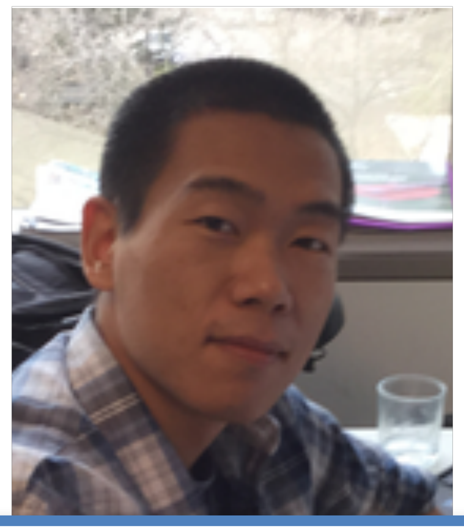

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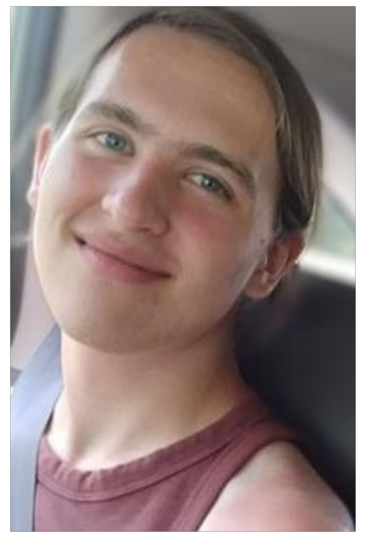

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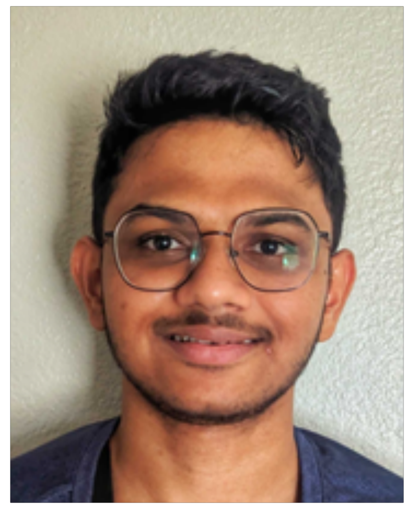

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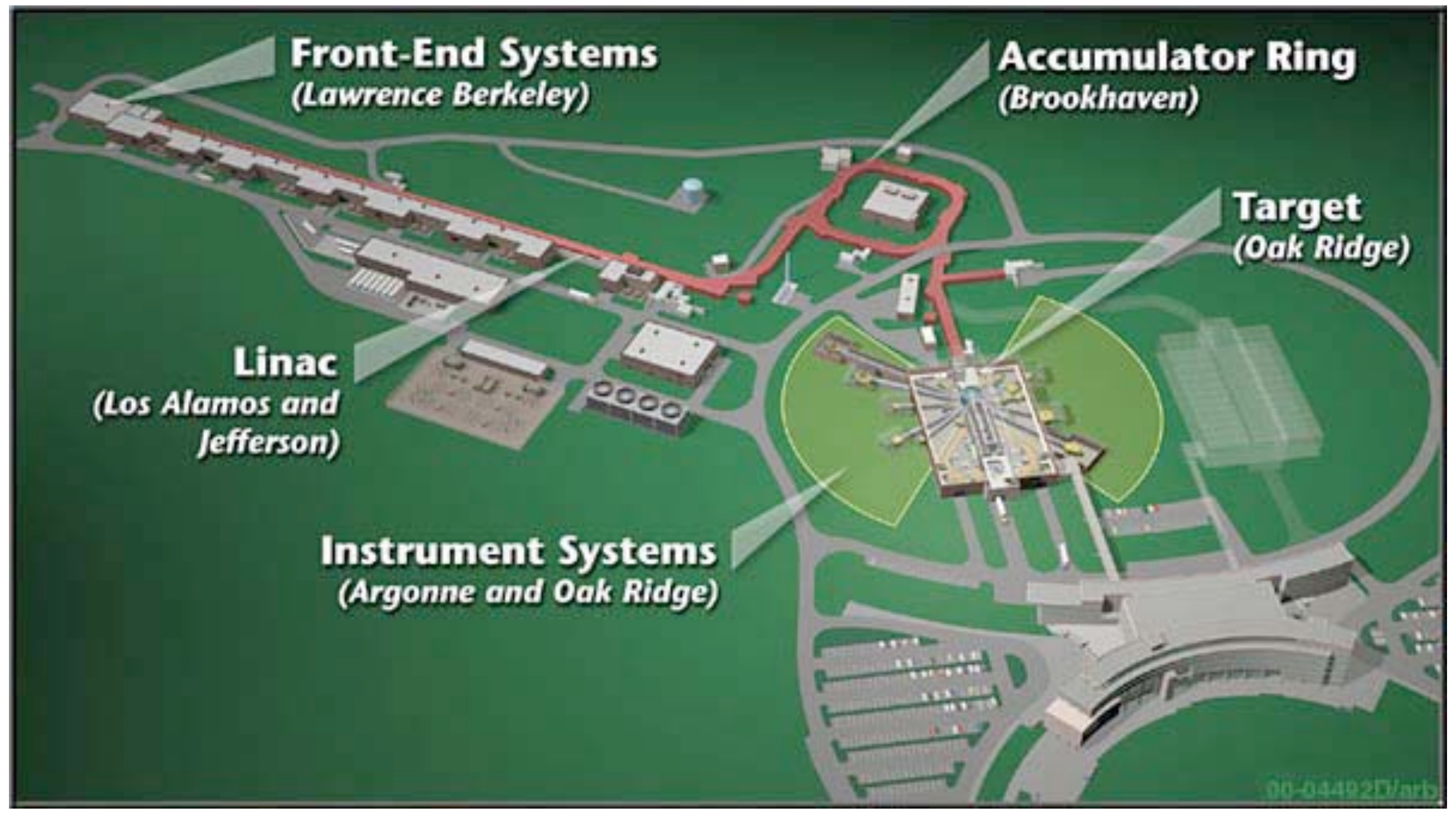
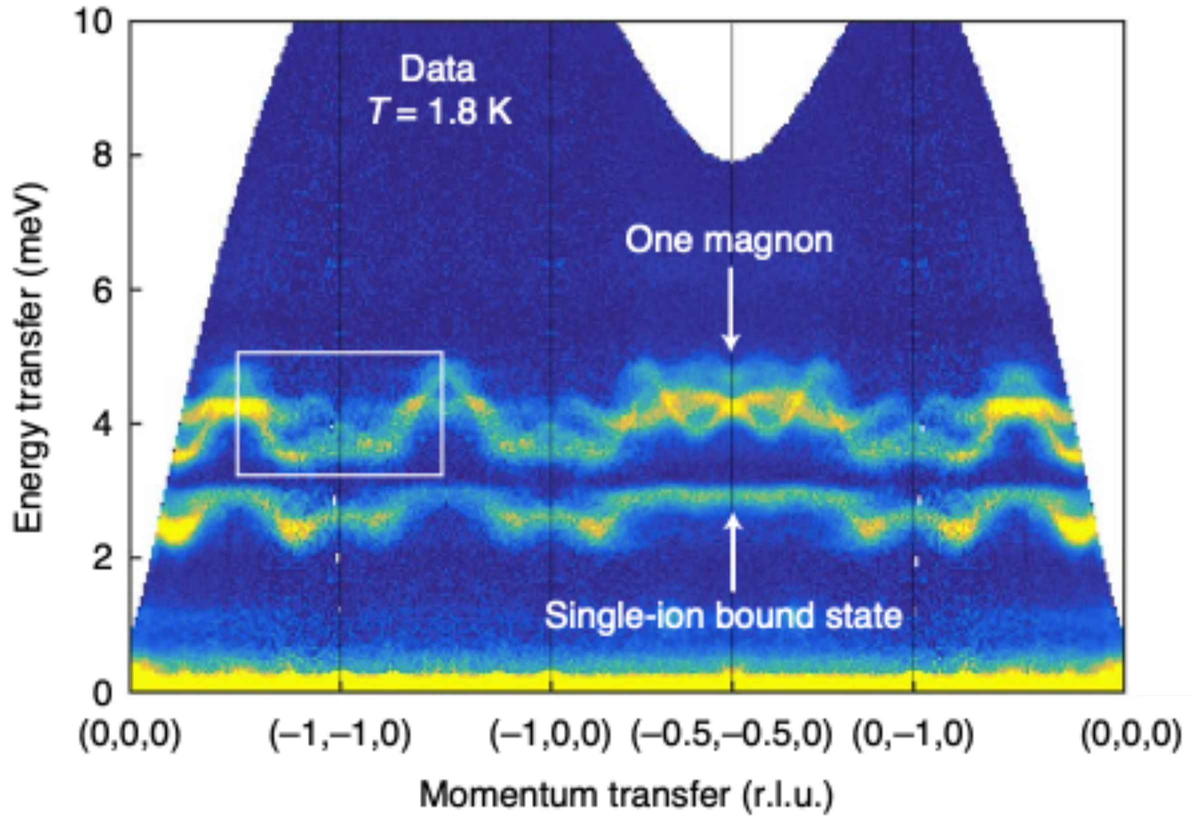
Motivation for developing Sunny

Experiment

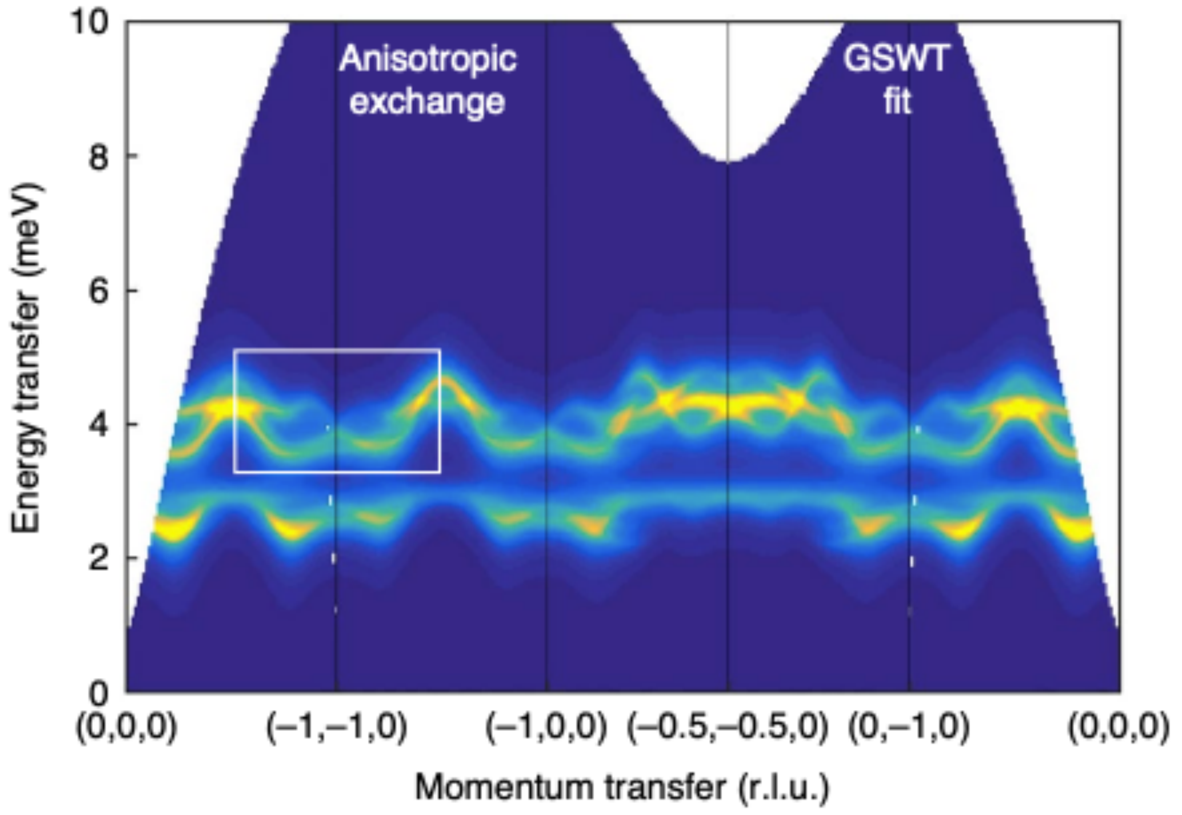




Theory

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

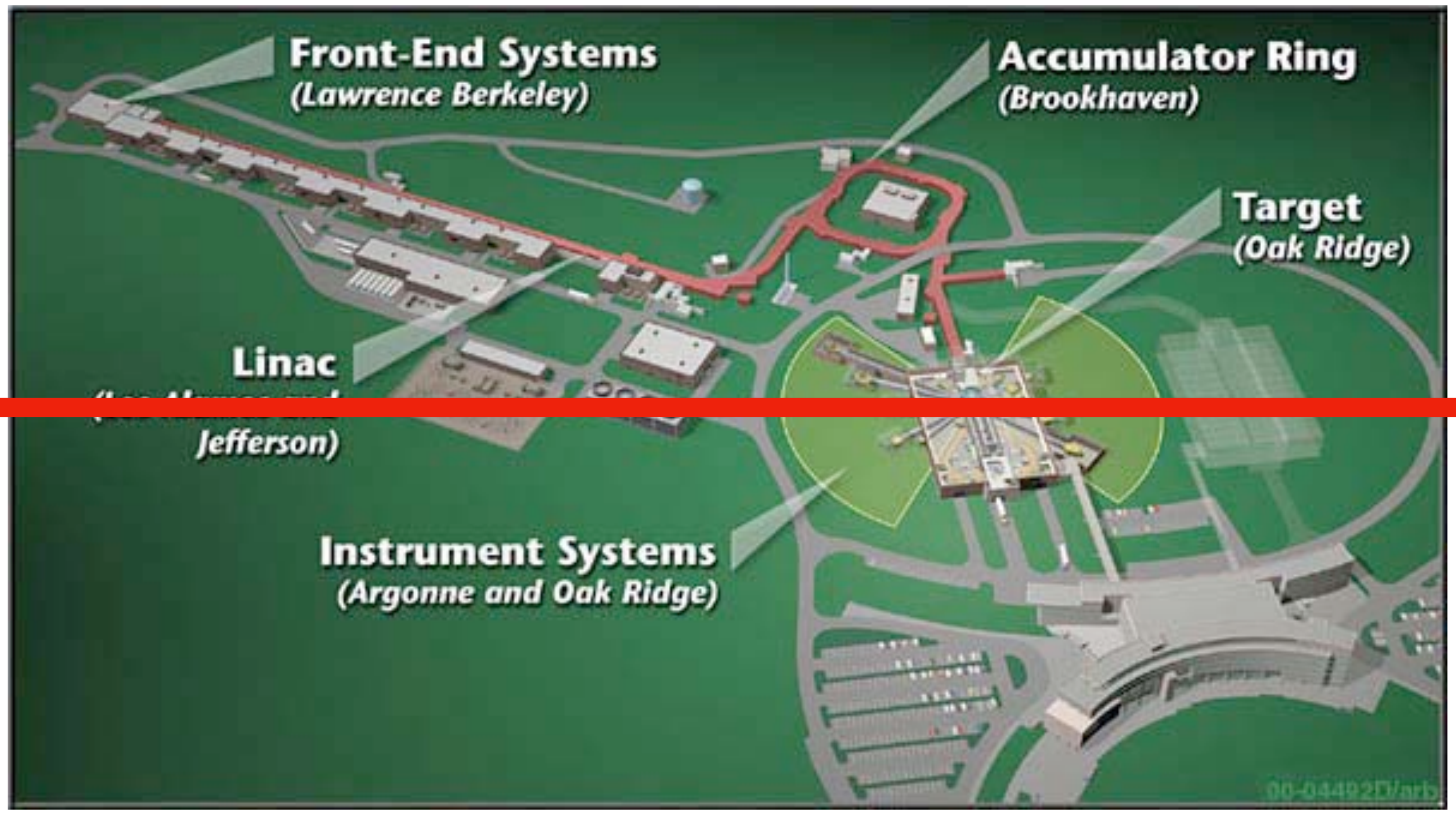
$$i\hbar \frac{d}{dt} |\Psi\rangle = \hat{\mathcal{H}} |\Psi\rangle$$

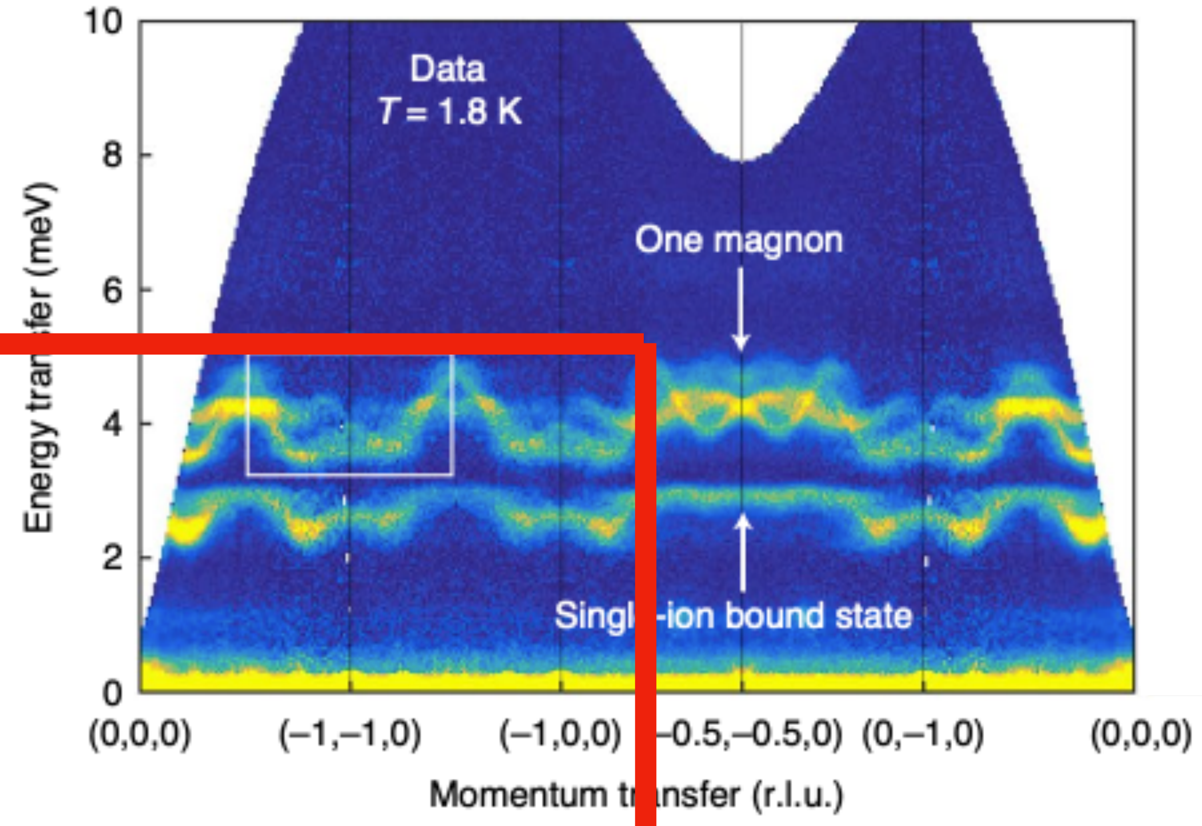


Xiaojian Bai, et al. Nature Physics, 17, 467-472 (2021)

Motivation for developing Sunny

Experiment





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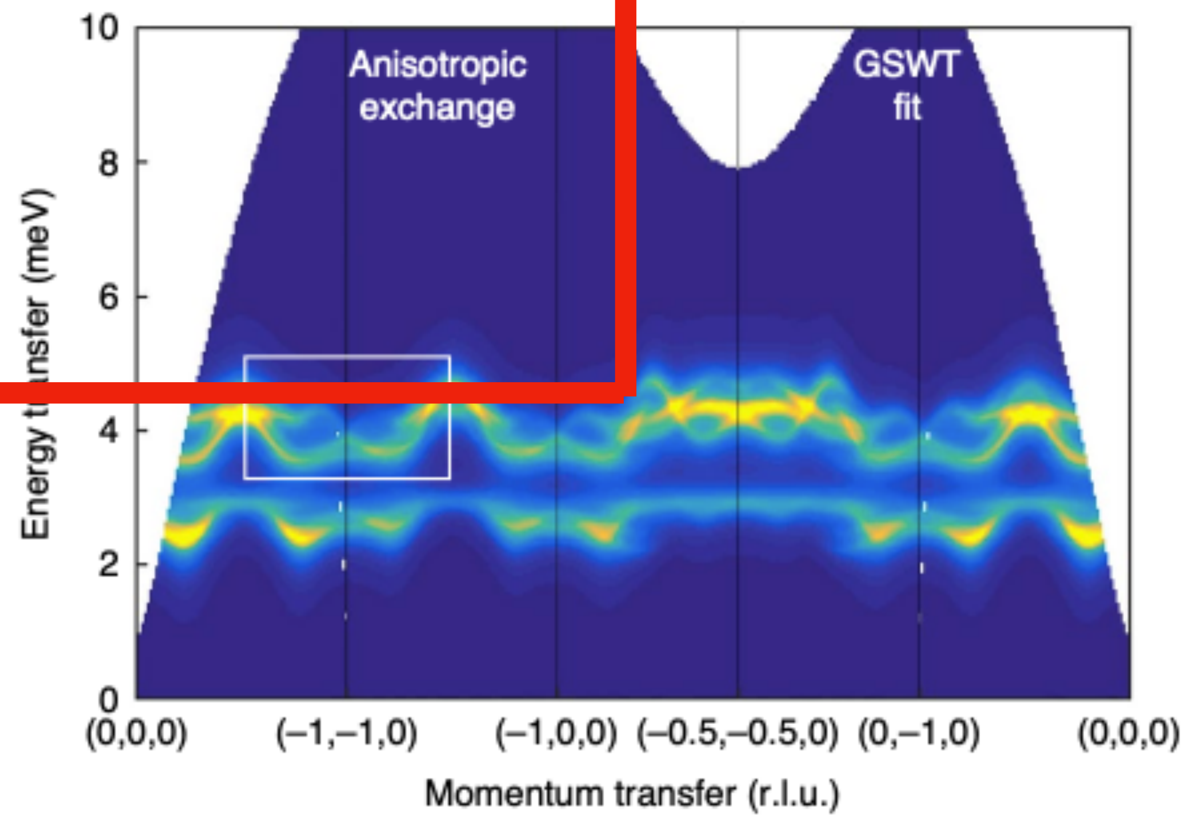
$$i\hbar \frac{d}{dt} |\Psi\rangle = \hat{\mathcal{H}} |\Psi\rangle$$



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Motivation for developing Sunny

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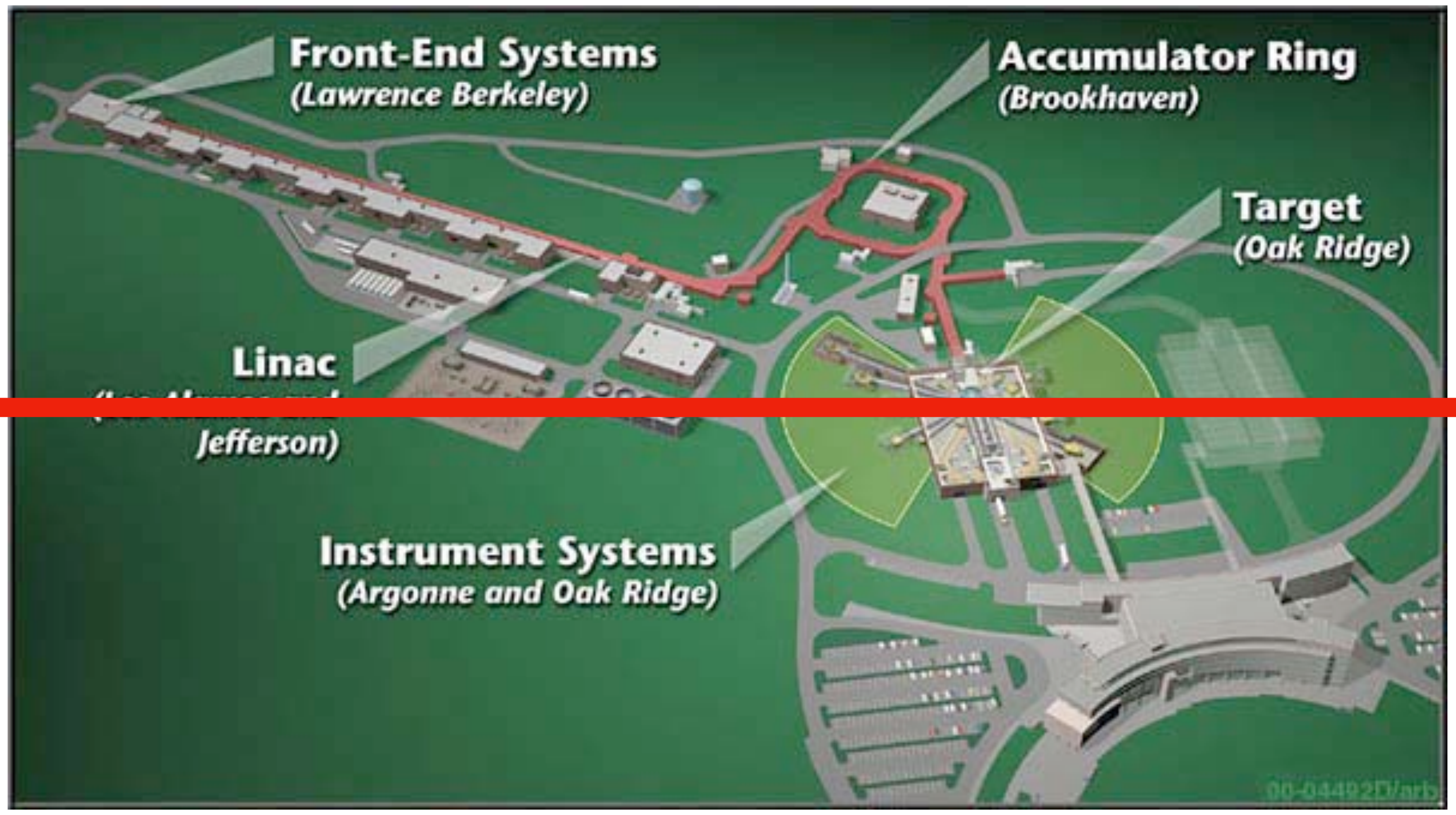
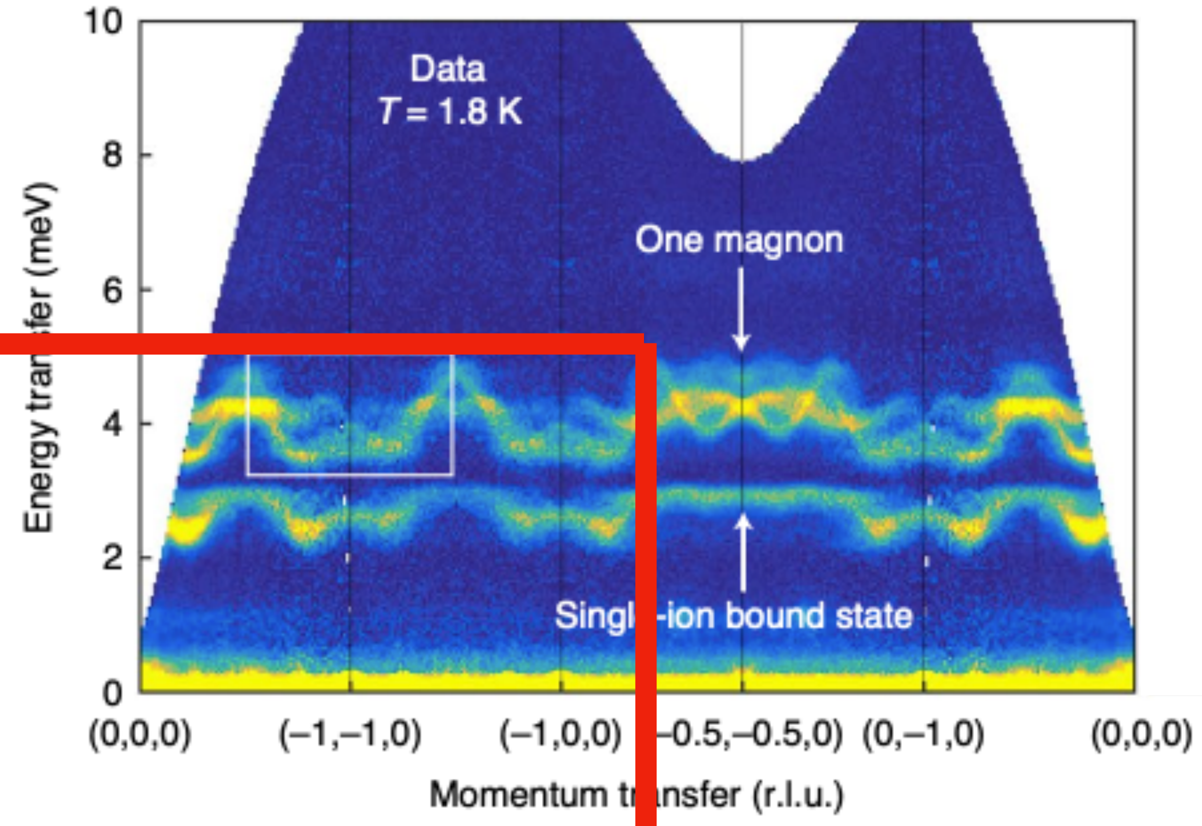


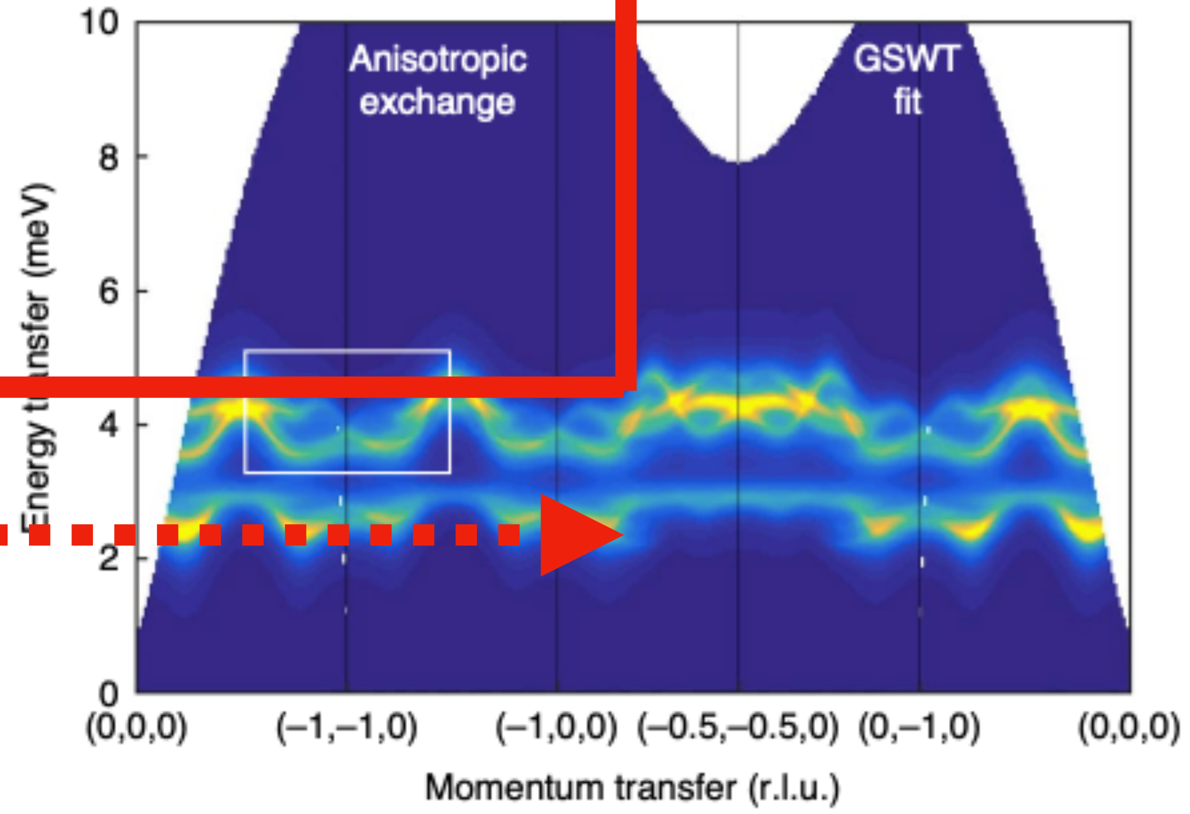
$\propto \mathcal{S}^{\alpha\beta}(\mathbf{q},\omega)$



Theory

$\hat{\mathcal{H}}$

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



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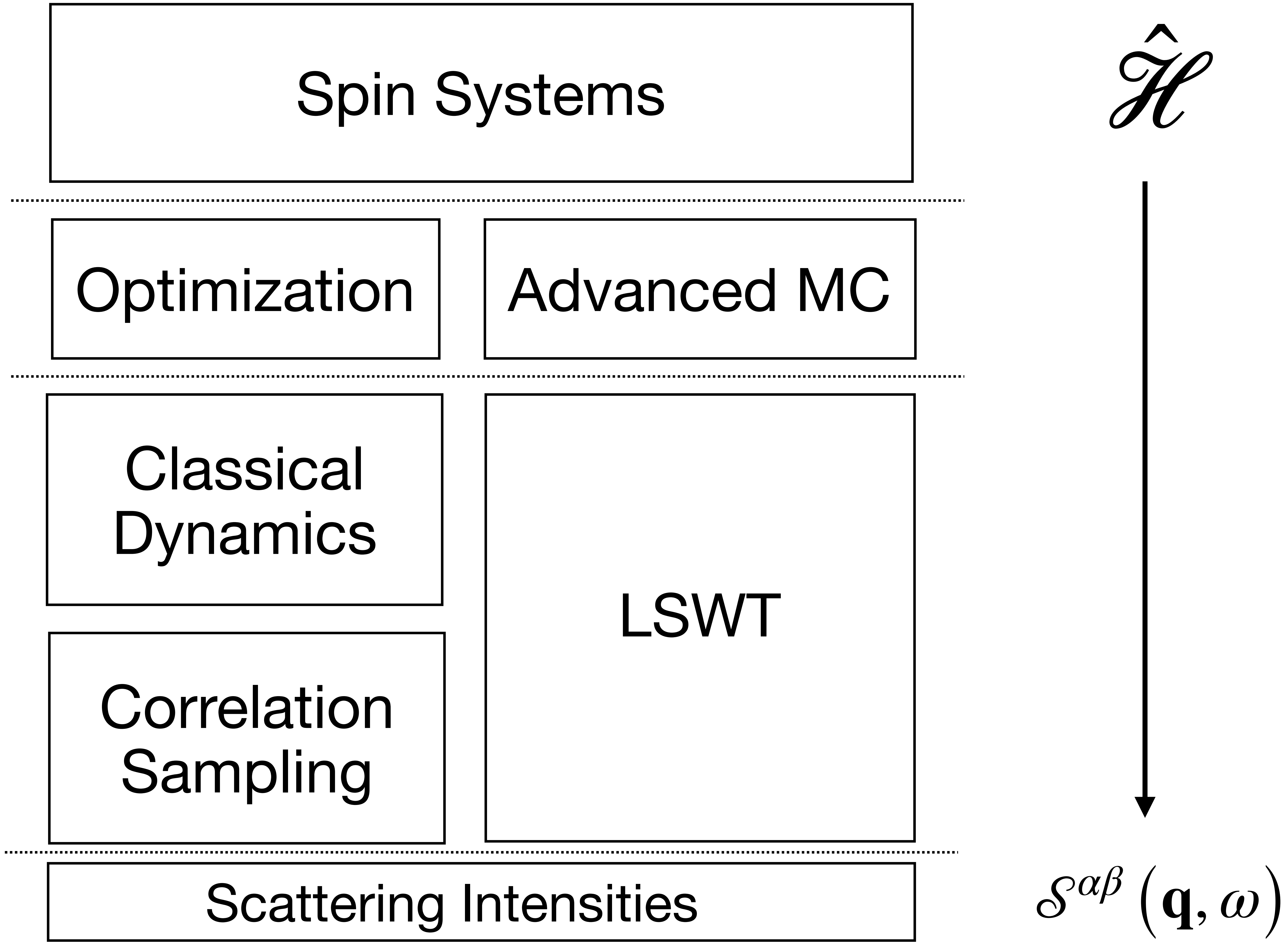
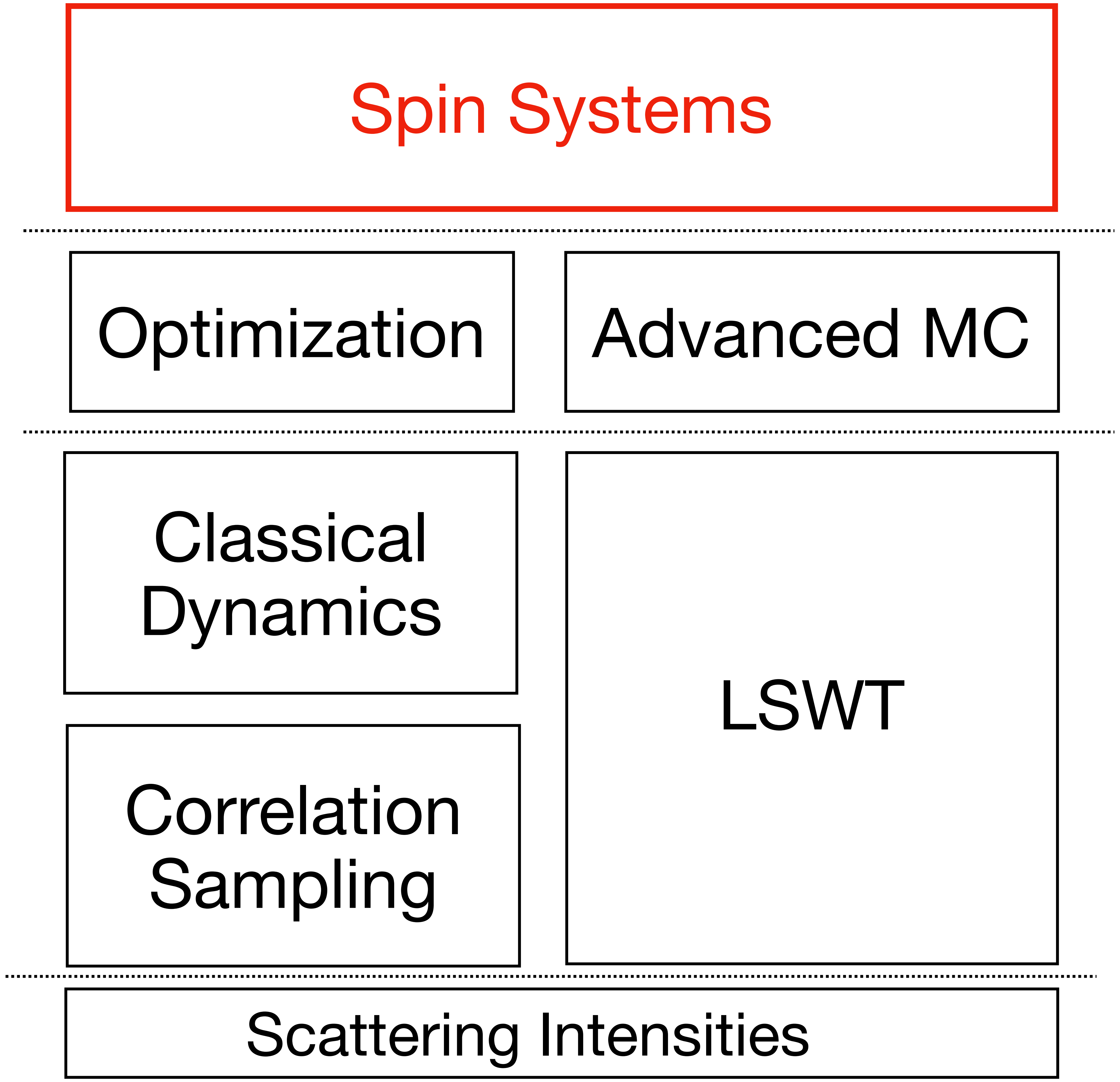
Structure of Sunny

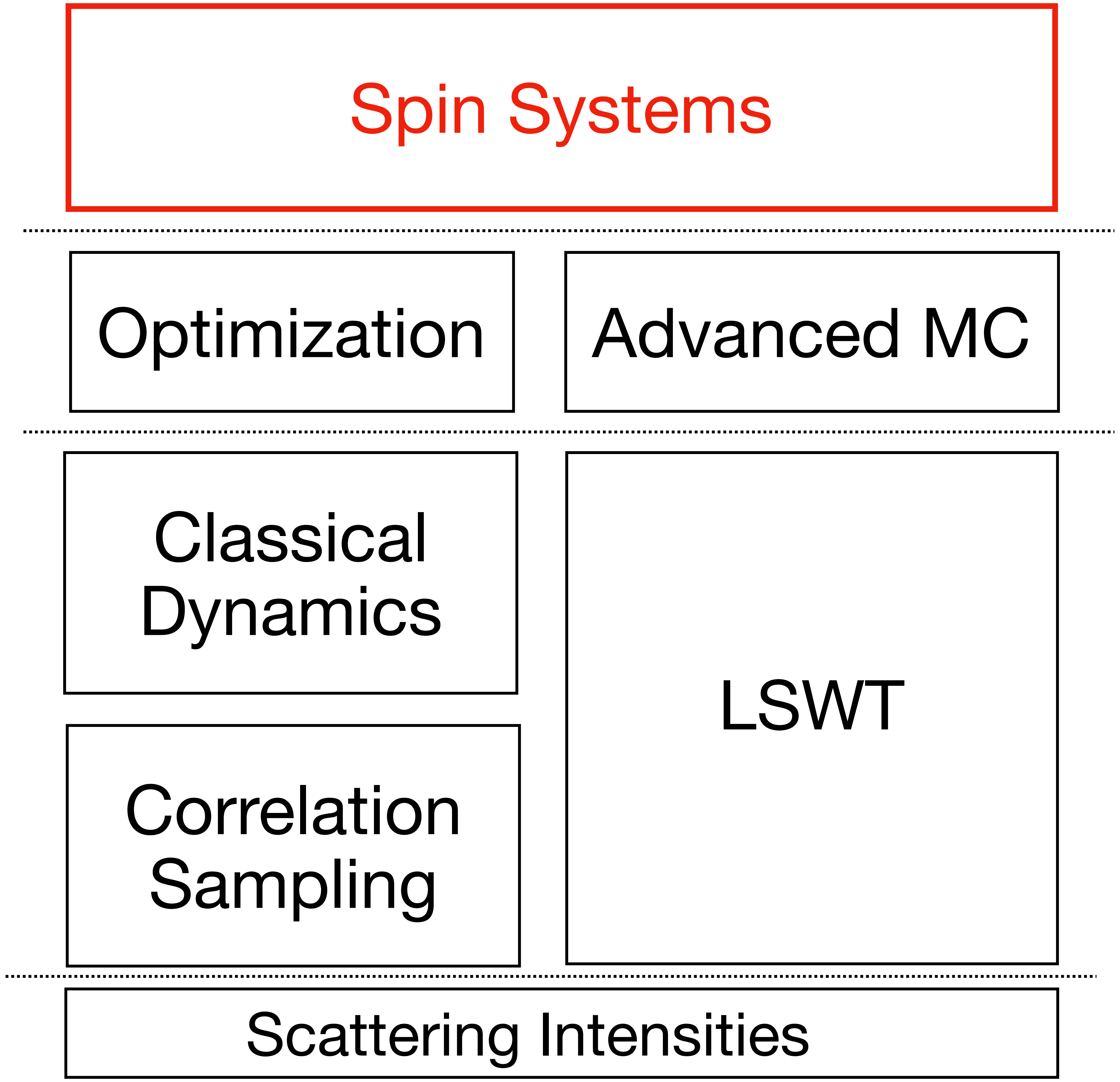


Structure of Sunny



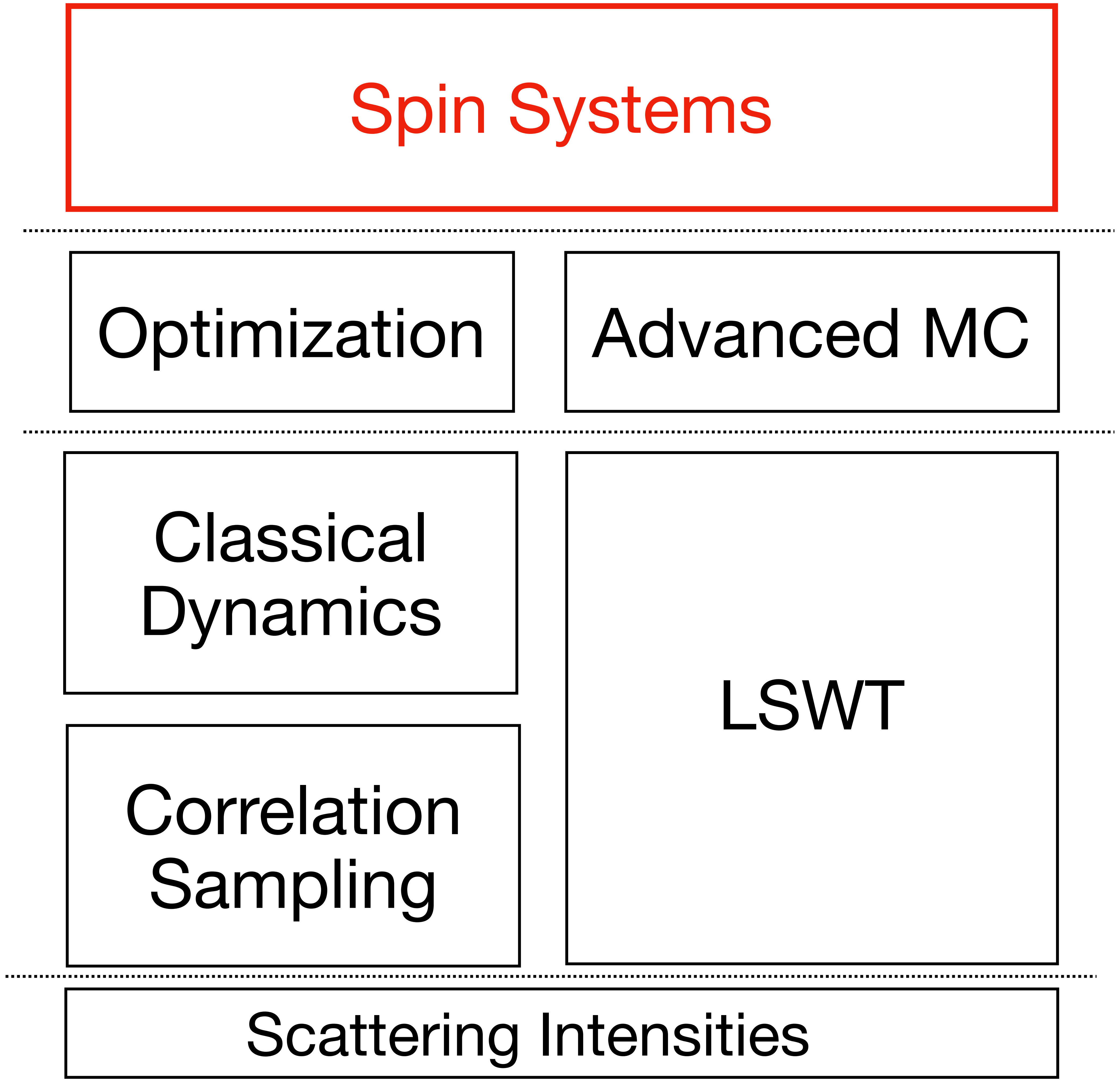
- Crystals and symmetry analysis
- Visualization
- Hamiltonian specification
  - General pair-wise interactions
  - Single-ion anisotropies (and renormalizations)
- Storage of product states (dipoles or SU(*N*) coherent states)

Structure of Sunny



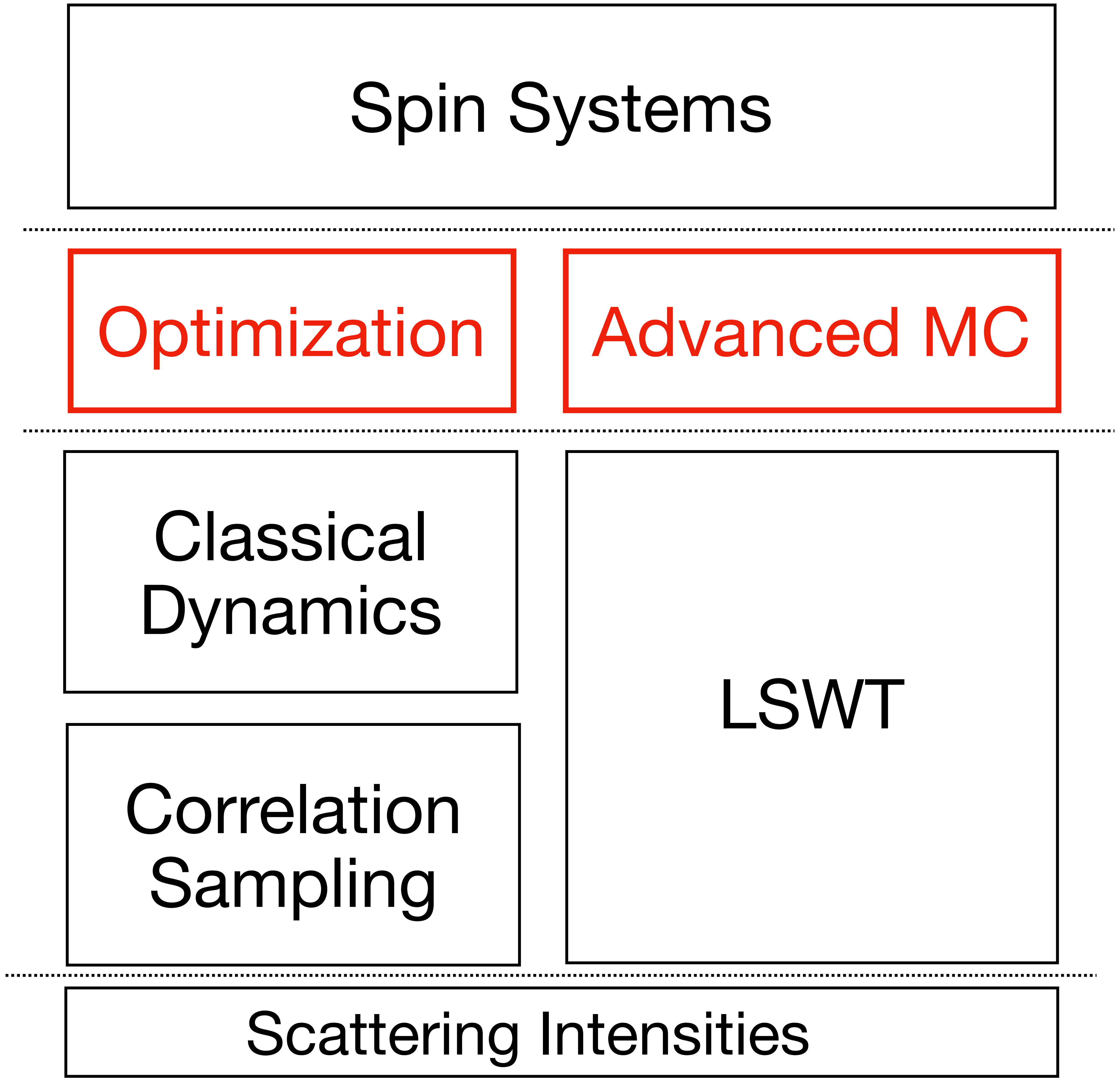
- Symmetry analysis
  - `Crystal`
  - `print_symmetry_table`
  - `view_crystal`

Structure of Sunny



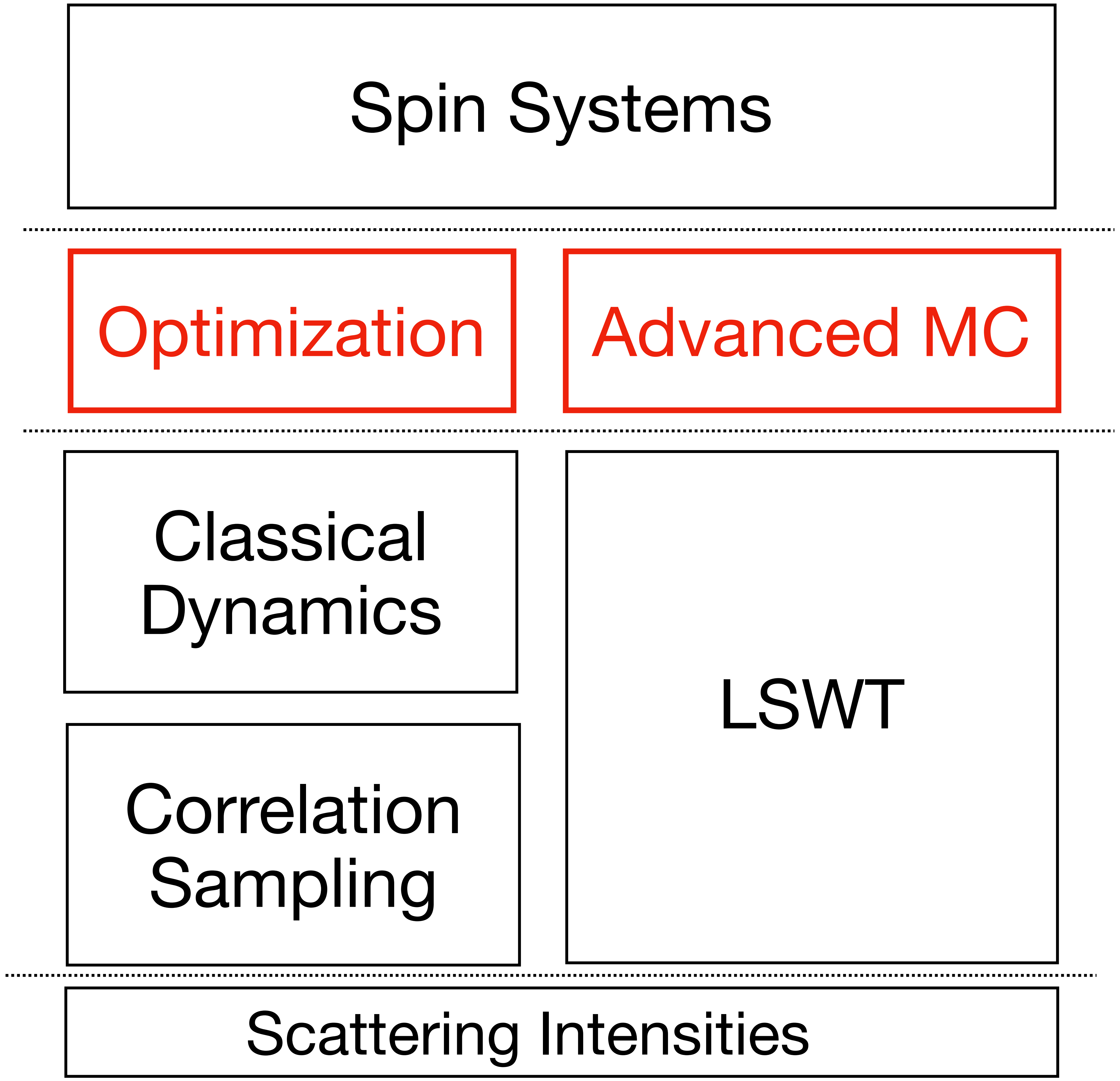
- System and Hamiltonian specification
  - `System`
  - `SpinInfo`
  - `set_exchange!`
  - `set_pair_coupling!`
  - `set_onsite_coupling!`

Structure of Sunny



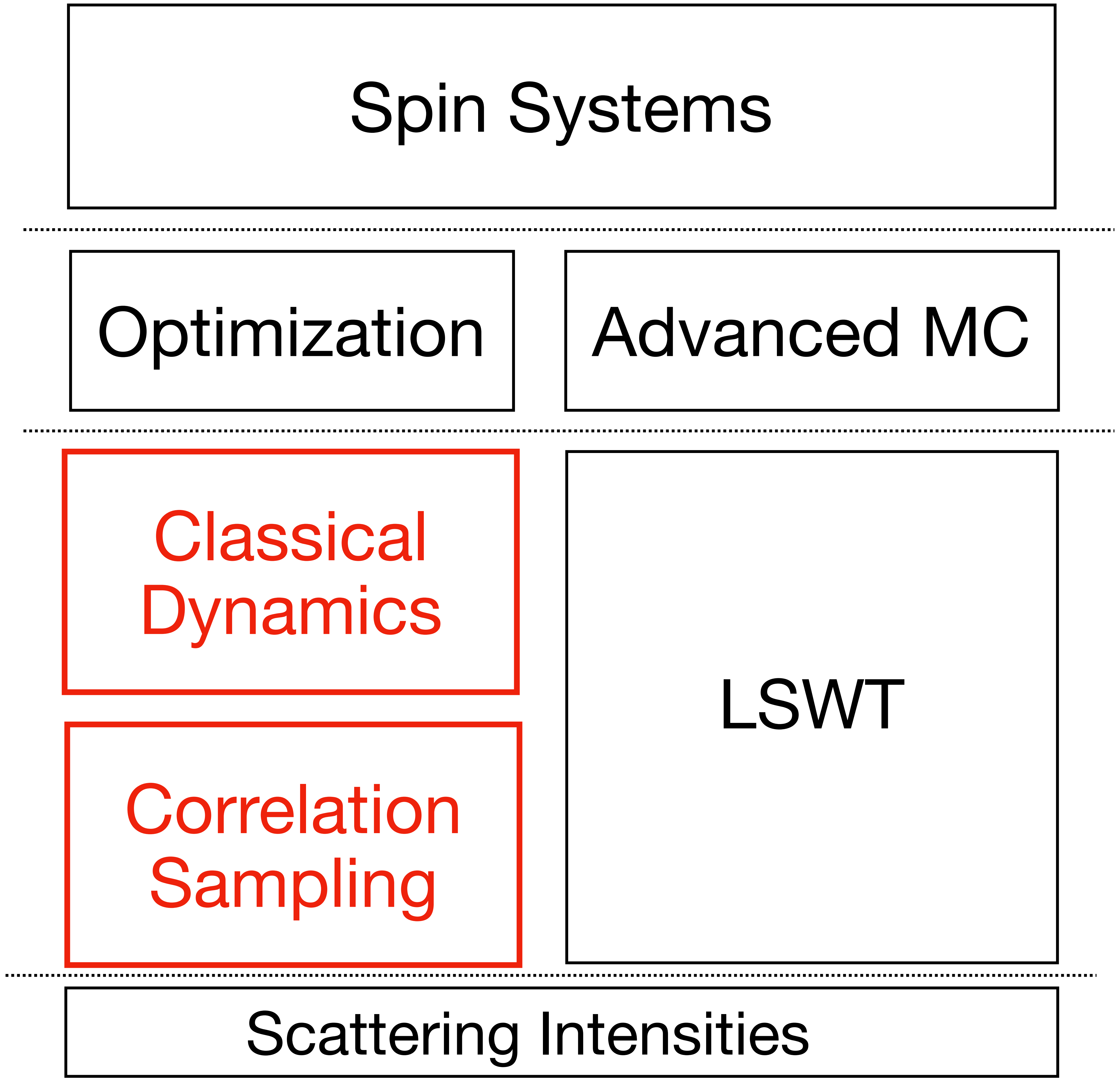
- Gradient-based optimizers to find ground states
  - Work for both dipoles and SU(*N*) coherent states
- Advanced Monte Carlo classical spin systems
  - Parallel tempering
  - Wang-Landau

Structure of Sunny



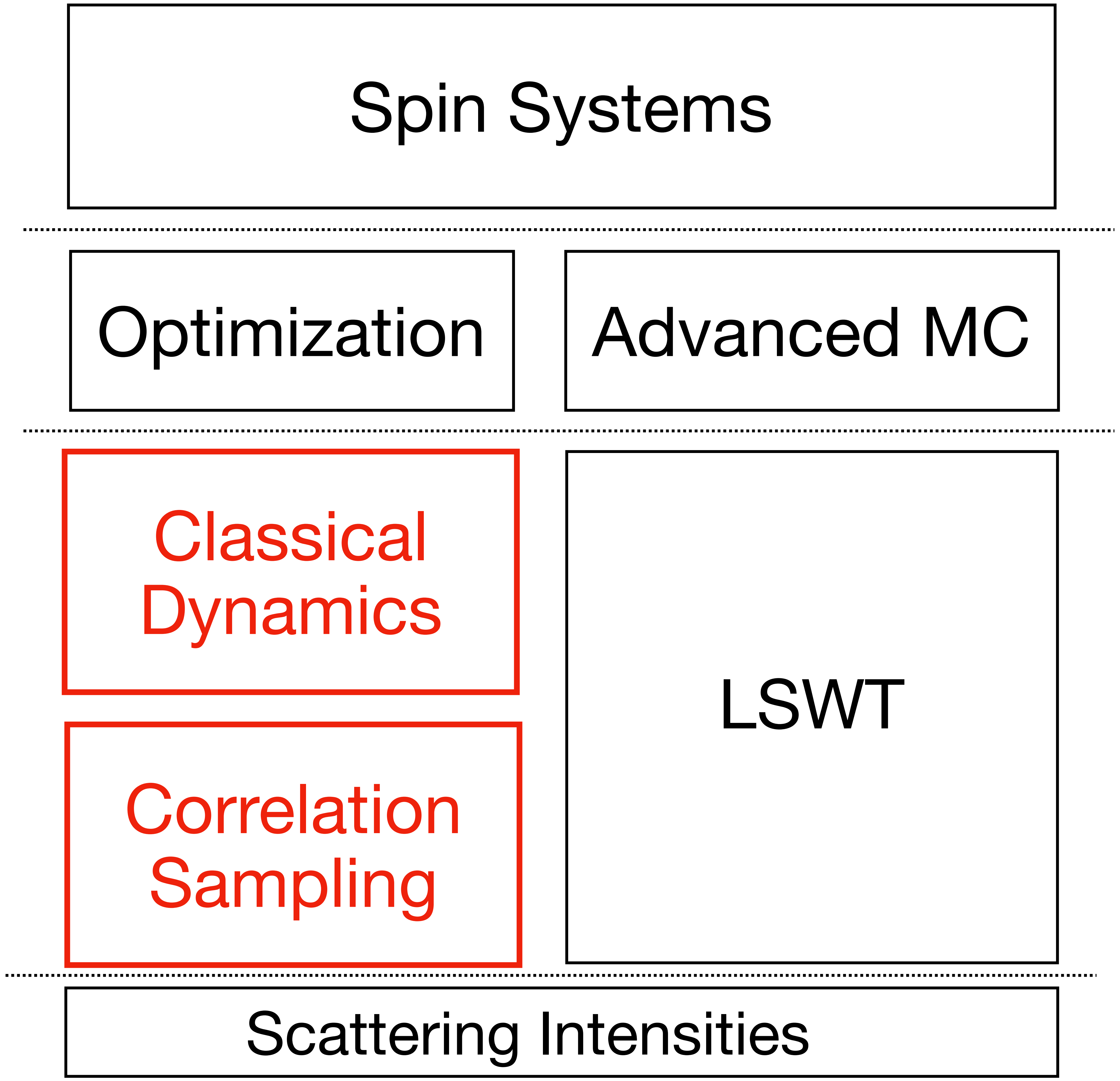
- Optimization
  - `randomize_spins!`
  - `minimize_energy!`
- Annealing via
  - `Langevin` and `step!`
  - `LocalSampler` and `step!`

Structure of Sunny



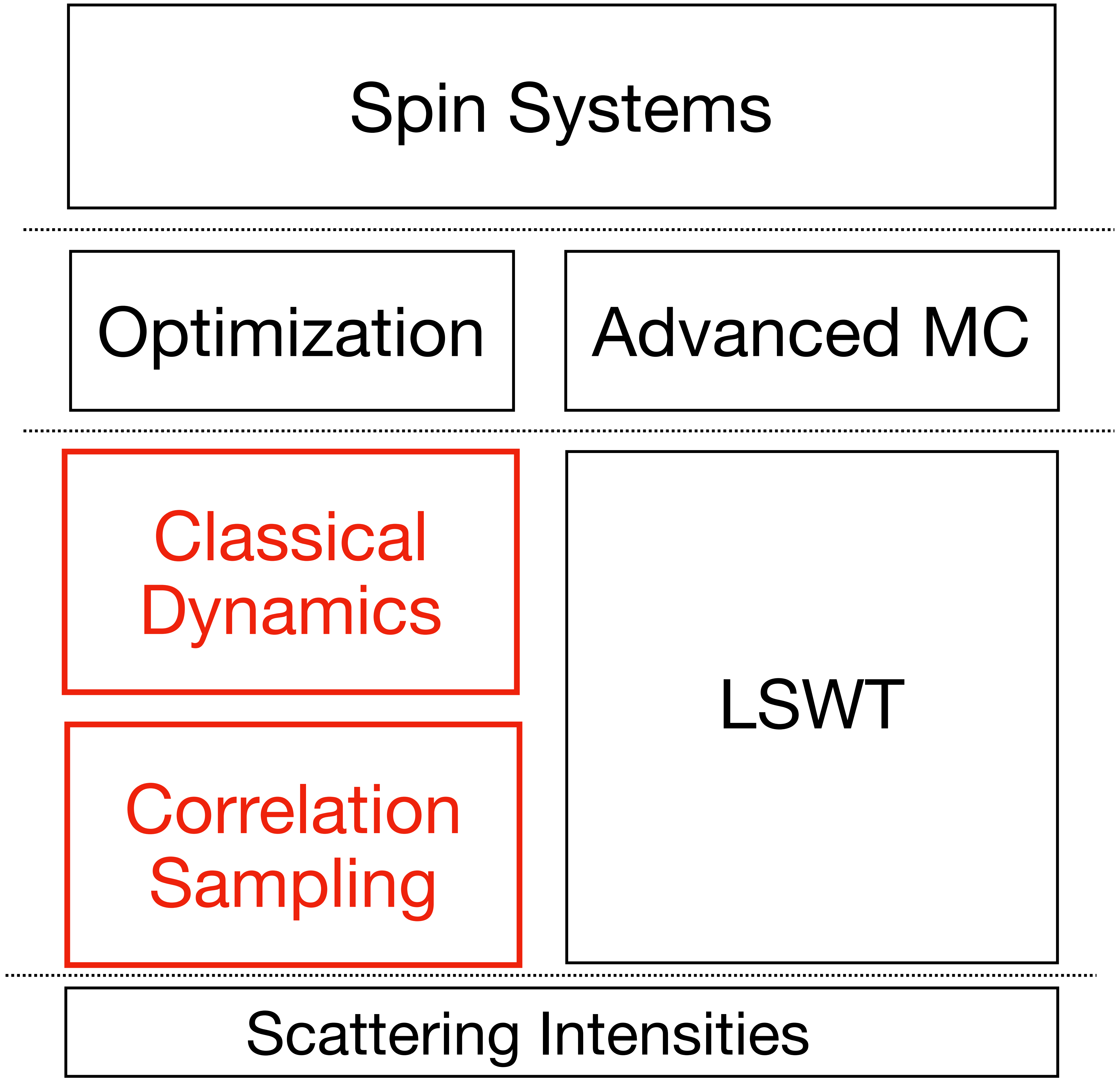
- Traditional Landau-Lifshitz and generalized SU(N) classical dynamics
- Advanced integration techniques
  - Symplectic integrators for energy-conserving dynamics
- Dynamics with presence of thermal bath (both dipole and SU(N)).

Structure of Sunny



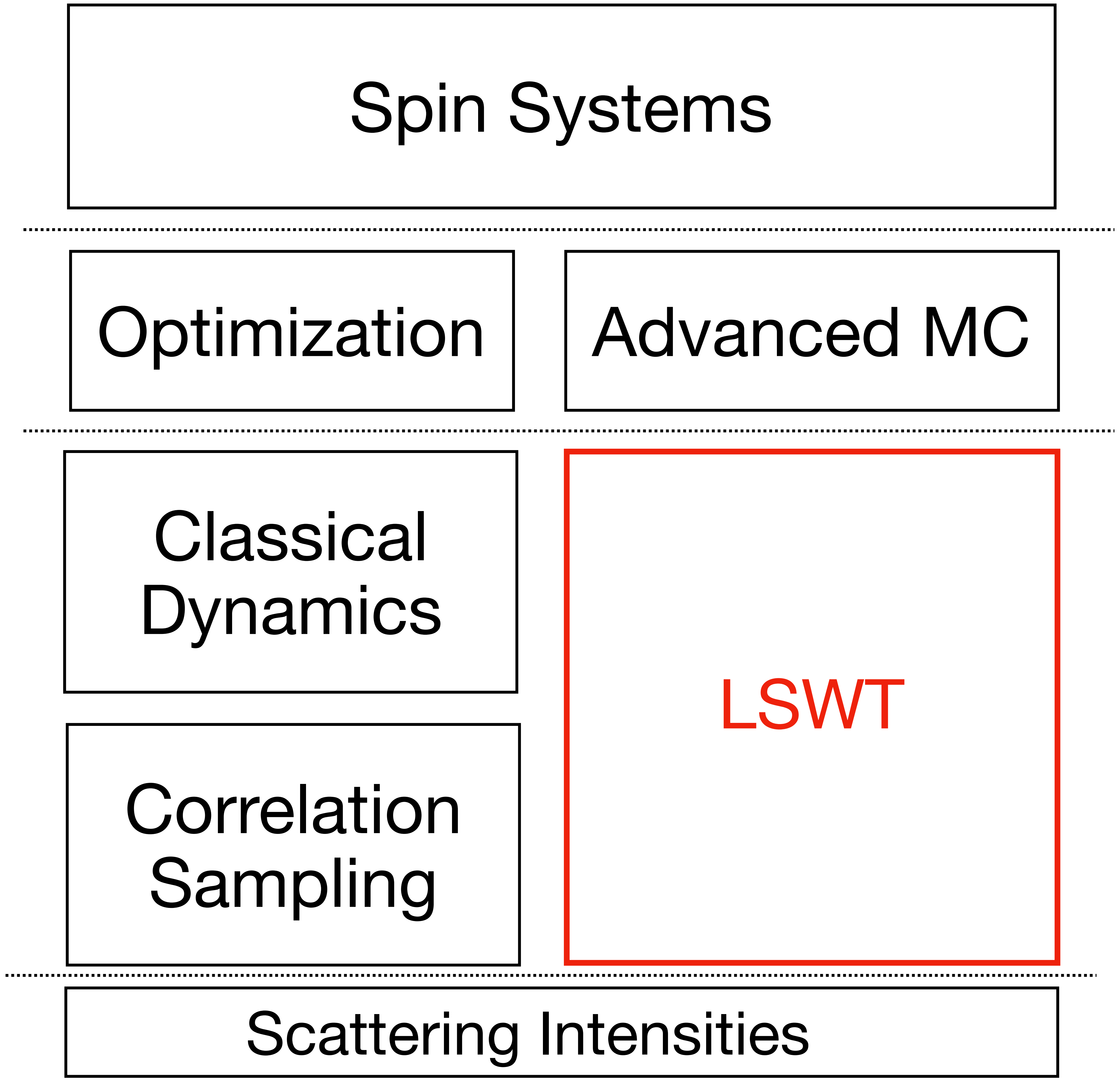
- Classical dynamics
  - `ImplicitMidpoint` and `step!`
  - `Langevin` and `step!`
  - `suggest_timestep`

Structure of Sunny



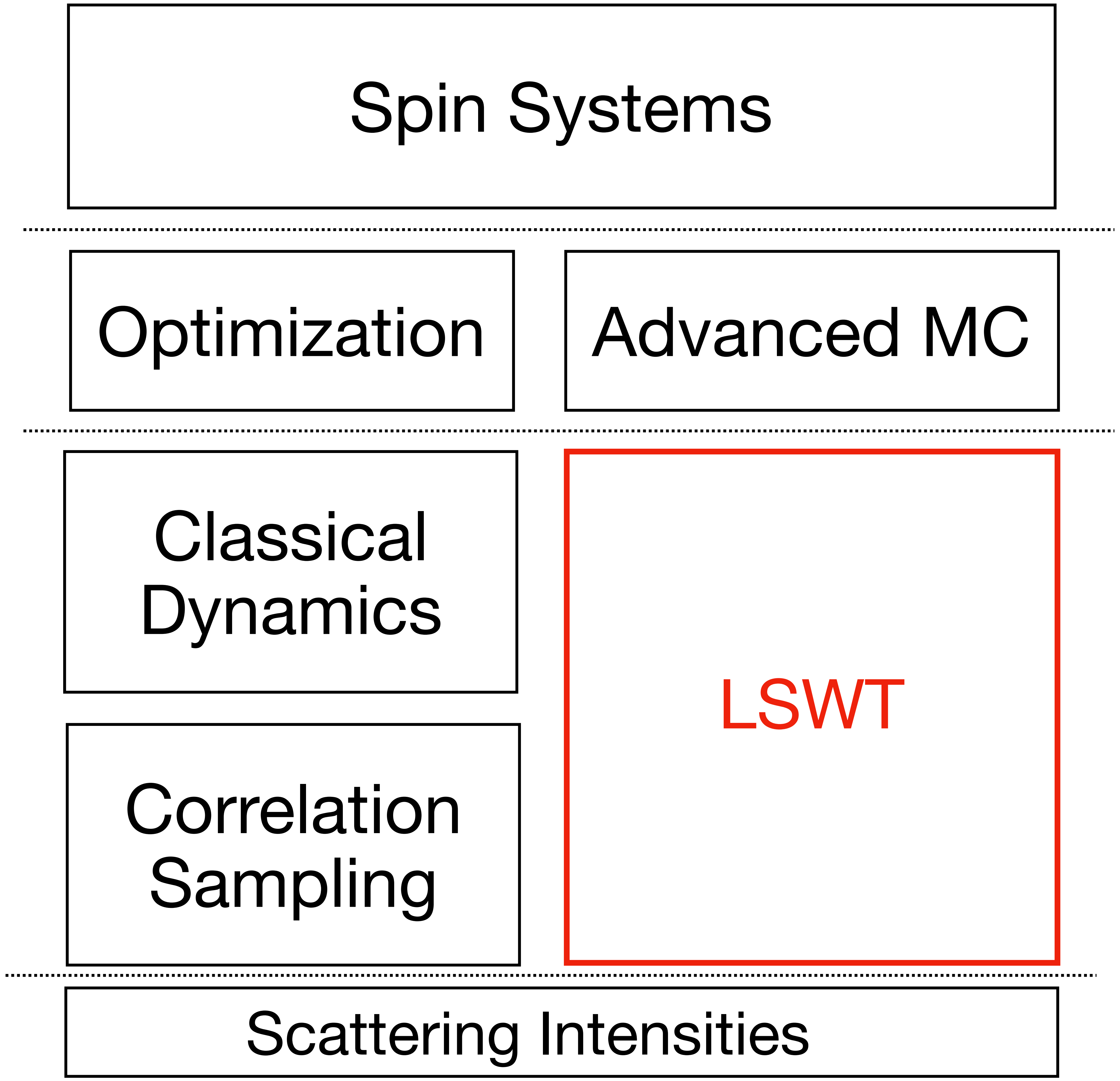
- Correlation sampling, S(q,ω)
  - **`dynamical_correlations`**
  - **`instant_correlations`**
  - **`Langevin`** and **`step!`**
  - **`add_sample!`**

Structure of Sunny



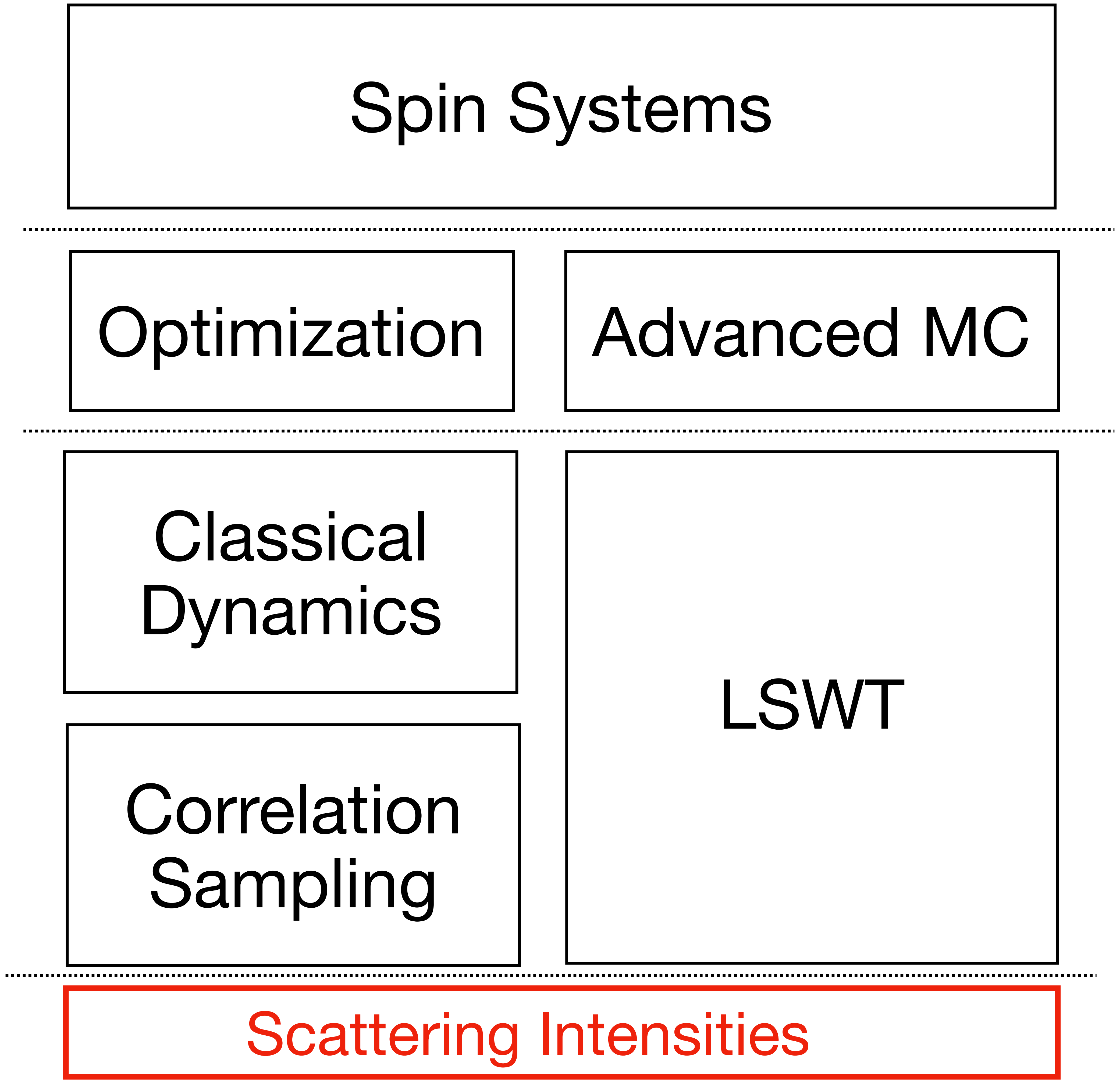
- Construct and diagonalize LSWT Hamiltonian
- Both traditional *S*-based formalism and generalization based on SU(*N*) coherent states.

Structure of Sunny



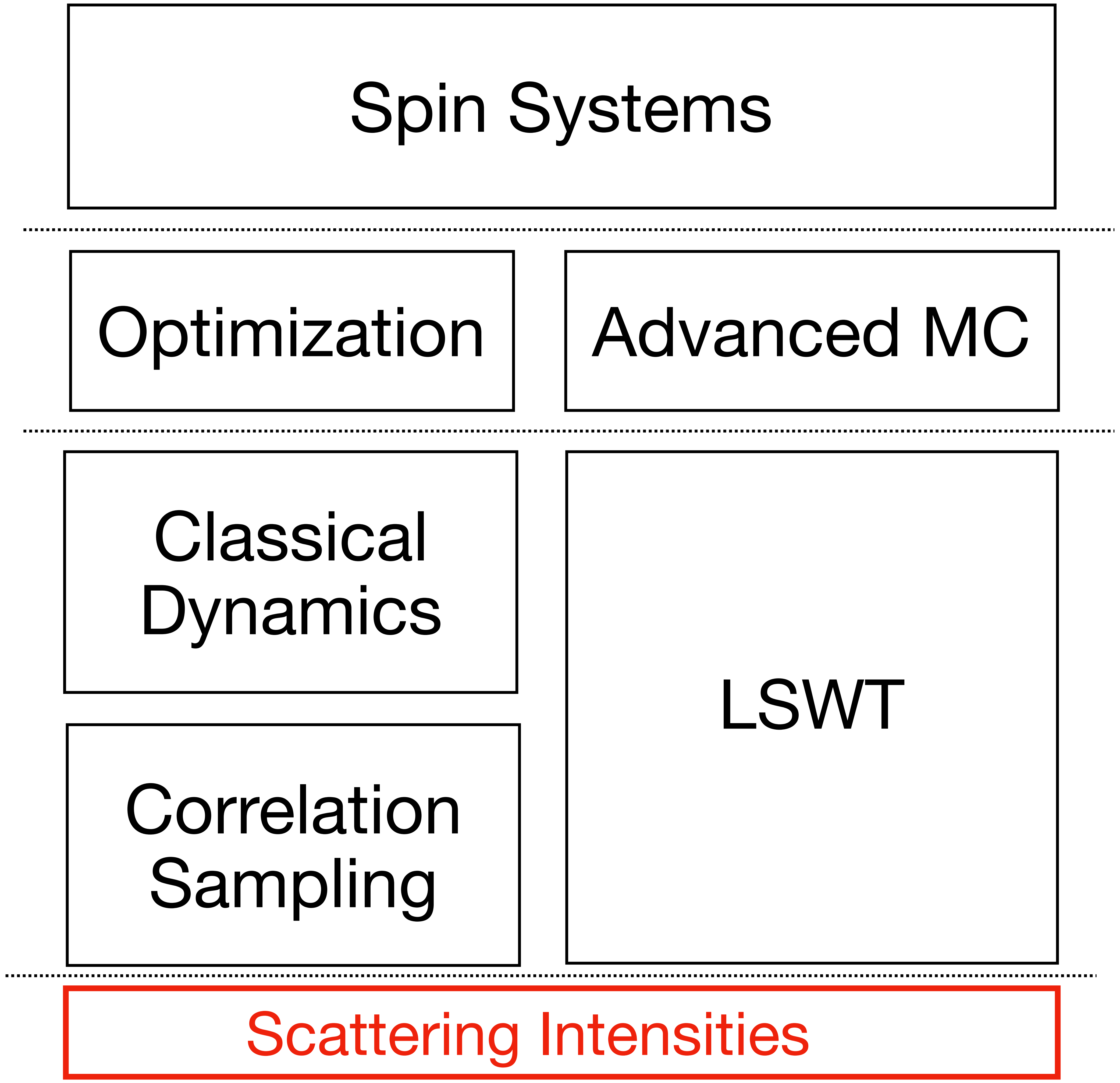
- LSWT
  - `SpinWaveTheory`

Structure of Sunny



- Tools for extracting scattering intensities for comparison with experiment.
- Polarization, form factors, convolution kernels.

Structure of Sunny



- Intensity calculations
  - **`intensity_formula`**
  - **`intensities_bands`**
  - **`intensities_broadened`**
  - **`intensities_interpolated`**

Typical workflow

1) Specify a system

Specify a crystal, supercell, local Hilbert space information, and interactions

- `Crystal`
- `view_crystal`
- `print_symmetry_table`
- `System`
- `SpinInfo`
- `set_exchange!`
- `set_onsite_coupling!`

Typical workflow

2) Find a ground state

Thermalize system or randomize spins, then find lowest energy configuration

- **`randomize_spins!`**
- **`minimize_energy!`**
- **`Langevin`** `or` **`LocalSampler`** and **`step!`** with an annealing schedule

Typical workflow

3a) Classical structure factors

Build a **`SampledCorrelations`** object that accumulates spin-spin correlation information.

- **`dynamical_correlations`**
- **`Langevin`** and **`step!`**
- **`add_sample!`**

Typical workflow

3b) LSWT structure factors

Specify a magnetic unit cell and build a `SpinWaveTheory`. This stores observables and information for constructing the spin wave Hamiltonian.

- `print_wrapped_intensities`
- `suggest_magnetic_supercell`
- `reshape_supercell`
- `SpinWaveTheory`

Typical workflow

4) Retrieve intensities

For both classical and LSWT calculations, specify a “formula”

- **`intensity_formula`**

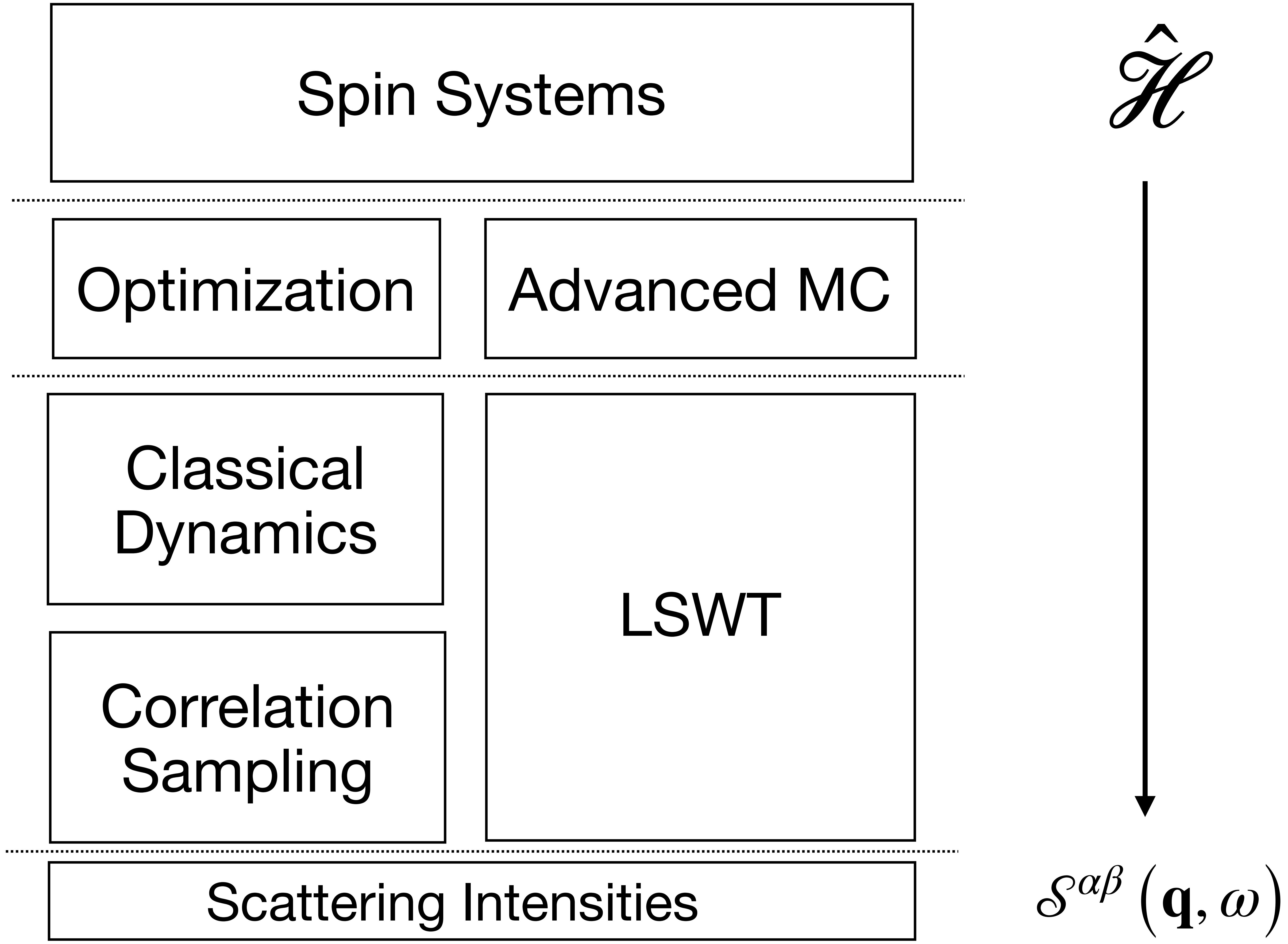
For classical calculations

- **`intensities_interpolated`**

For LSWT calculations

- **`intensities_bands`**, **`intensities_broadened`**, **`dispersion`**

Structure of Sunny



Advantages of Sunny

1. Provides tools for calculating **classical phase diagrams** in addition to spin wave calculations.

2. Can perform spin wave calculations both **classically** (at finite temperature) and **semi-classically** (SWT).

3. Generalizes both the classical and SWT calculations in corresponding ways with **SU(*N*) coherent states**.

4. Is written is a language with dynamic features (as easy as Python) that is nonetheless compiled (as fast as C++) — both **fast** and **interactive.**

Summary of Sunny “modes”

Modes when creating a system

- `:dipole_large_S`
  - Both LL and LSWT are performed using the traditional $S \to \infty$ limit
  - 1 mode per site
- `:SUN`
  - Both LL and LSWT are performed using the $SU(N)$ formalism
  - $(N-1)$ modes per site
- `:dipole`
  - Use $SU(N)$ formalism but constrain to dipolar states, leading to renormalizations
  - 1 mode per site

Summary of Sunny “modes”

Guidance about when to use each mode

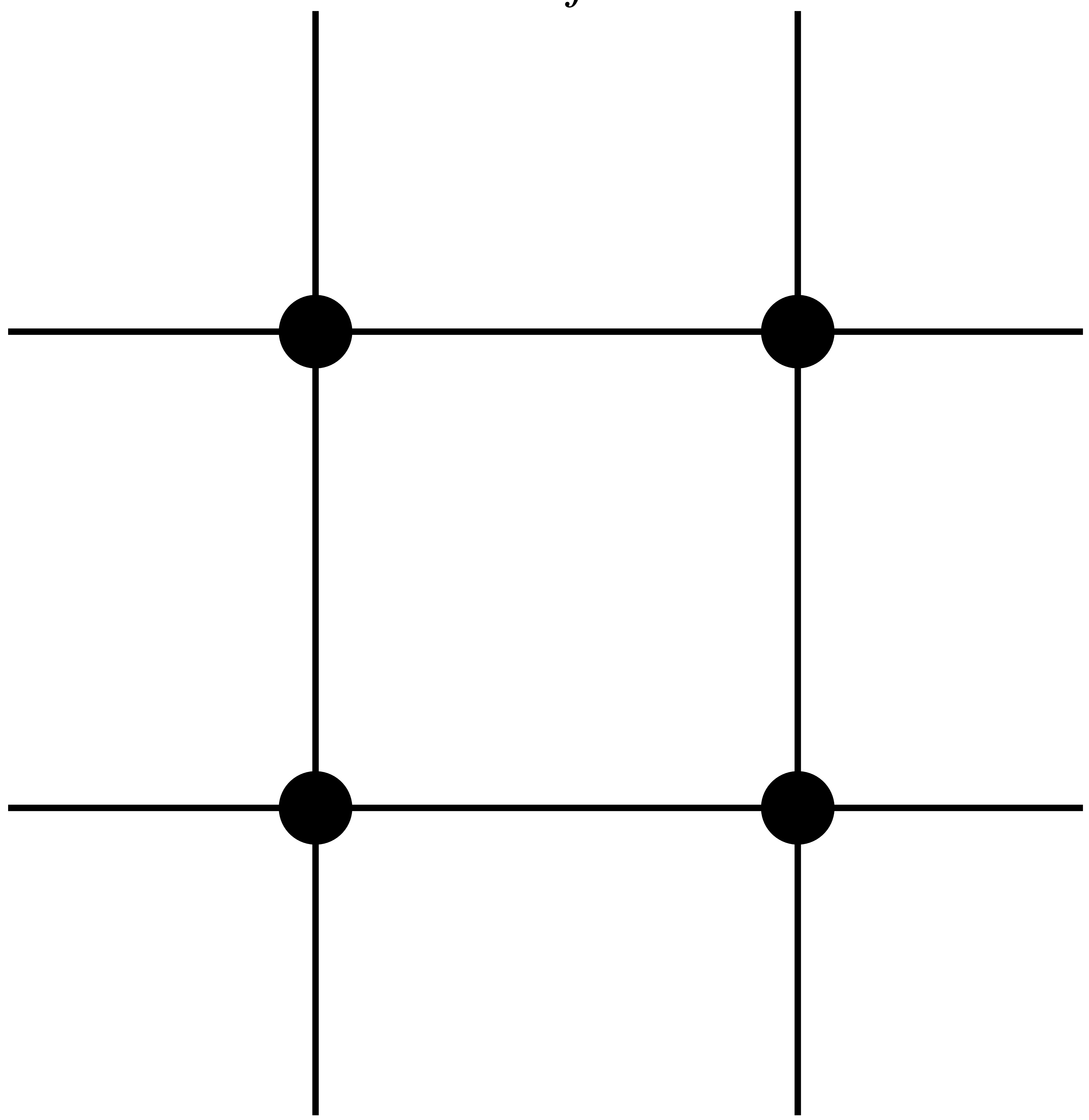
- **`:dipole_large_S`**
  - For reproducing existing results (verification)
  - Will differ from `:dipole` mode only when there are nonlinear terms
- **`:SUN`**
  - When you have large spins with nonlinear terms
  - When you want to model “localized” entanglement
- **`:dipole`**
  - For Hamiltonians that have a predominantly dipolar character
  - Nonlinear terms small compared to exchange terms.

General structure of SU(2) methods

Product State Assumption

- In traditional (large-*S*) theories, decompose into product of SU(2) coherent states.

$$|\Psi\rangle = \bigotimes_j |\Psi_j\rangle$$



General structure of SU(2) methods

Product State Assumption

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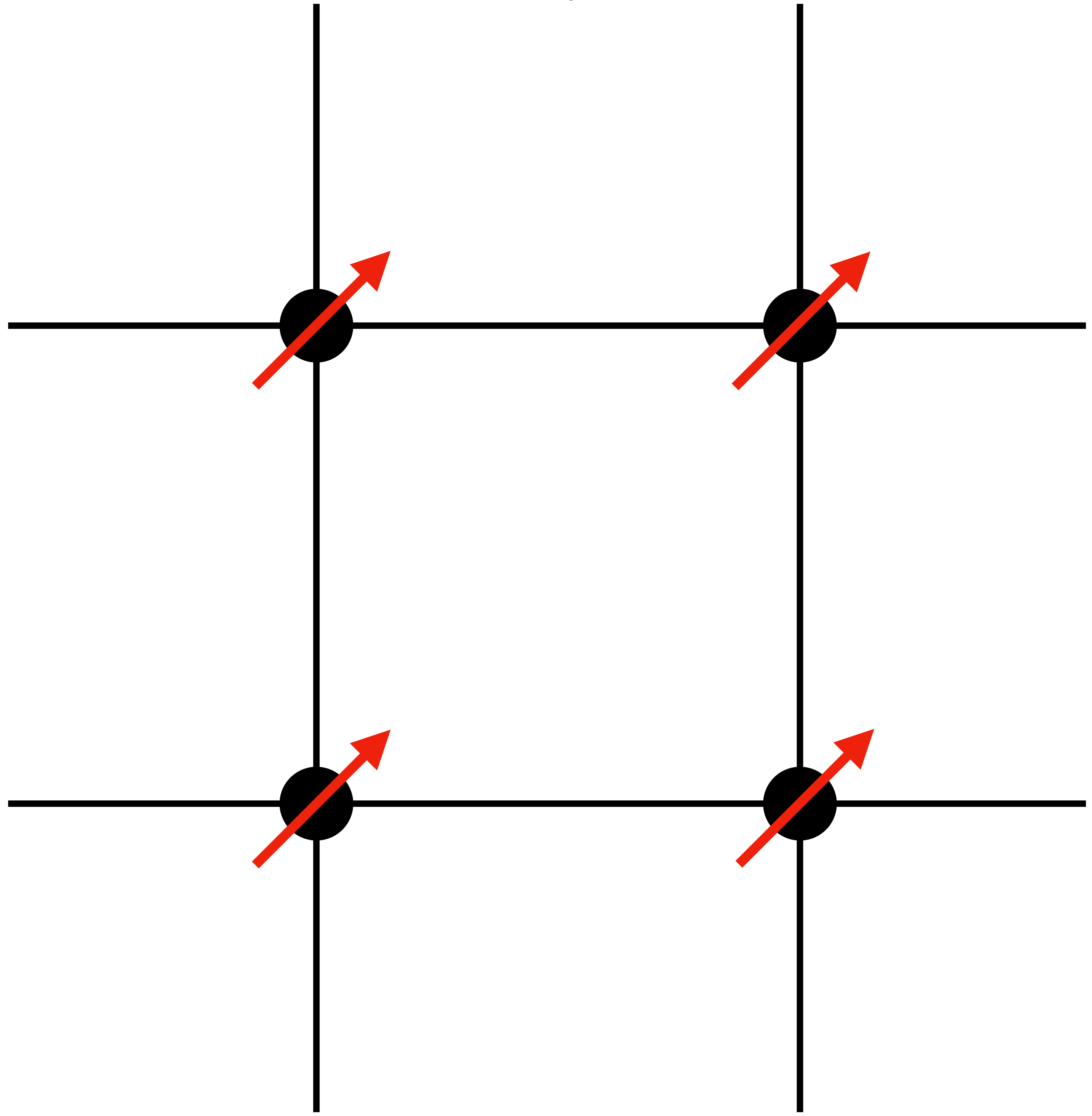
- SU(2) coherent states can always be put into one-to-one correspondence with points on a sphere



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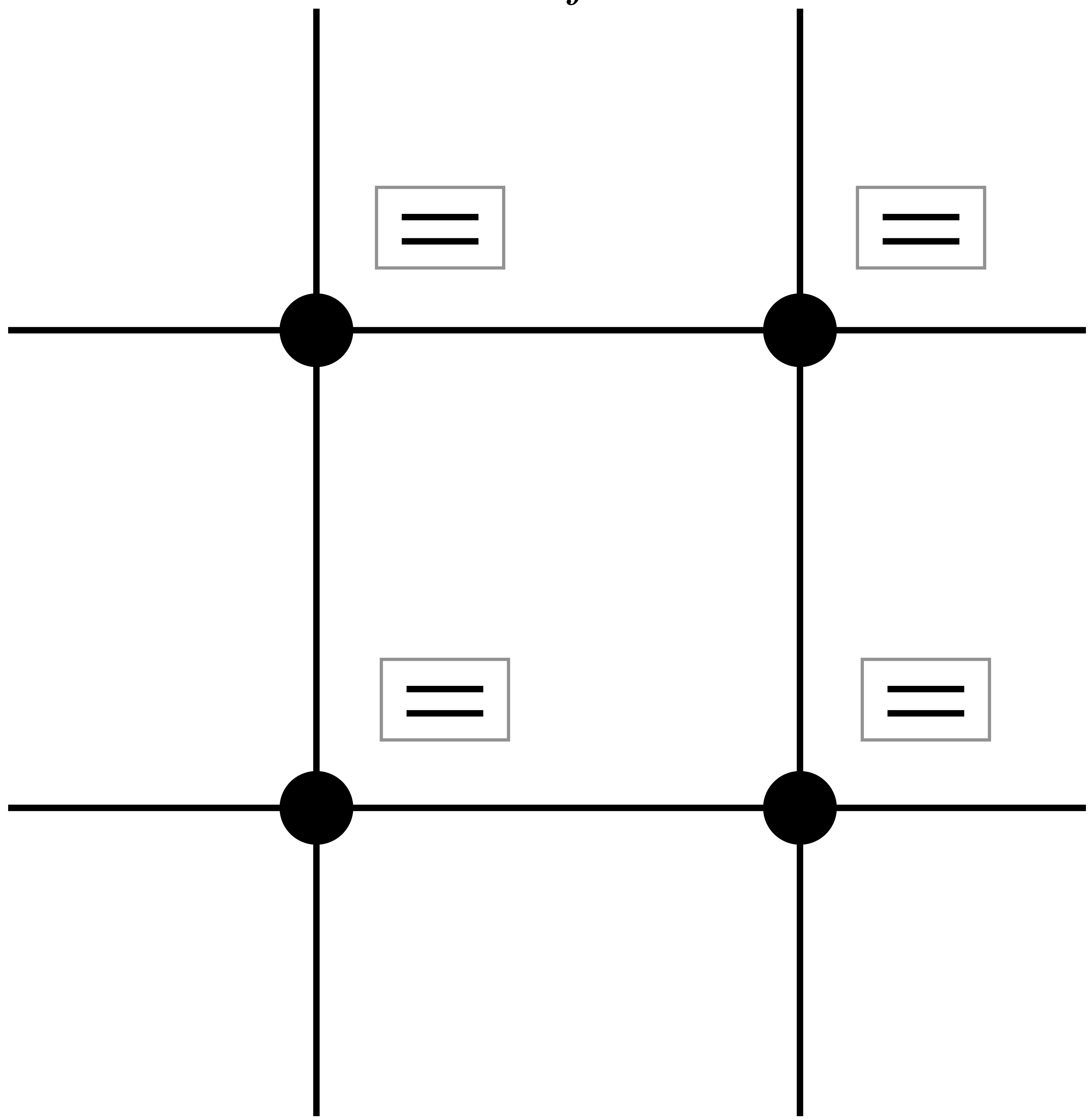


- In traditional (large-S) theories, decompose into product of SU(2) coherent states.
- SU(2) coherent states can always be put into one-to-one correspondence with points on a sphere
- This is isomorphic to the state space for a 2-level system

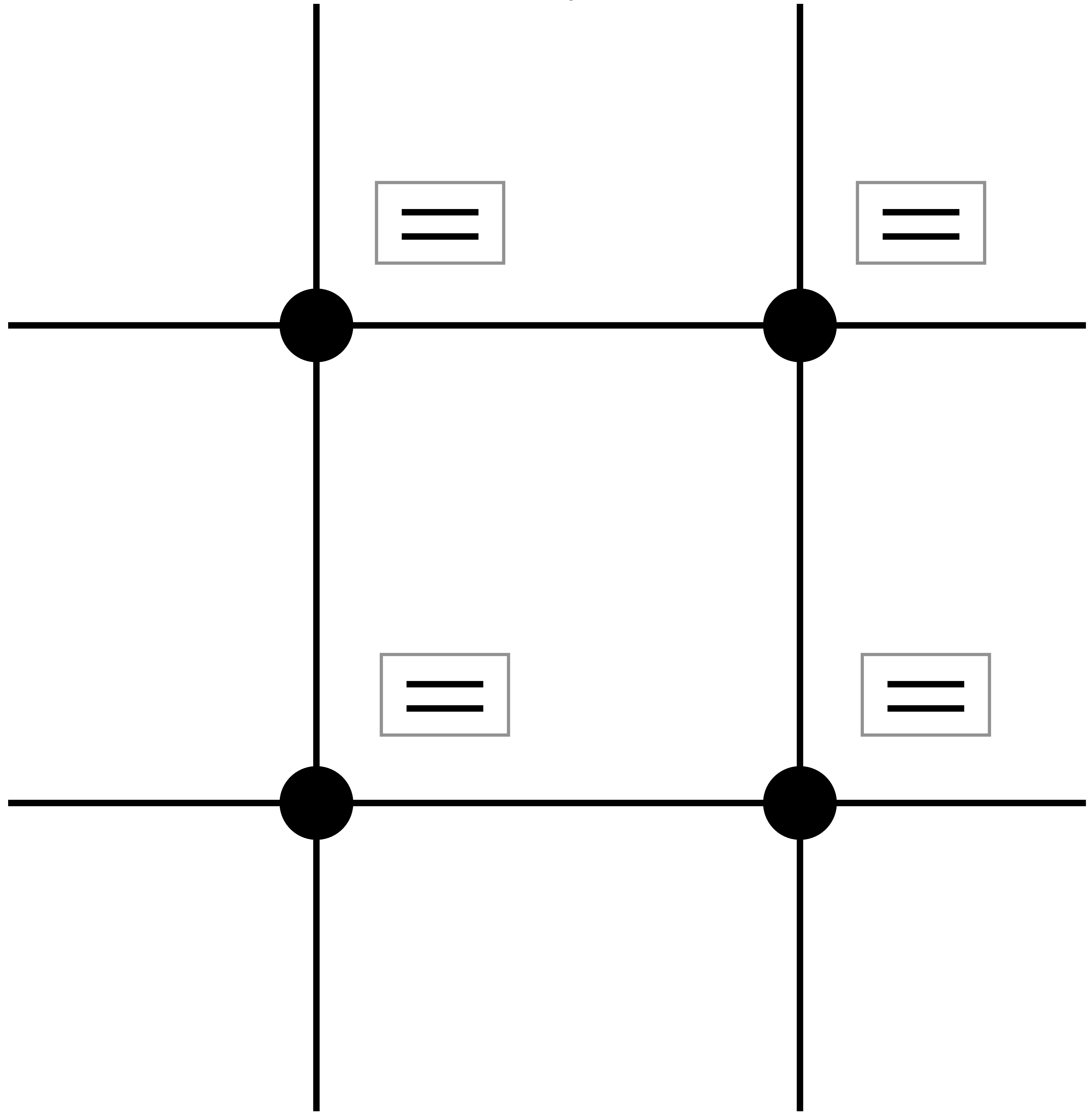
General structure of SU(2) methods

Classical dynamics

$$|\Psi\rangle = \bigotimes_j |\Psi_j\rangle$$

- Well defined procedures for deriving **classical dynamics** ($S \to \infty$)

$$\boxed{\frac{d\mathbf{s_j}}{dt} = -\,\mathbf{s_j} \times \nabla_{\mathbf{s_j}} \mathbf{H}_{\mathrm{SU}(\mathbf{2})}}$$



General structure of SU(2) methods

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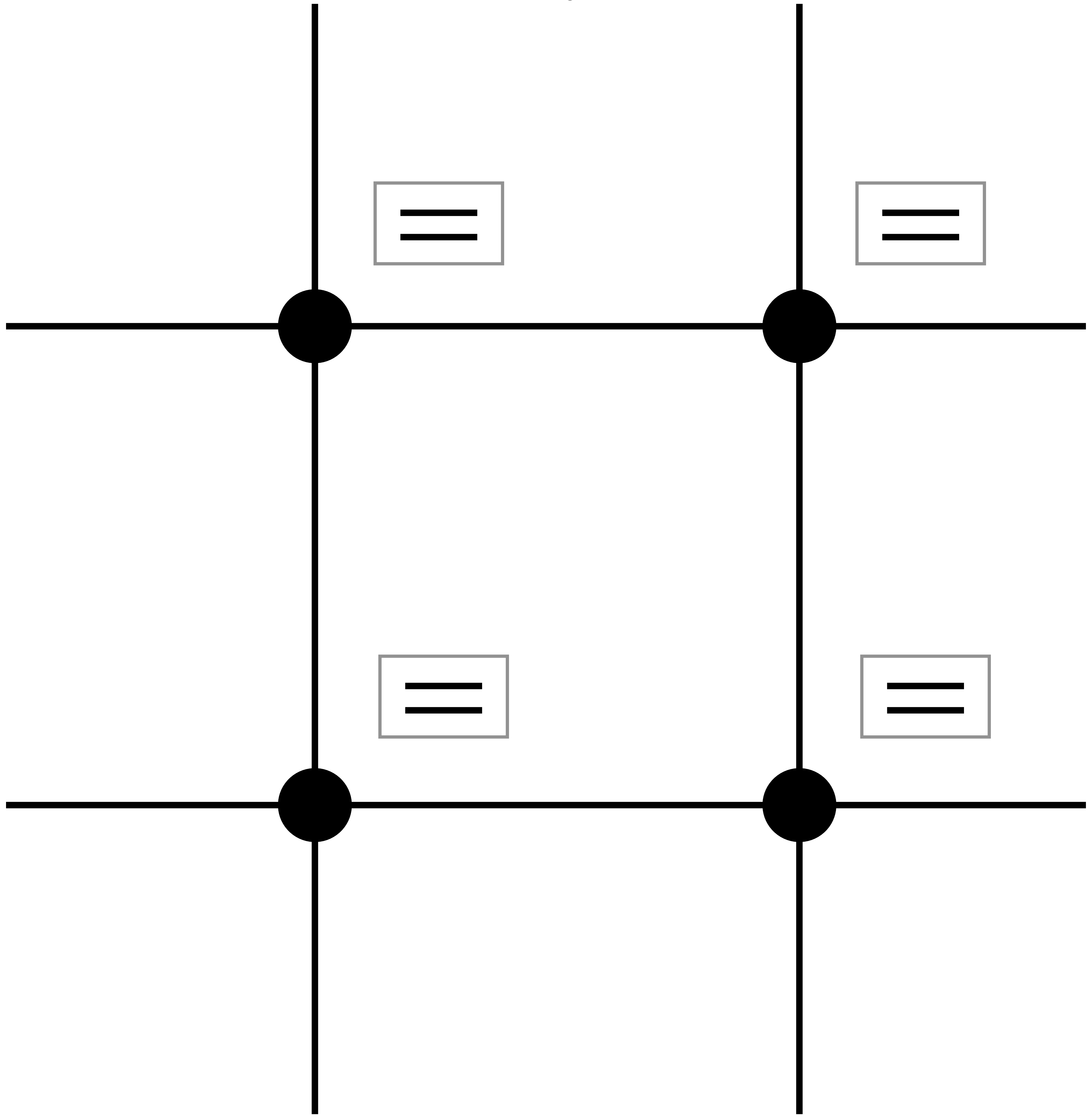


General structure of SU(2) methods

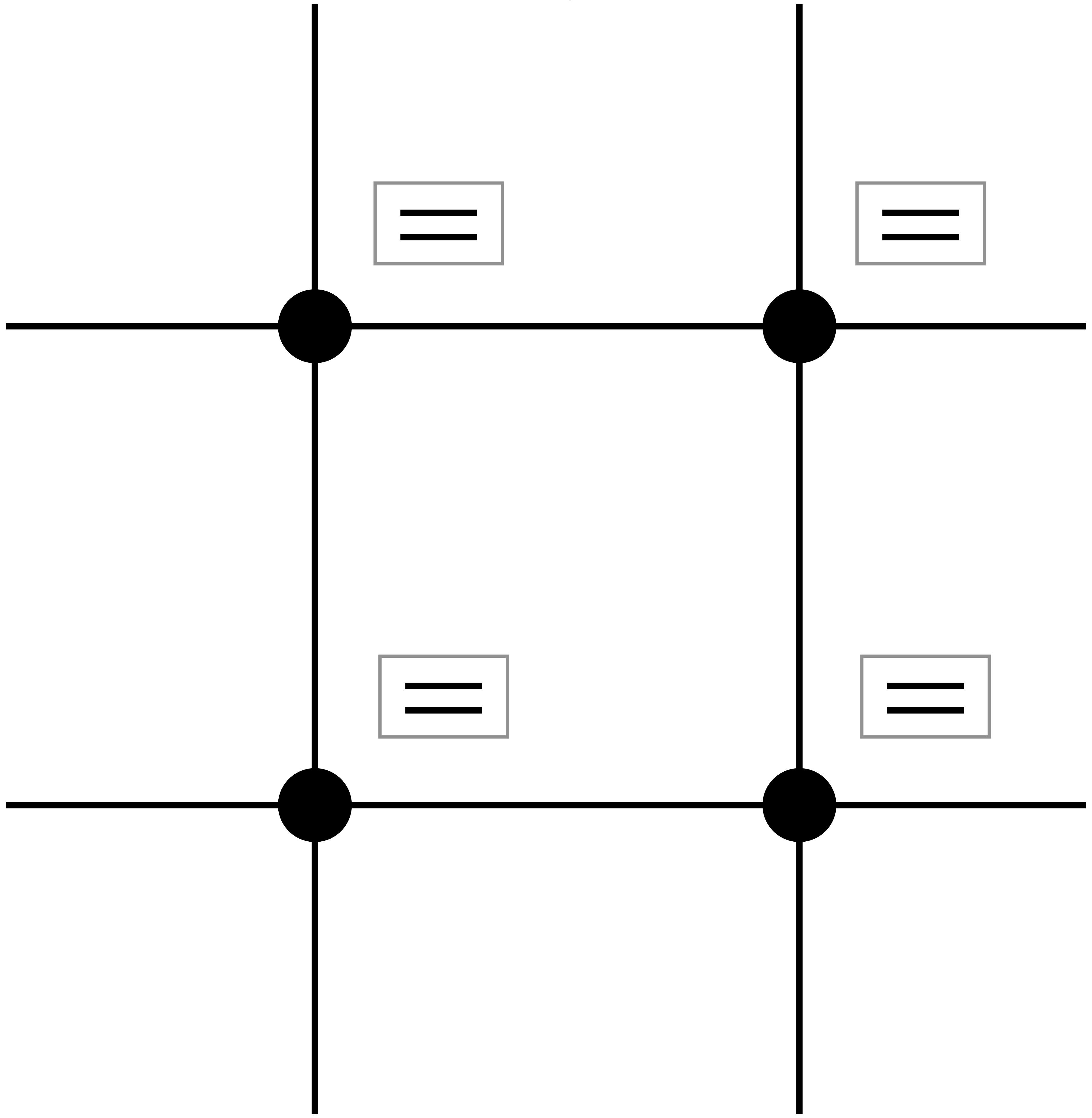
Semiclassical dynamics

$$|\Psi\rangle = \bigotimes_j |\Psi_j\rangle$$

- Well defined procedures **bosonizing a Hamiltonian** (expansion in $1/S$)

$$\left\{ b_{j,0}, b_{j,1} \right\} \qquad b^\dagger_{0,j} b_{0,j} + b^\dagger_{1,j} b_{1,j} = 2S$$

$$b^\dagger_{j,0} = b_{j,0} = \sqrt{2S}\sqrt{1 - \frac{b^\dagger_{j,1} b_{j,1}}{2S}}$$

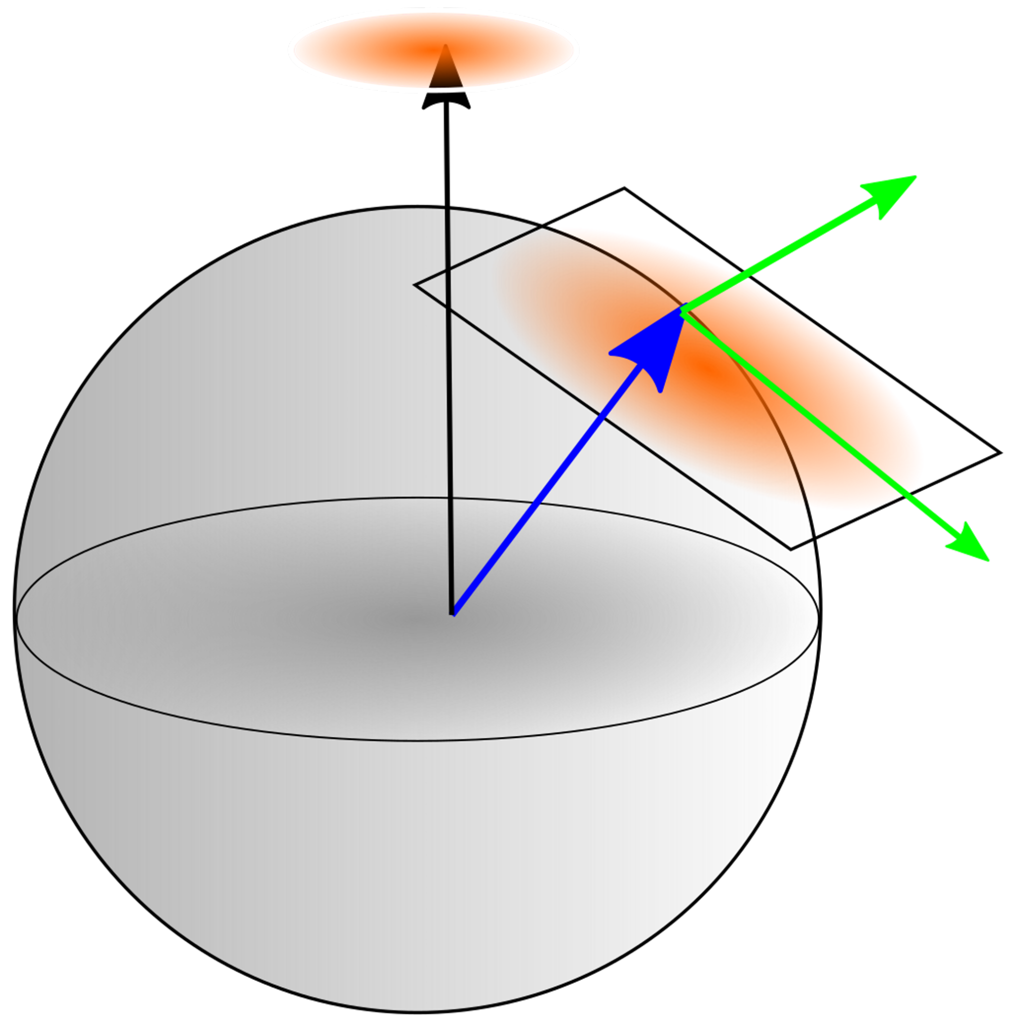


Correspondence between LL and LSWT

A few assertions

- LL and LSWT connected by SU(2) coherent states and the use of *S* as a control parameter.
- Linearized LL about the ground state yields same dispersion as LSWT
- Can recover quantum behavior by quantizing the normal modes of the classical solution

$$\mathbf{s}_j = \mathbf{s}_{0,j} + \delta\mathbf{s}_j$$



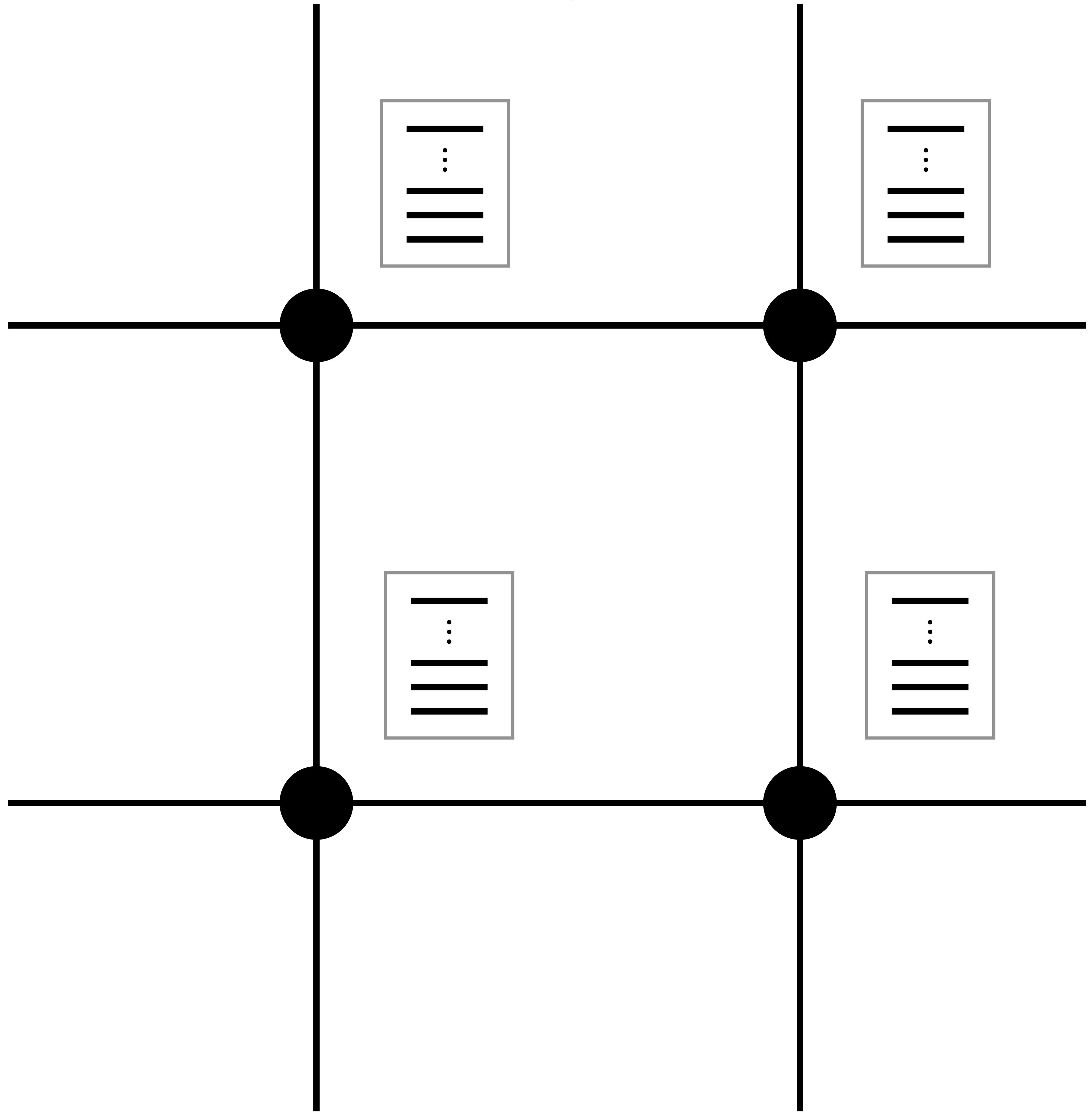
$$\mathcal{S}^{\mathrm{H}}_{\mathrm{Q}}(\mathbf{q},\omega) = \frac{\hbar\omega}{k_{\mathrm{B}}T}\left[1 + n_{\mathrm{B}}(\omega/T)\right]\mathcal{S}^{\mathrm{H}}_{\mathrm{cl}}(\mathbf{q},\omega)$$

General structure of SU(*N*) methods

Product State Assumption

- Again decompose into a product state.
- This time put an SU(*N*) coherent state on each site
- Retain all the richness of an *N*-level system — don't reduce to a dipole.

$$|\Psi\rangle = \bigotimes_j |\Psi_j\rangle$$



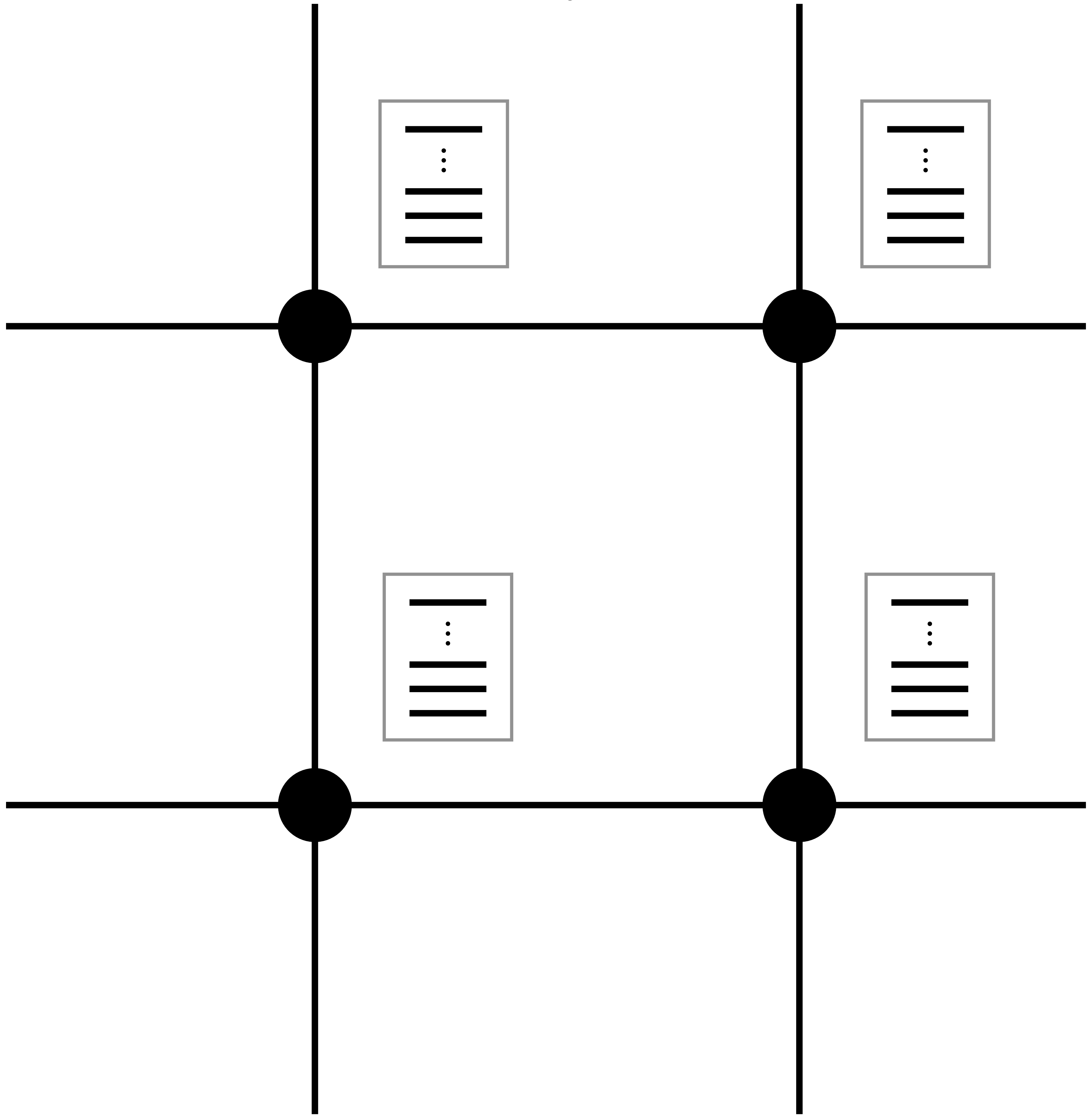
General structure of SU(*N*) methods

Classical dynamics

- Well defined procedure for defining a classical dynamics.

$$\frac{d\mathbf{n_j}}{dt} = -\,\mathbf{n_j} \star \nabla_{\mathbf{n_j}} \mathbf{H}_{\mathrm{SU(N)}}$$

$$|\Psi\rangle = \bigotimes_j |\Psi_j\rangle$$



H. Zhang and C. Batista, "Classical spin dynamics based on SU(*N*) coherent states," PRB **96** (2022).

General structure of SU(*N*) methods

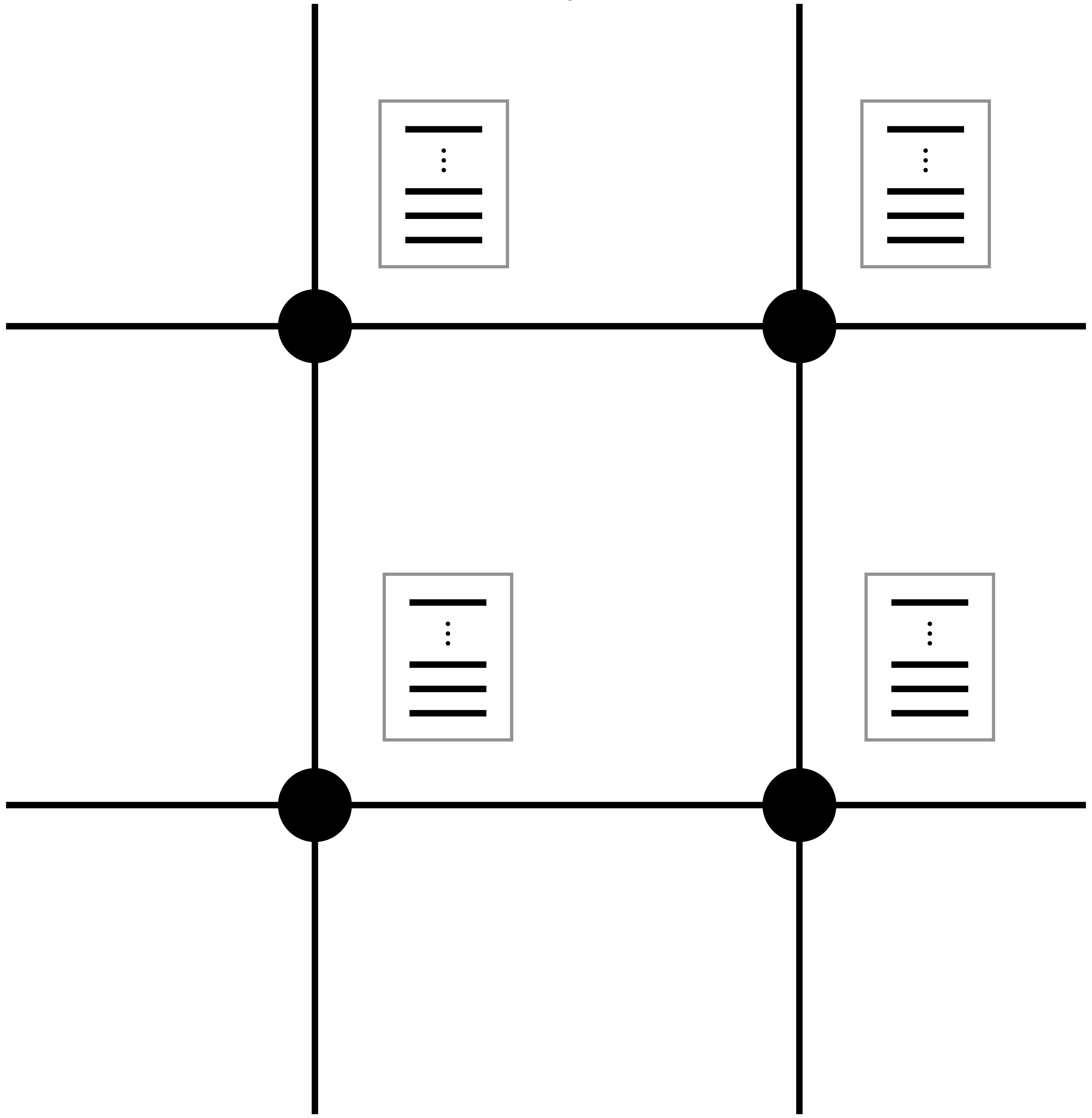
Classical dynamics

$$|\Psi\rangle = \bigotimes_j |\Psi_j\rangle$$

- Well defined procedure for bosonizing a Hamiltonian in *N*-flavors

$$\left\{ b_{j,0}, \ldots, b_{j,N-1} \right\} \qquad \sum_{m=0}^{N-1} b_{j,m}^{\dagger} b_{j,m} = M$$

$$b_{j,0}^{\dagger} = b_{j,0} = \sqrt{M}\sqrt{1 - \frac{\sum_{m=1}^{N-1} b_{j,m}^{\dagger} b_{j,m}}{M}}$$



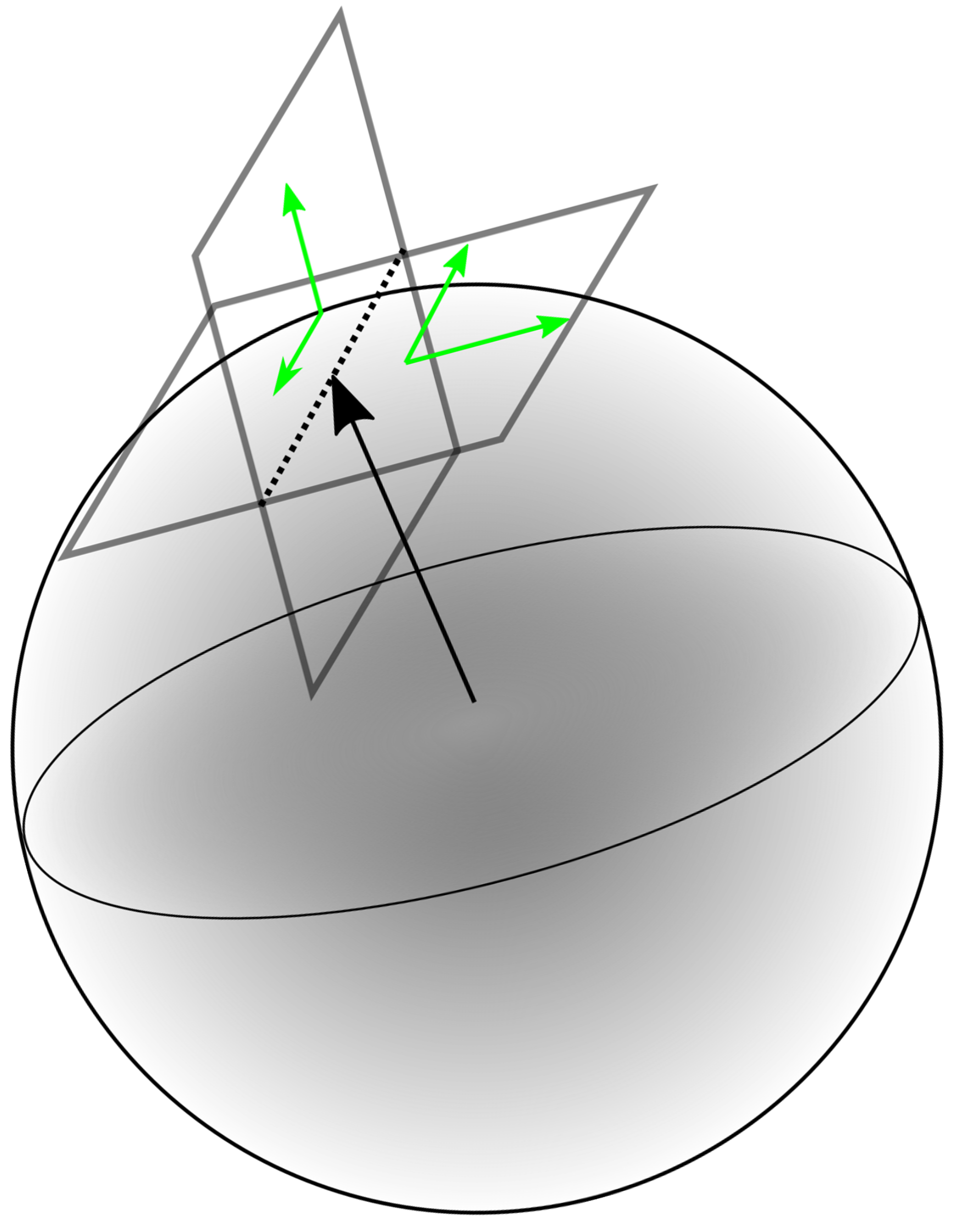
R. Muniz, Y. Kato, C. Batista, "Generalized spin-wave theory," Prog. Theor. Exp. Phys., (2014).

Correspondence between LL and LSWT

SU(*N*) generalization

- Generalized LL (GLL) and multi-flavor LSWT (GLSWT) are connected by SU(*N*) coherent states and the use of *M* as a control parameter.
- Linearized GLL about the ground state yields same dispersion as GLSWT
- The generalizations of both the classical and semiclassical theories yield $N-1$ modes per site

$$\mathbf{n}_j = \mathbf{n}_{0,j} + \delta\mathbf{n}_j$$



SU(*N*) generalization

Motivation: Ground states

- Consider a simple single-site problem.

$$\mathcal{H} = D\left(S^z\right)^2 = D\begin{pmatrix}1 & 0 & 0\\ 0 & 0 & 0\\ 0 & 0 & 1\end{pmatrix}$$

$$\langle \pm 1|\,\mathcal{H}\,|\pm 1\rangle = D$$

$$\langle 0|\,\mathcal{H}\,|0\rangle = 0$$

SU(*N*) generalization

Motivation: Ground states

- The ground state is clearly $|0\rangle$, which is non-magnetic:

$$\langle 0 | S^x | 0 \rangle = \langle 0 | S^y | 0 \rangle = \langle 0 | S^z | 0 \rangle = 0$$

- But $|0\rangle$ is not an $SU(2)$ coherent state. Recall the $S = 1$ parameterization:

$$\left| \Omega(\theta, \phi) \right\rangle = e^{i\phi} \cos^2\left(\frac{\theta}{2}\right) | 1 \rangle + \sqrt{2} \cos\left(\frac{\theta}{2}\right) \sin\left(\frac{\theta}{2}\right) | 0 \rangle + e^{-i\phi} \sin^2\left(\frac{\theta}{2}\right) | -1 \rangle$$

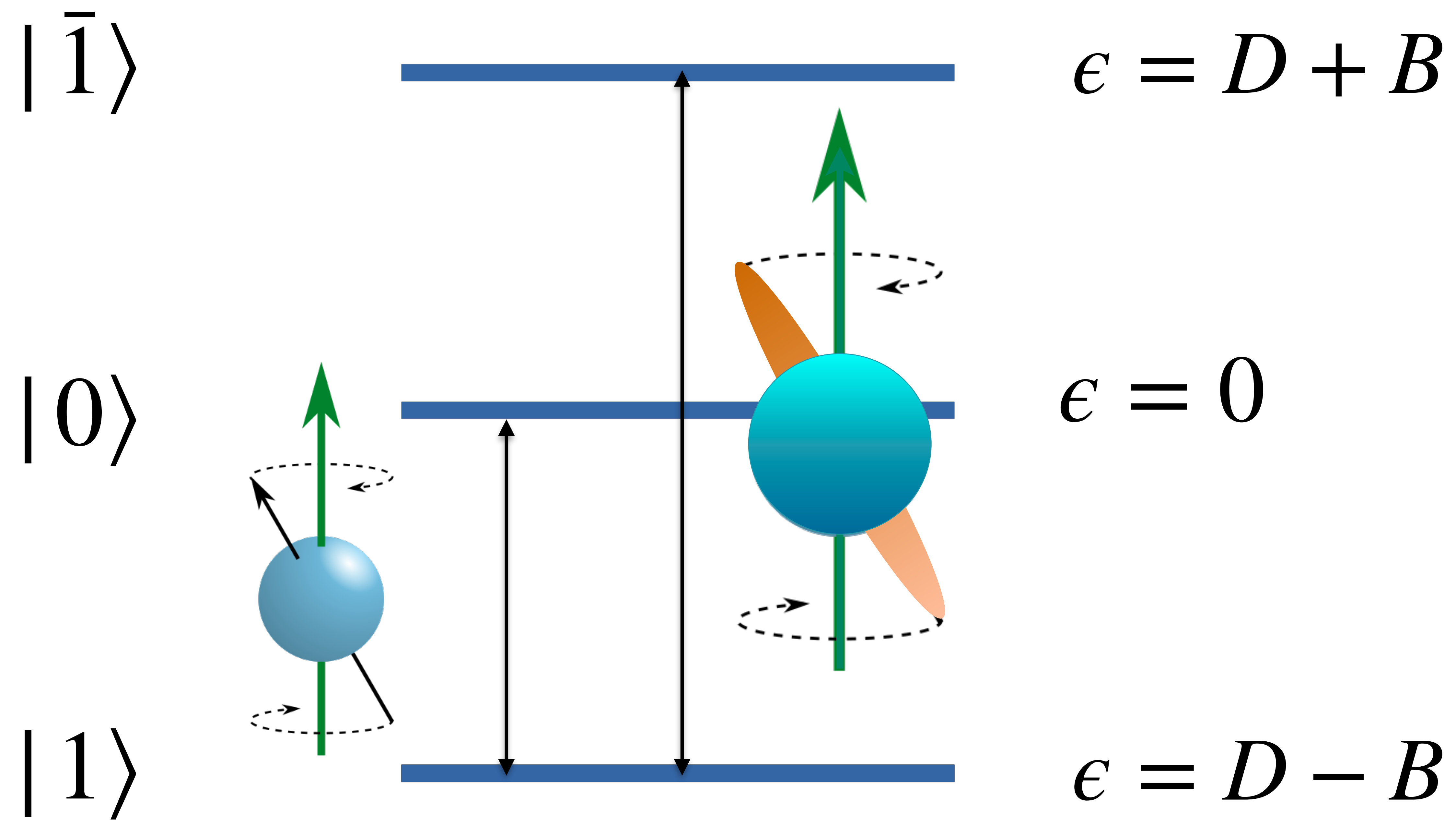
SU(*N*) generalization

Motivation: Dynamics

$$\boxed{\hat{\mathscr{H}}_{SI} = D(\hat{S}^z)^2 - BS^z}$$

Dipolar precession $\omega_D = (D + B)/\hbar$

Quadrupolar precession $\omega_Q = 2B/\hbar$

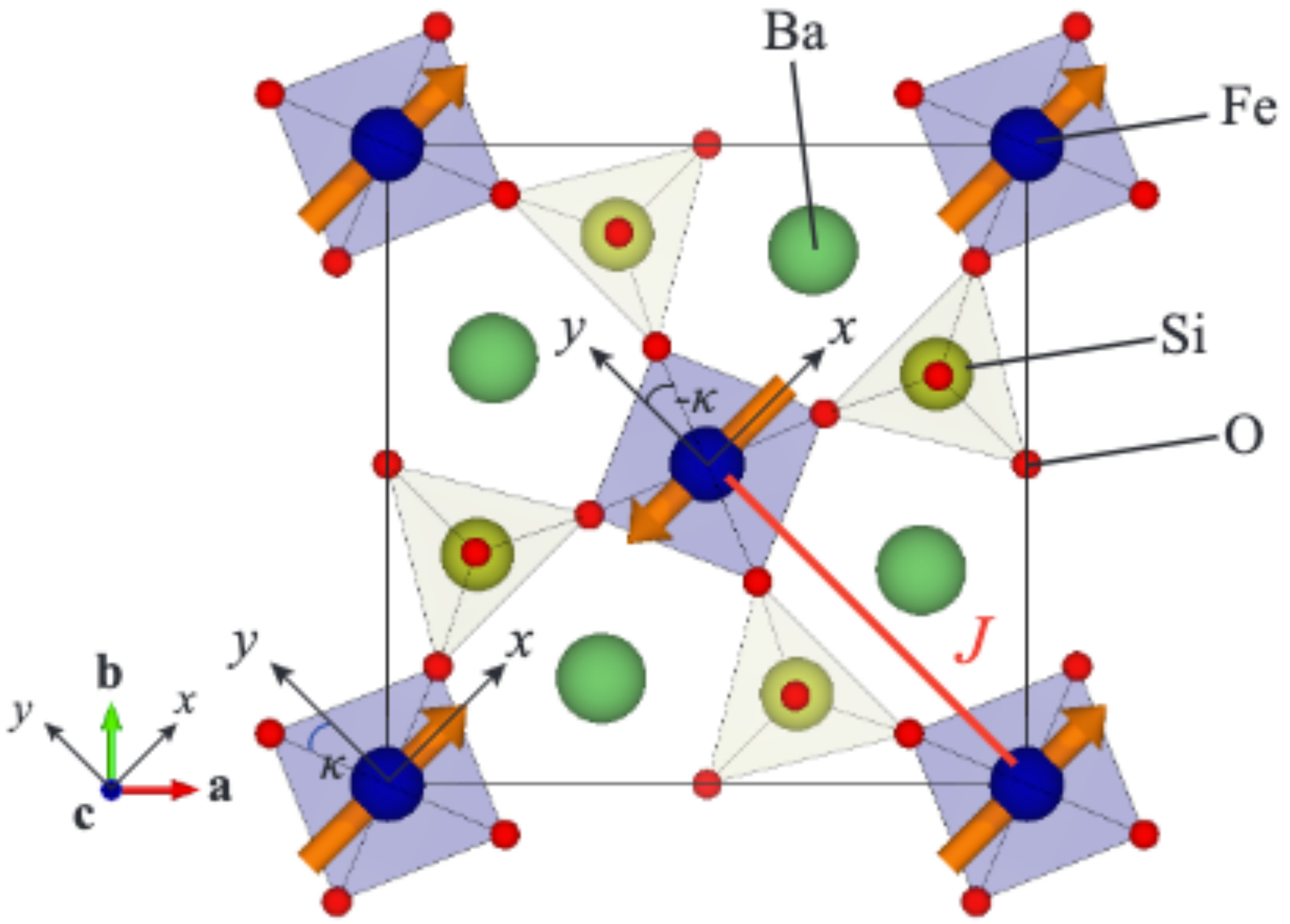


SU(*N*) use case: $Ba_2FeSi_2O_7$

Rich behavior of $S = 2$ spins

- AFM exchange and hard-axis anisotropy on a square lattice.
- Quasi-2D — weak AFM coupling between layers.
- Effective $S = 2$, so use SU(5) with local basis

$$|2\rangle\,, |1\rangle\,, |0\rangle\,, |-1\rangle\,, |-2\rangle$$



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- Quasi-2D — weak AFM coupling between layers.
- Effective $S = 2$, so use SU(5) with local basis

$$|2\rangle \, , |1\rangle \, , |0\rangle \, , |-1\rangle \, , |-2\rangle$$

$$\begin{aligned}
\mathcal{H} \;=\;& J \sum_{i,j} \mathbf{S}_i \cdot \mathbf{S}_j + J' \sum_{\langle\langle i,j \rangle\rangle} \mathbf{S}_i \cdot \mathbf{S}_j \\
&+ D \sum_i (S_i^z)^2 - h \sum_i S_i^z \\
&+ A \sum_{i \in A} \left[\left(\mathbf{S}_i \cdot \mathbf{n}_1^A \right)^4 + \left(\mathbf{S}_i \cdot \mathbf{n}_2^A \right)^4 \right] \\
&+ A \sum_{j \in B} \left[\left(\mathbf{S}_j \cdot \mathbf{n}_1^B \right)^4 + \left(\mathbf{S}_j \cdot \mathbf{n}_2^B \right)^4 \right] \\
&+ C \sum_i (S_i^z)^4 ,
\end{aligned}$$

SU(N) use case: $Ba_2FeSi_2O_7$

Rich behavior of $S = 2$ spins

- Magnetization versus field

  *PRB **107** 144427 (2023)*

Field-induced spin level crossings within a quasi-XY antiferromagnetic state in $Ba_2FeSi_2O_7$

Minseong Lee,[1,*] Rico Schönemann,[1] Hao Zhang,[2,3] David Dahlbom,[3] Tae-Hwan Jang,[4] Seung-Hwan Do,[2] Andrew D. Christianson,[2] Sang-Wook Cheong,[4,5] Jae-Hoon Park,[4,6] Eric Brosha,[7] Marcelo Jaime,[1] Kipton Barros,[8] Cristian D. Batista,[3,†] and Vivien S. Zapf[1,‡]

- Generalized LSWT calculations

  Nature Communications 12:5331 (2021)

Decay and renormalization of a longitudinal mode in a quasi-two-dimensional antiferromagnet

Seung-Hwan Do[1,9✉], Hao Zhang[1,2,9], Travis J. Williams[3], Tao Hong[3], V. Ovidiu Garlea[3], J. A. Rodriguez-Rivera[4,5], Tae-Hwan Jang[6], Sang-Wook Cheong[6,7], Jae-Hoon Park[6,8], Cristian D. Batista[2] & Andrew D. Christianson[1]

- Finite temperature behavior

  npj quantum materials 5 (2023)

Understanding temperature-dependent SU(3) spin dynamics in the $S = 1$ antiferromagnet $Ba_2FeSi_2O_7$

Seung-Hwan Do[1,8], Hao Zhang[1,2,8], David A. Dahlbom[2], Travis J. Williams[3], V. Ovidiu Garlea[3], Tao Hong[3], Tae-Hwan Jang[4], Sang-Wook Cheong[4,5], Jae-Hoon Park[4,6], Kipton Barros[7], Cristian D. Batista[2✉] and Andrew D. Christianson[1✉]

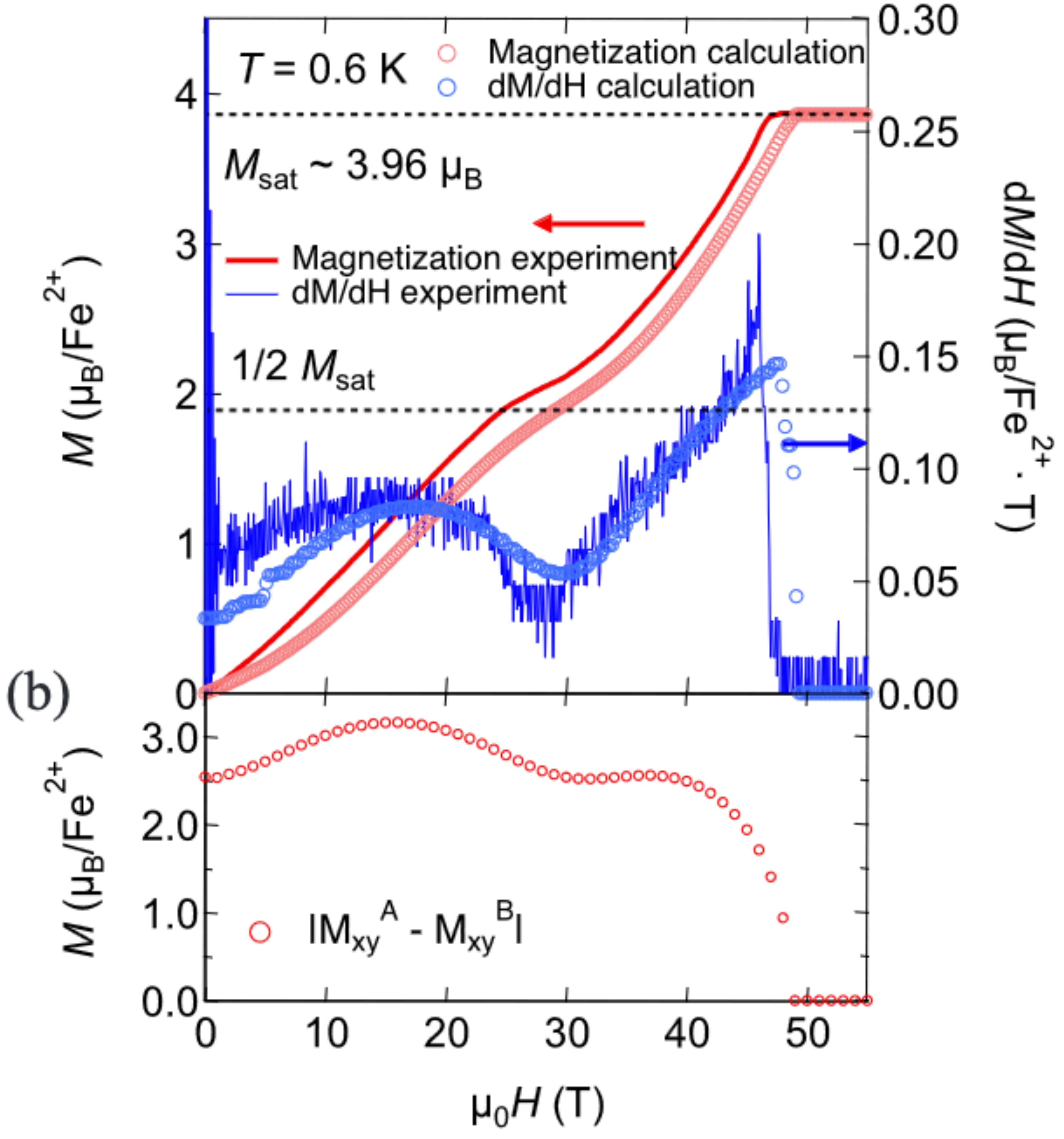
SU(N) use case: $Ba_2FeSi_2O_7$

M and staggered magnetization vs H

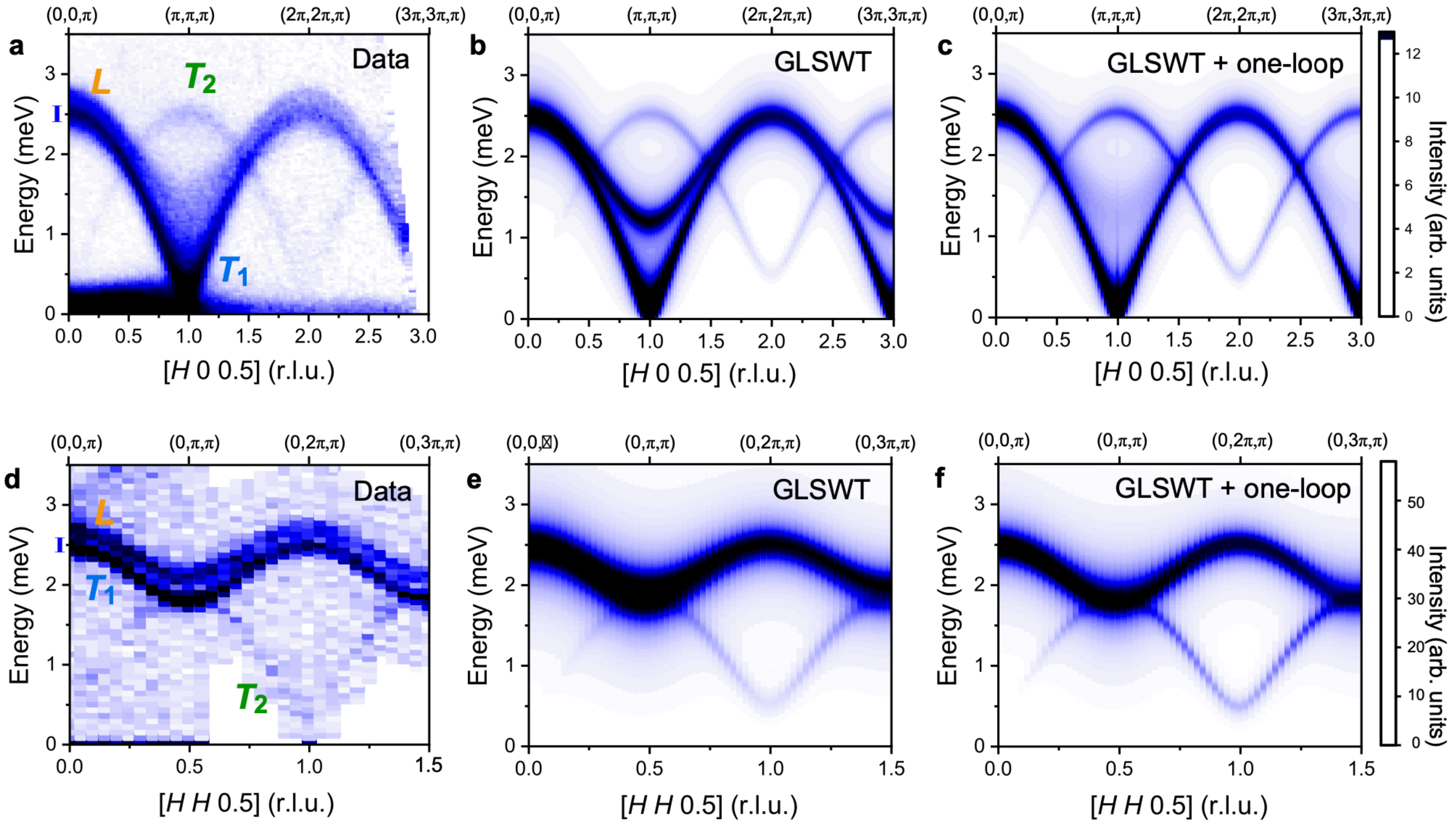
- Zero field: $|1\rangle\,,|0\rangle$

- Applied field: $|2\rangle\,,|0\rangle$

- Fully saturated: $|2\rangle$

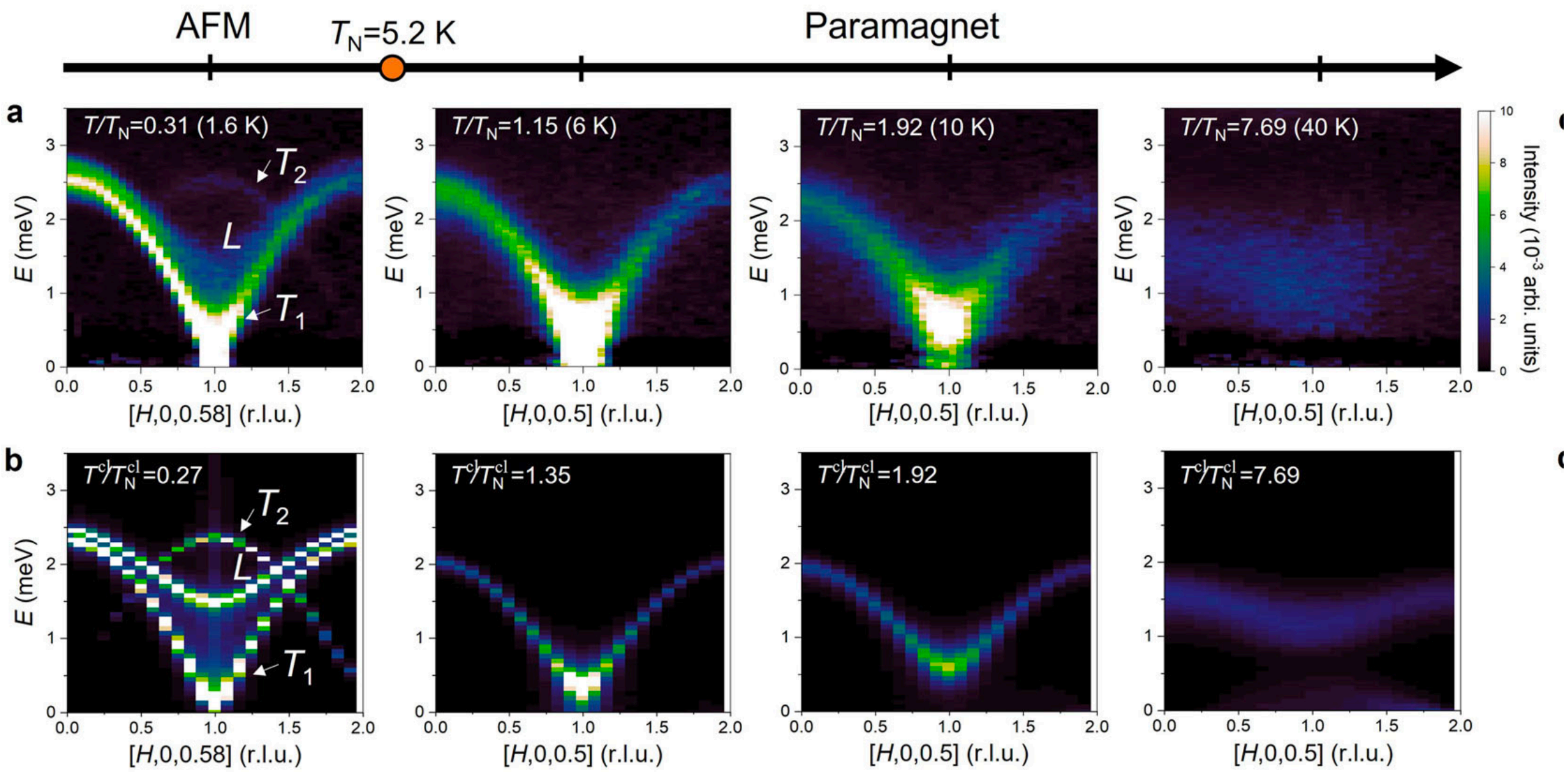


SU(*N*) use case: $Ba_2FeSi_2O_7$
Multi-flavor spin wave calculation



SU(*N*) use case: $Ba_2FeSi_2O_7$

Finite temperature



Takeaways

What Sunny is

- A collection of tools for
  - Performing **symmetry analysis** and specifying spin Hamiltonians

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  - Generating **intensity output** that can be compared directly to neutron scattering data
- It is also a broad collaboration dedicated to making general, high-quality implementations of theoretical techniques available to neutron scatterers.

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What SU(*N*) is good for

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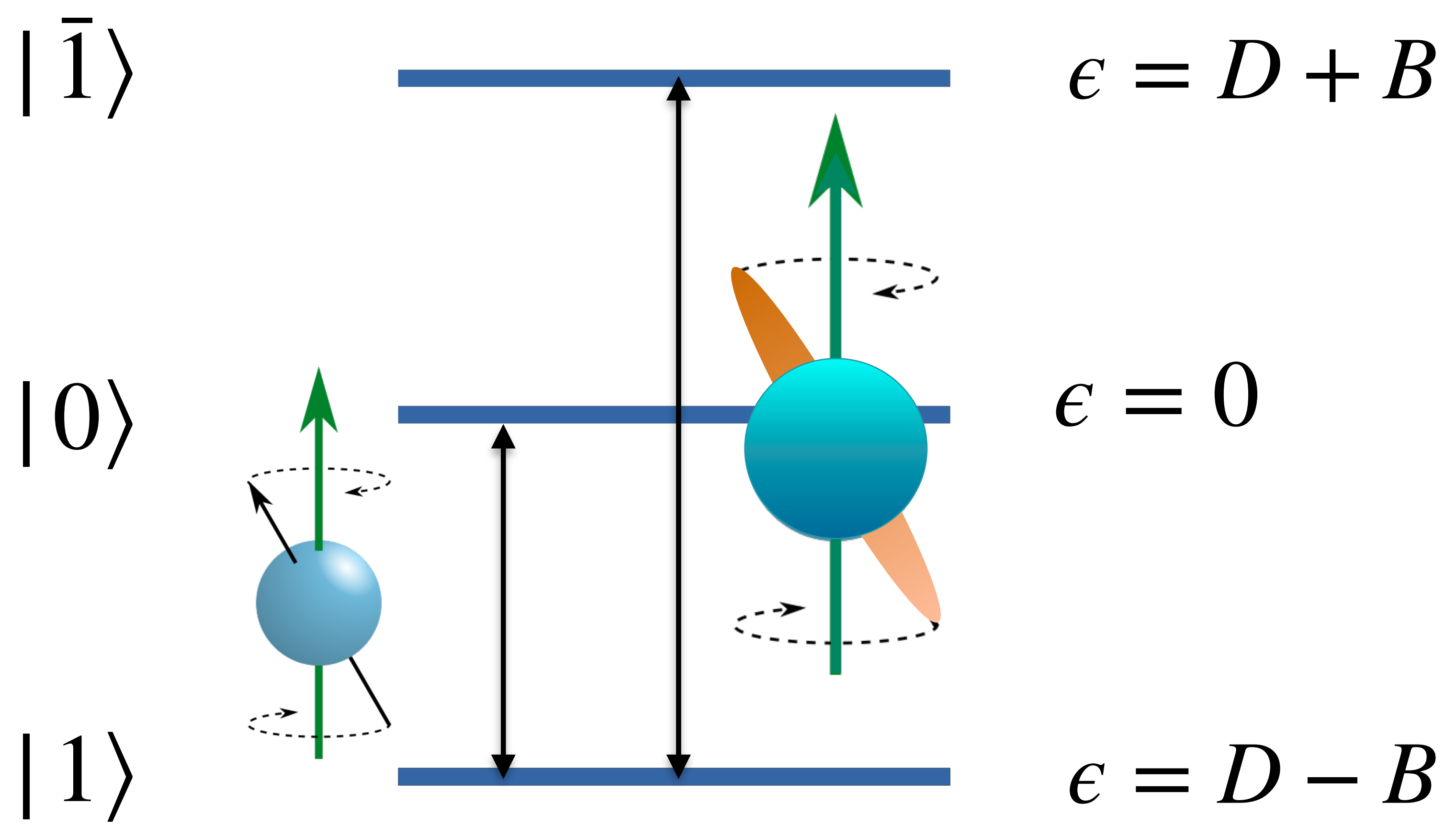

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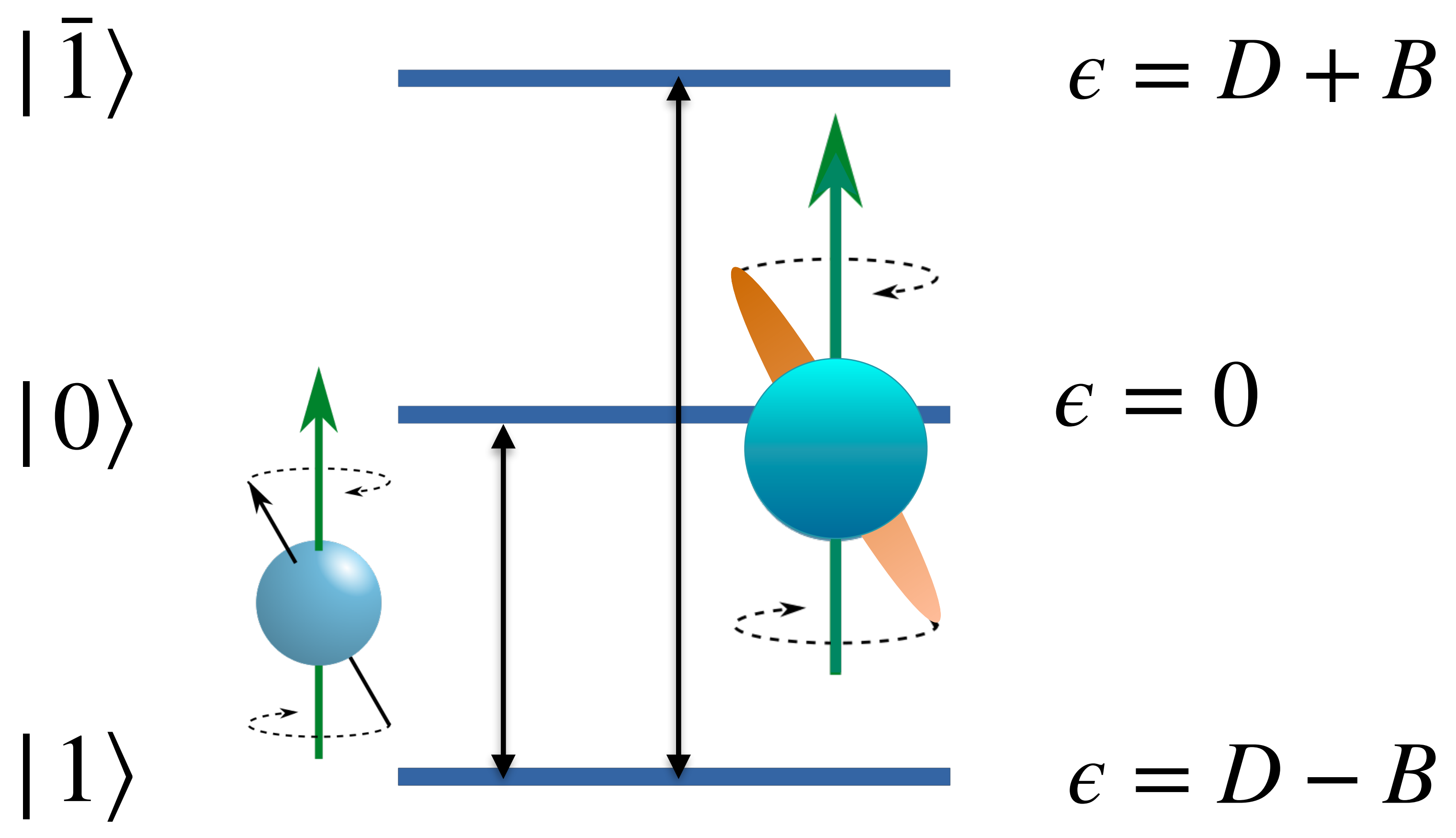
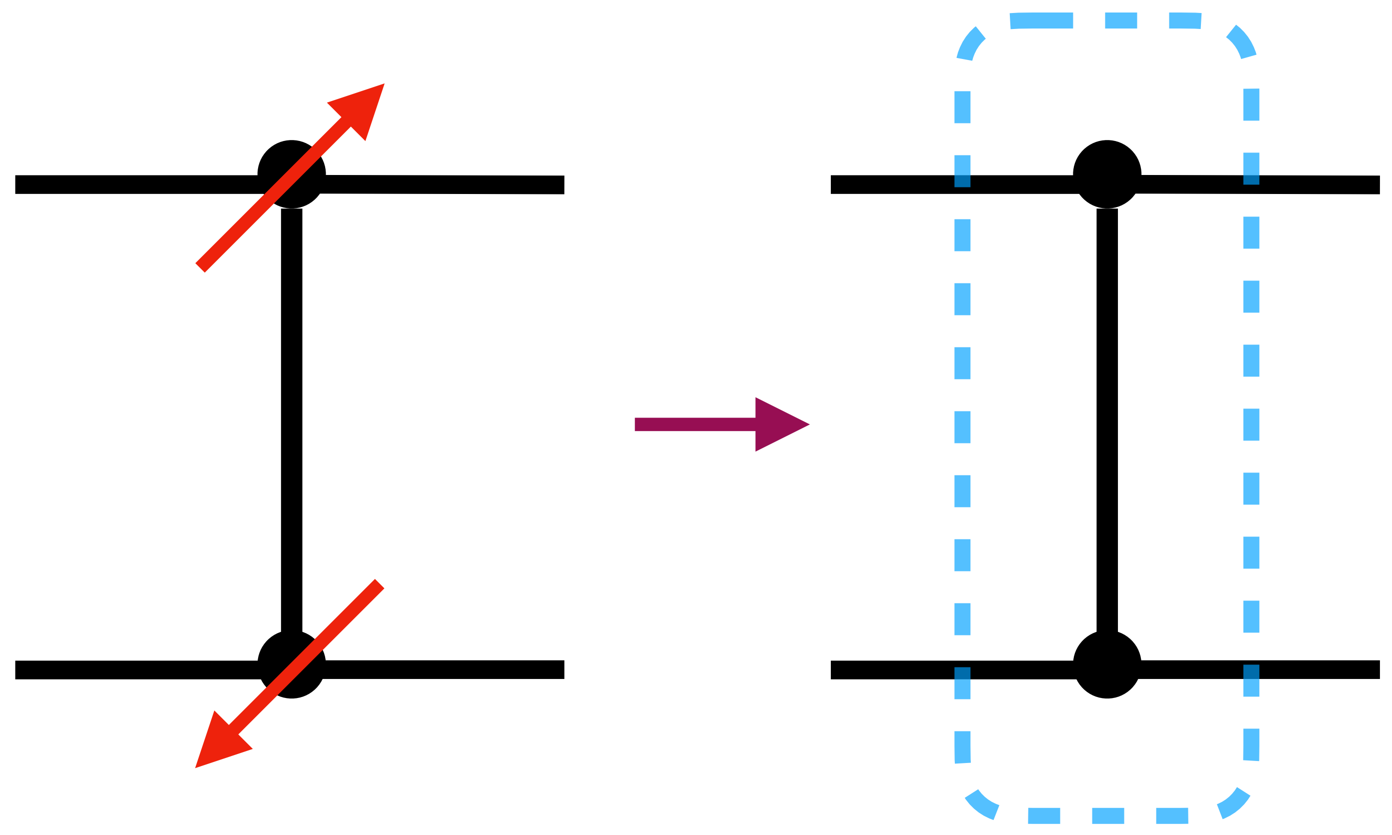
- Capture more **local physics** at the linear level
- Useful for **large spins** with “nonlinear” operators in your Hamiltonian (4d-5d, 4f-5f and some 3d materials).
- Model “localized” entanglement (dimers, trimers, tetramers, etc.).





Takeaways

What makes Sunny unique

- Powerful set of tools for analyzing symmetries, visualizing crystals, and specifying a **broad class of spin Hamiltonians**.
- Easy access to both **classical and semiclassical techniques**, which are coupled together productively.
- Generalization of both classical and semiclassical dynamics to **SU(*N*) coherent states**.
- Written in **Julia**, which is both interactive and fast.

Takeaways

How to get involved

- Visit the GitHub site (https://github.com/SunnySuite/Sunny.jl)
- Join the Sunny Slack (link on bottom of GitHub page)
- Talk to one of us!