OAK RIDGE National Laboratory

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Brief introduction to Classical and Semiclassical Spin Dynamics

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U.S. DEPARTMENT OF ENERGY

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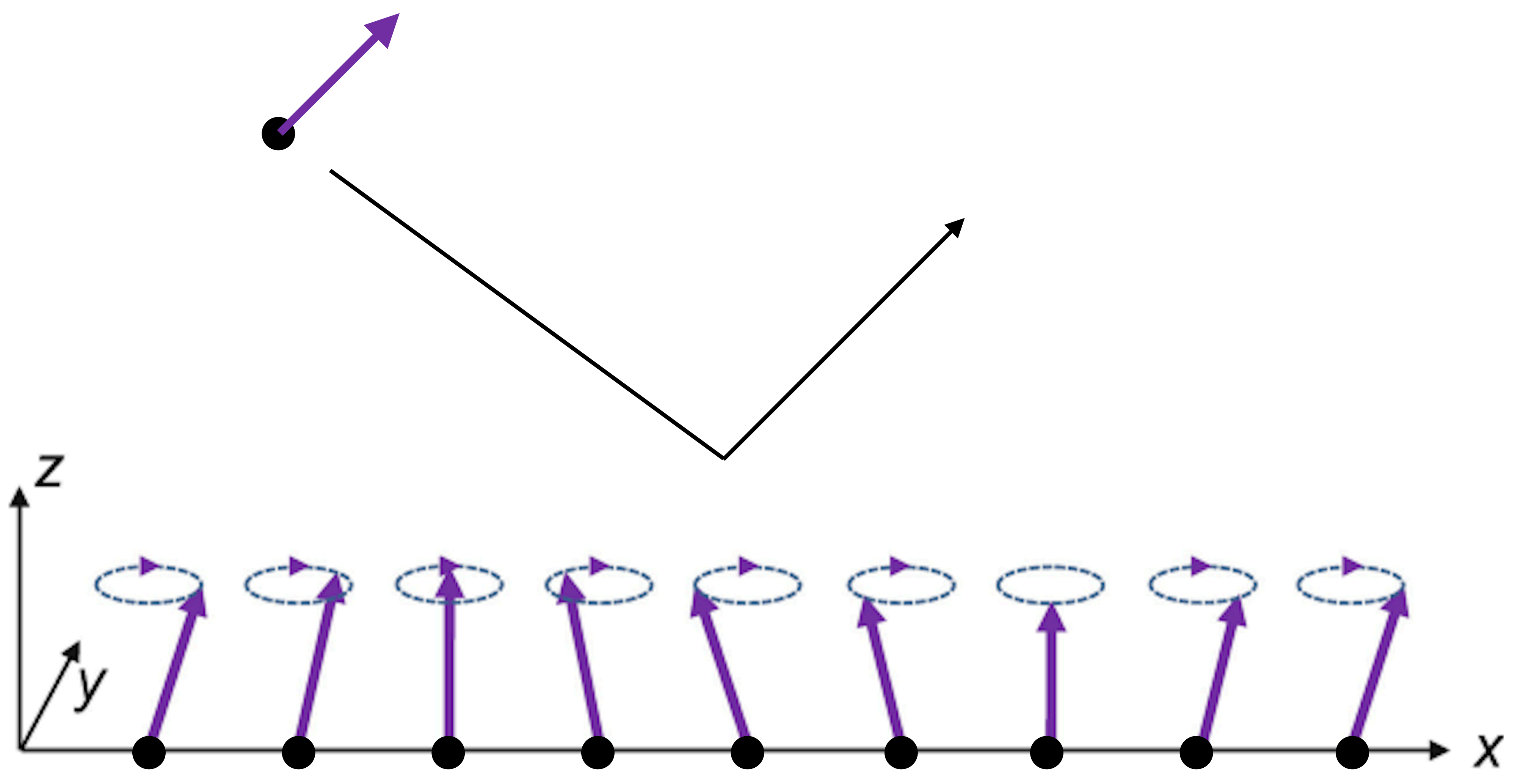
Part I
Introduction

- Briefly introduce the information that is obtained from neutron scattering experiments
- Describe spin Hamiltonians and their basic interactions
- Describe how to develop spin dynamics on top of ground states, classically and semiclassically

Inelastic Neutron Scattering

Overview

- Neutrons have (small) magnetic moments but no electrical charge.
- They can scatter either off of nuclei (strong force) or have their magnetic moment couple to the magnetic structure of material.
- The magnetic coupling is relative weak, meaning the measurement process does not strongly affect the sample.
- Scattering process can be treated perturbatively

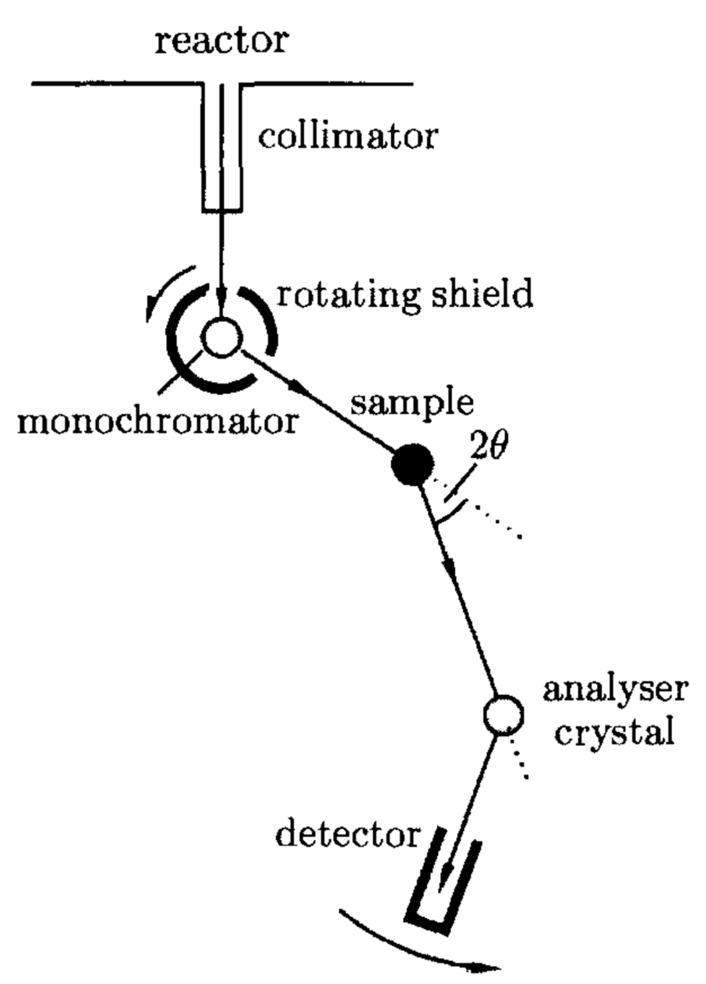


https://warwick.ac.uk/fac/sci/physics/research/condensedmatt/imr_cdt/students/kelvin_goh/ins/

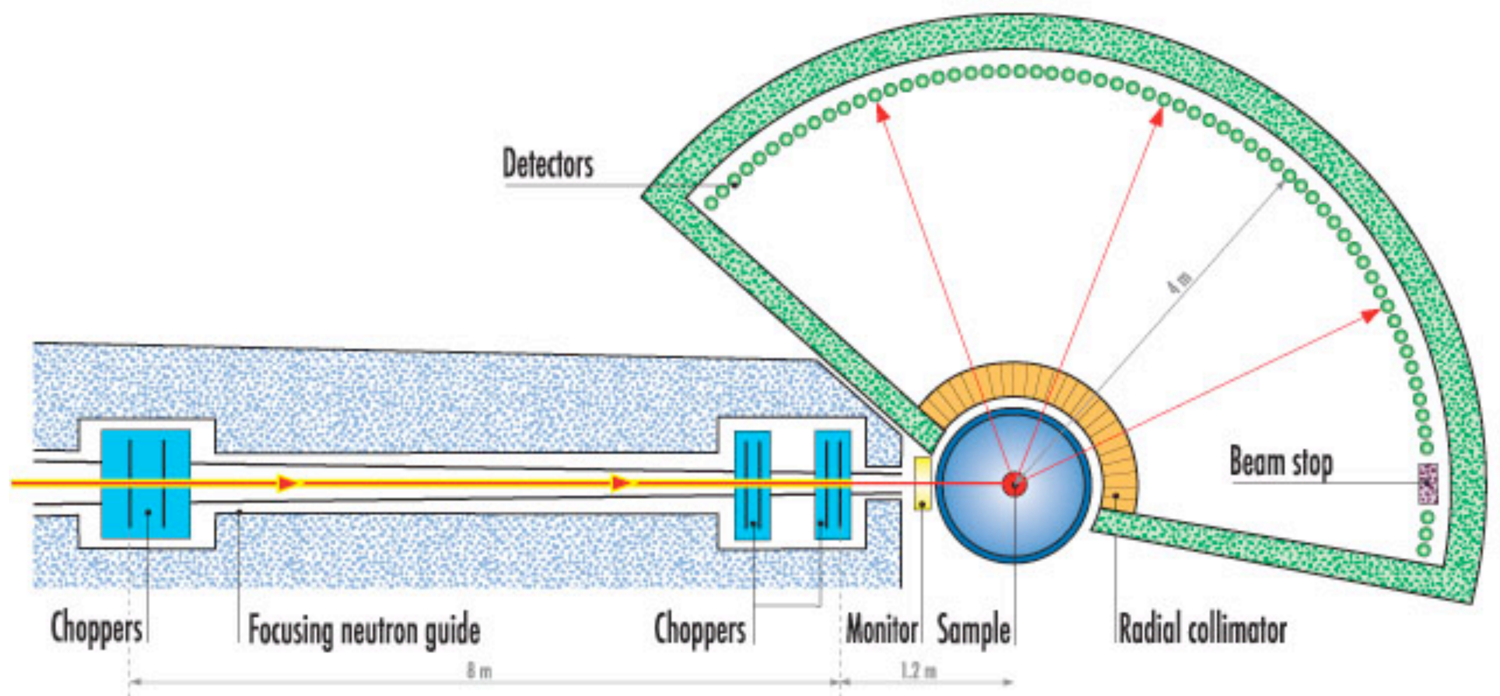
Inelastic Neutron Scattering

Sources and Instruments

- Neutrons typically generated as byproduct of nuclear reaction or “spalled” off of heavy ions with accelerated protons.
- Resulting neutrons are then filtered in various ways (moderated, “chopped," etc.) and directed at a sample.
- Some system of detectors is set up to measure the results of the scattering process.



S. Blundell, *Magnetism in Condensed*



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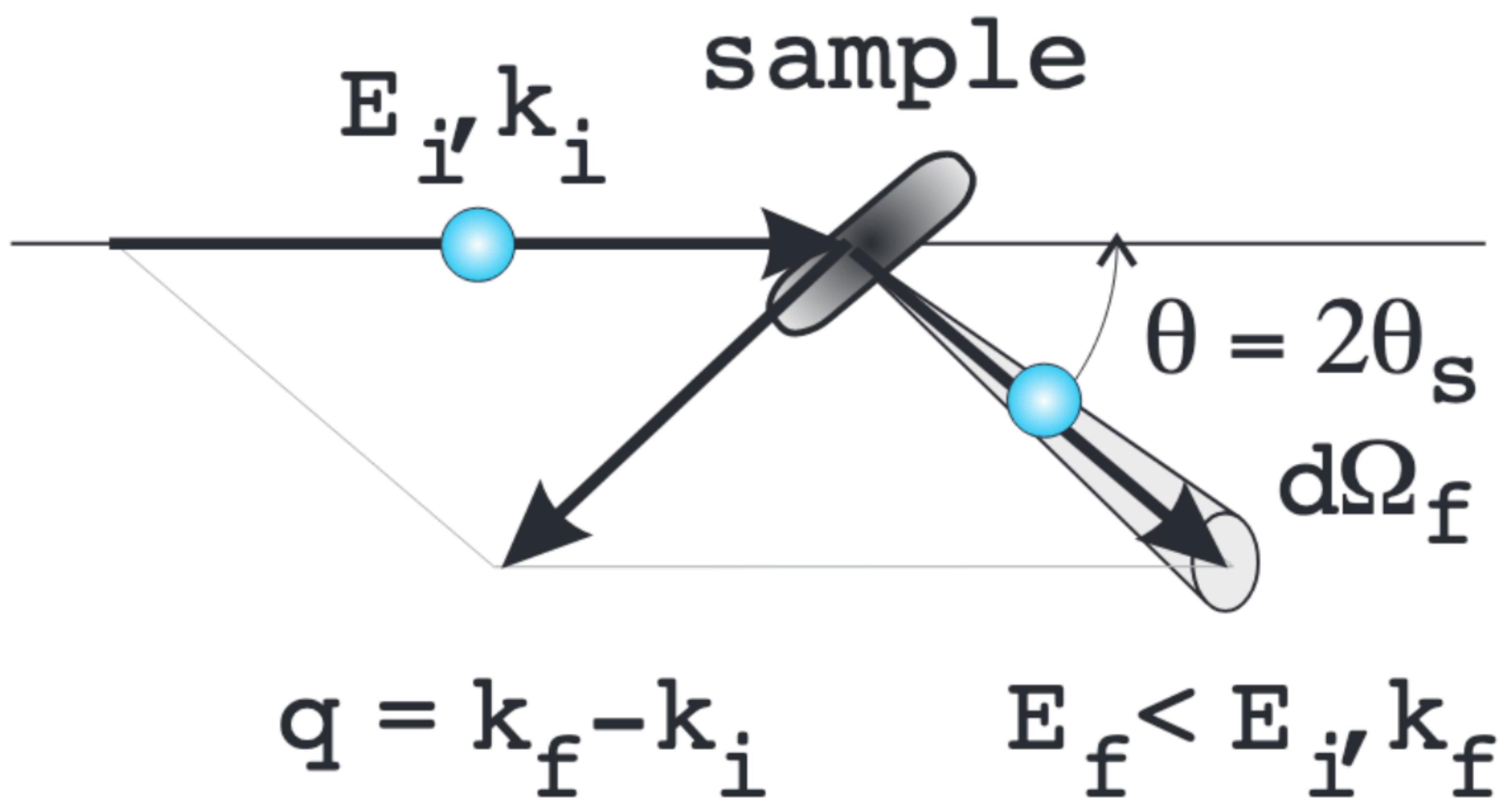
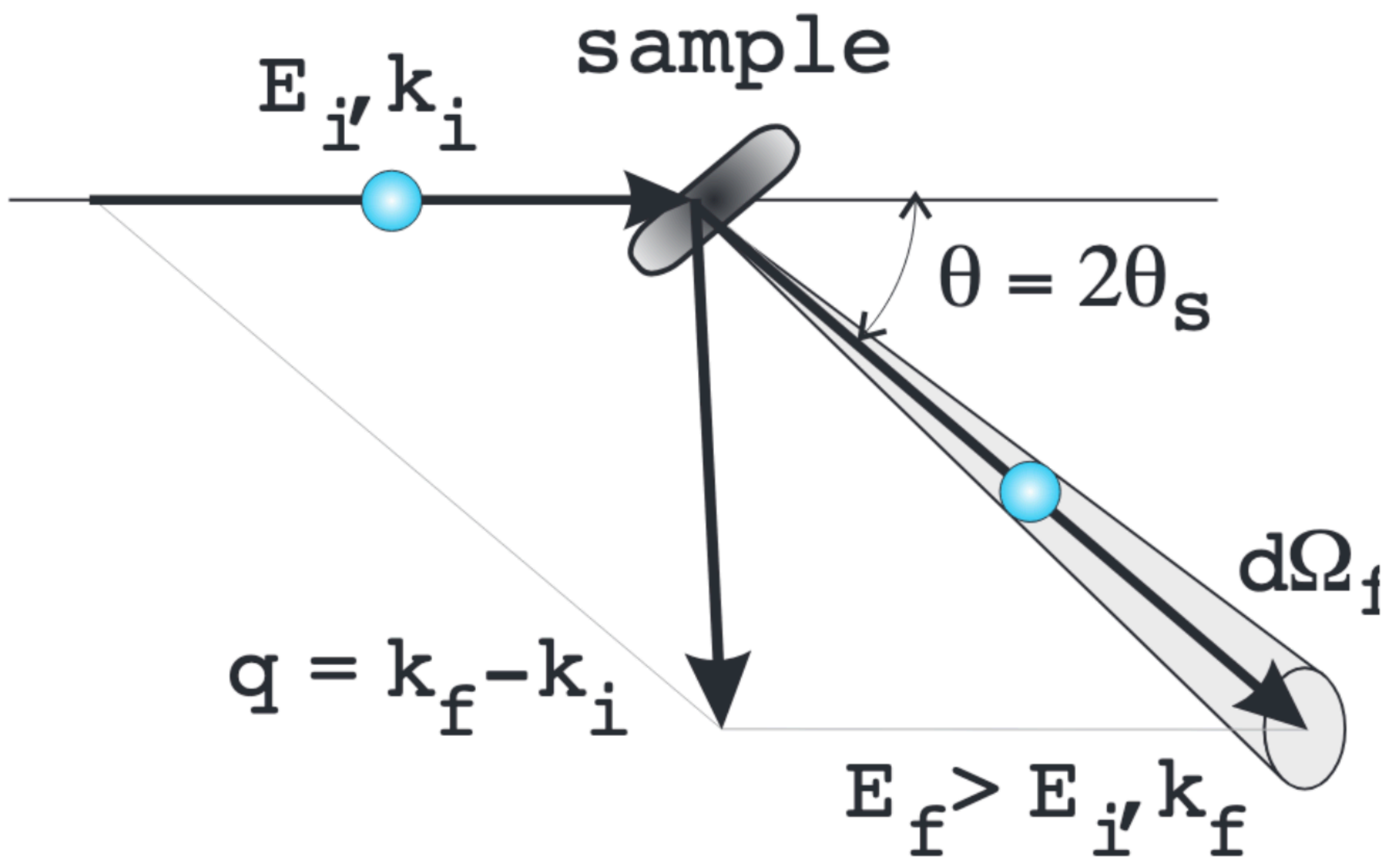
Inelastic Neutron Scattering

Basic picture of scattering process

- The conservation of energy and momentum allow us to infer information about the interaction of the neutron with the material.

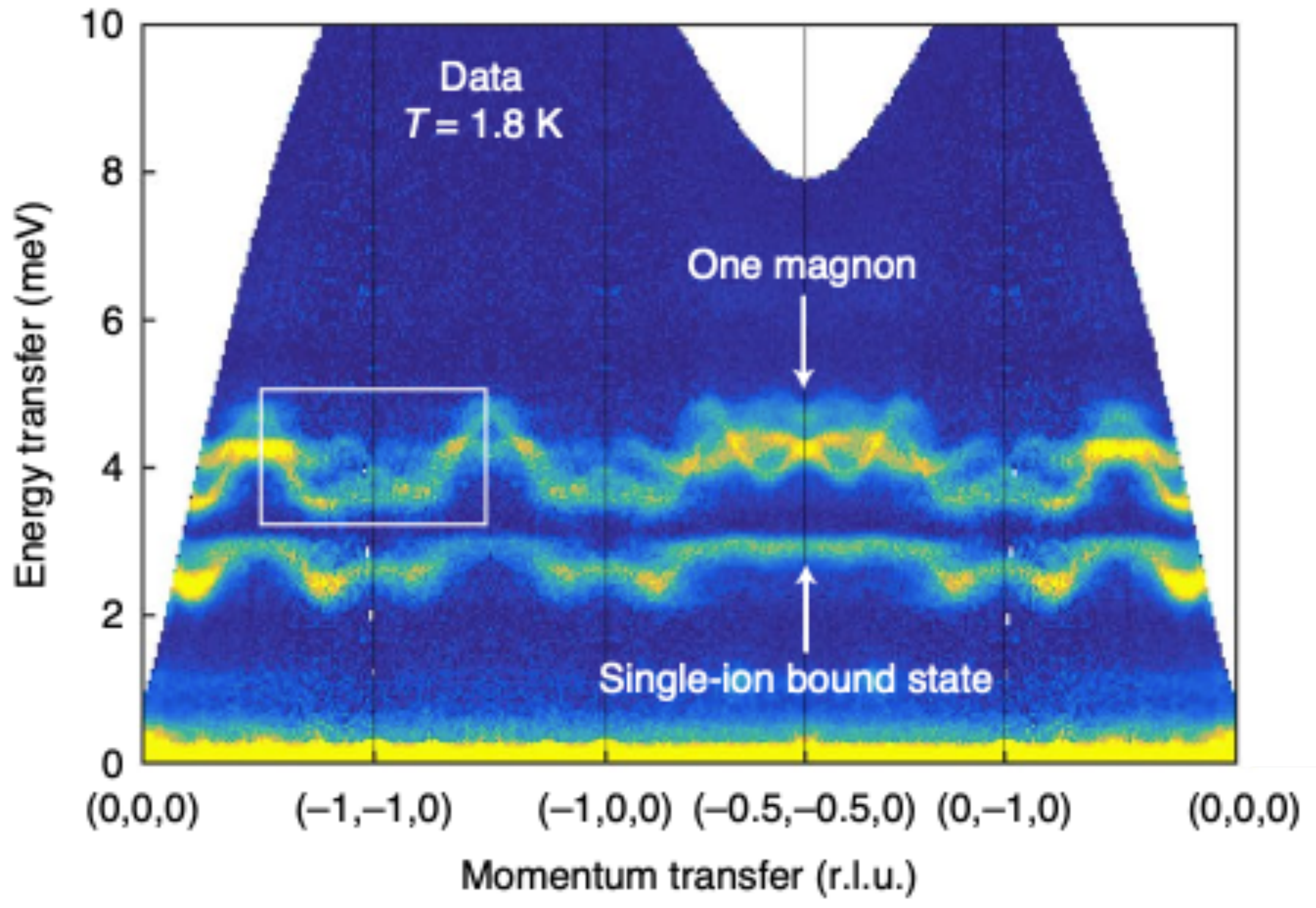




I.A. Zalyzniak and J.M. Tranquada, arXiv:1304.4214 (2013).

Inelastic Neutron Scattering

Scattering intensities

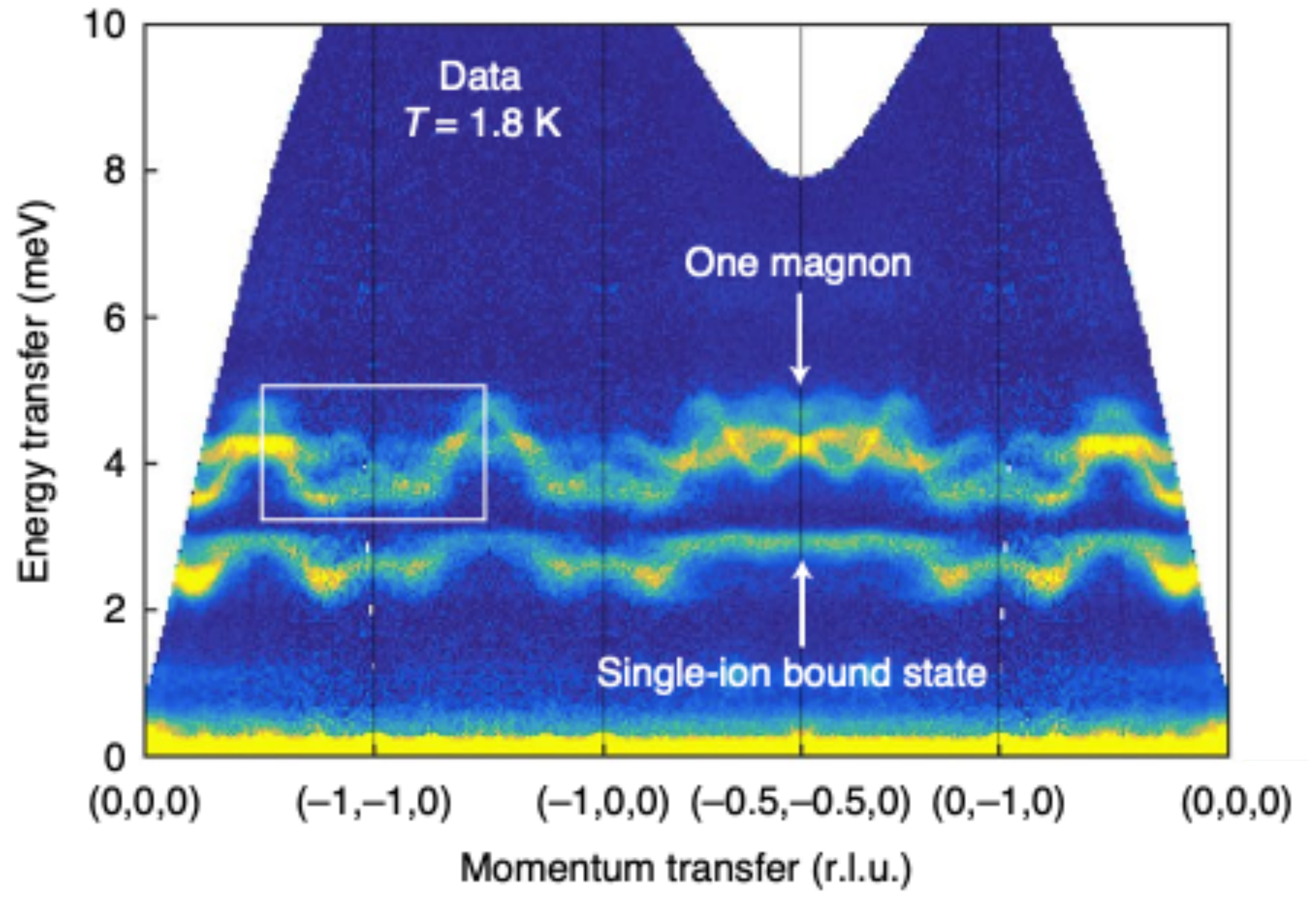


Xiaojian Bai, et al. Nature Physics, 17, 467-472 (2021)

$$\frac{d^2\sigma}{d\Omega dE} = \frac{\text{number of neutrons scattered per second into d}\Omega\text{ \& dE}}{\Phi\ \text{d}\Omega\ \text{dE}}$$

Inelastic Neutron Scattering

Scattering intensities



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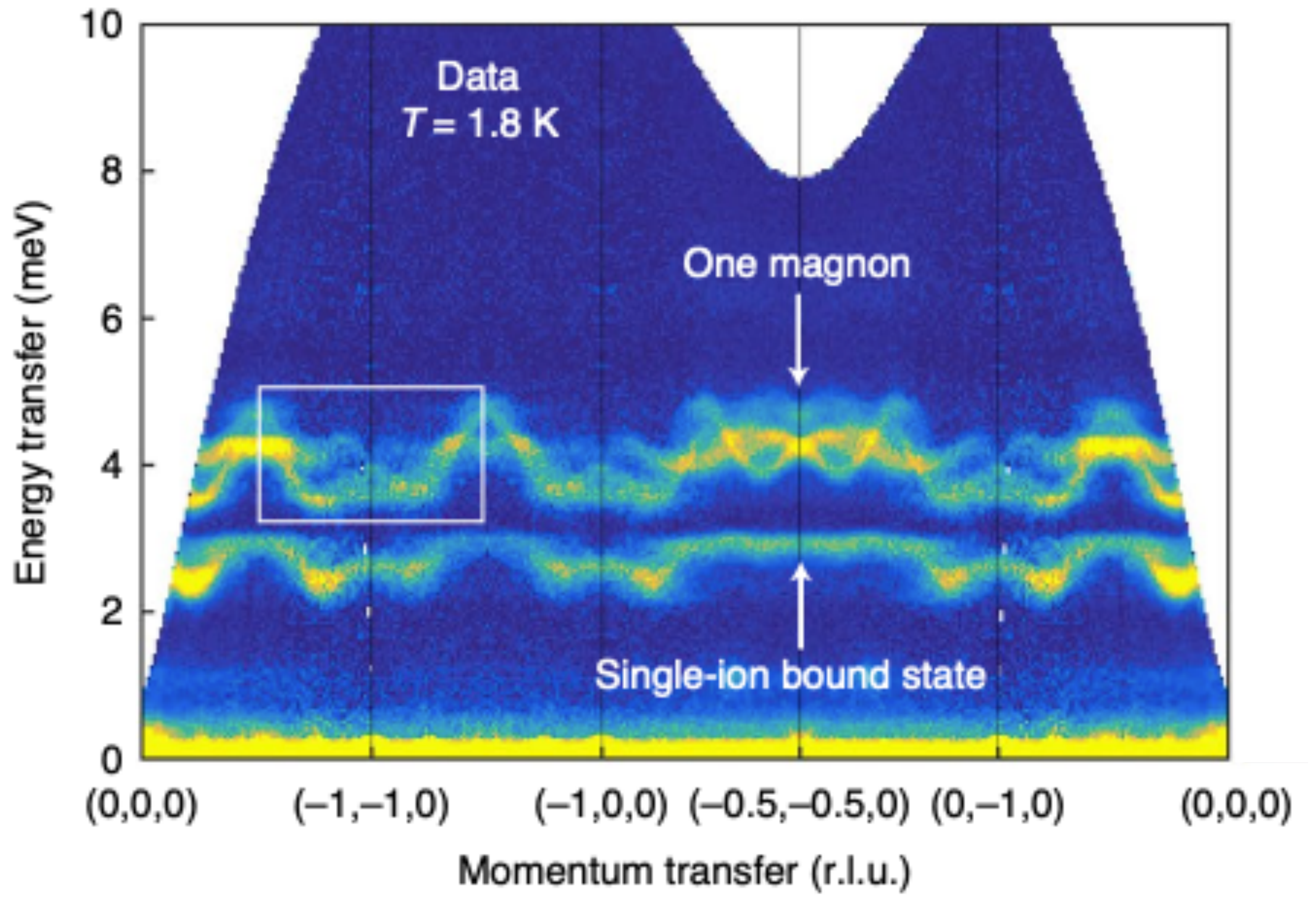

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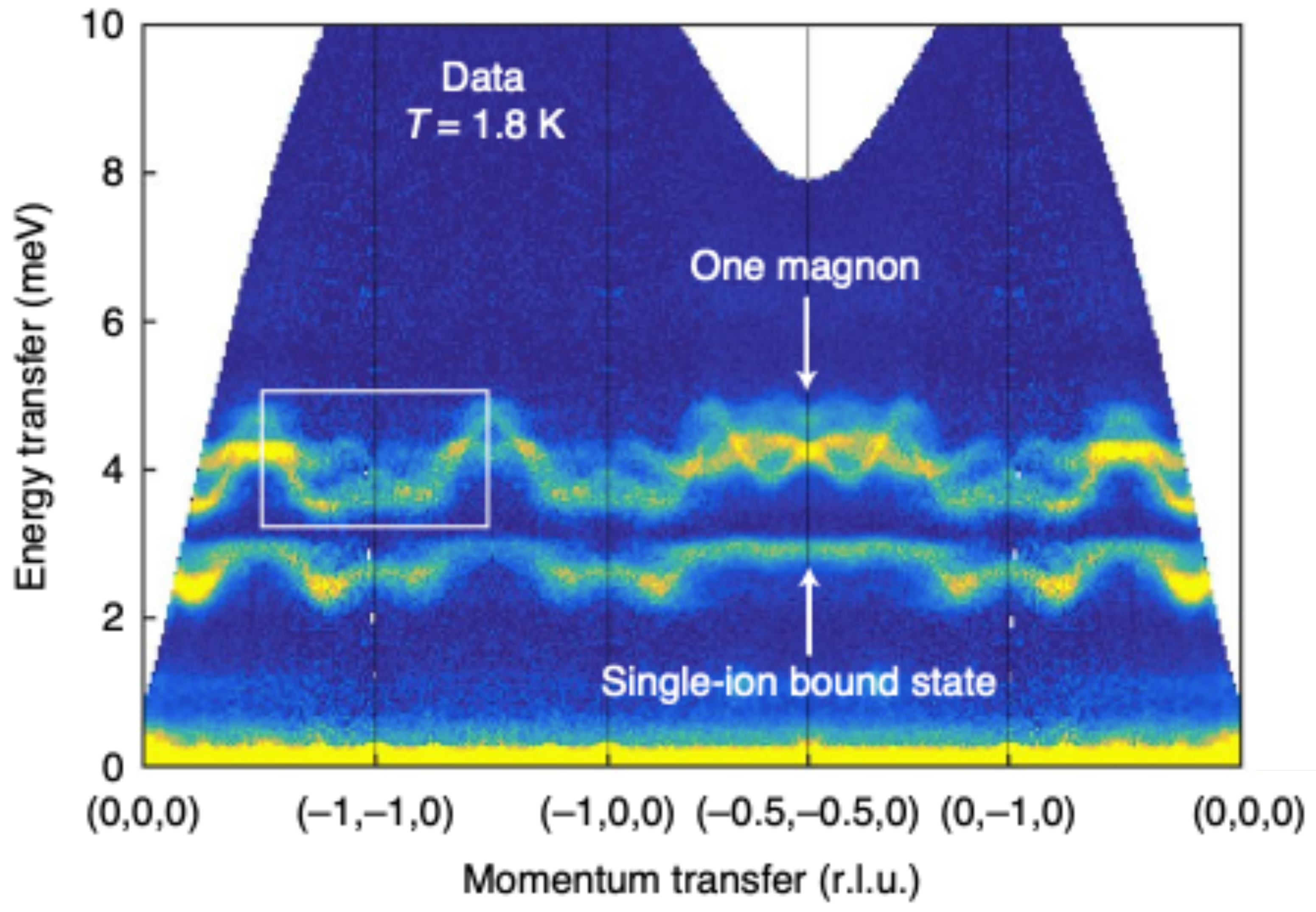

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← DSSF

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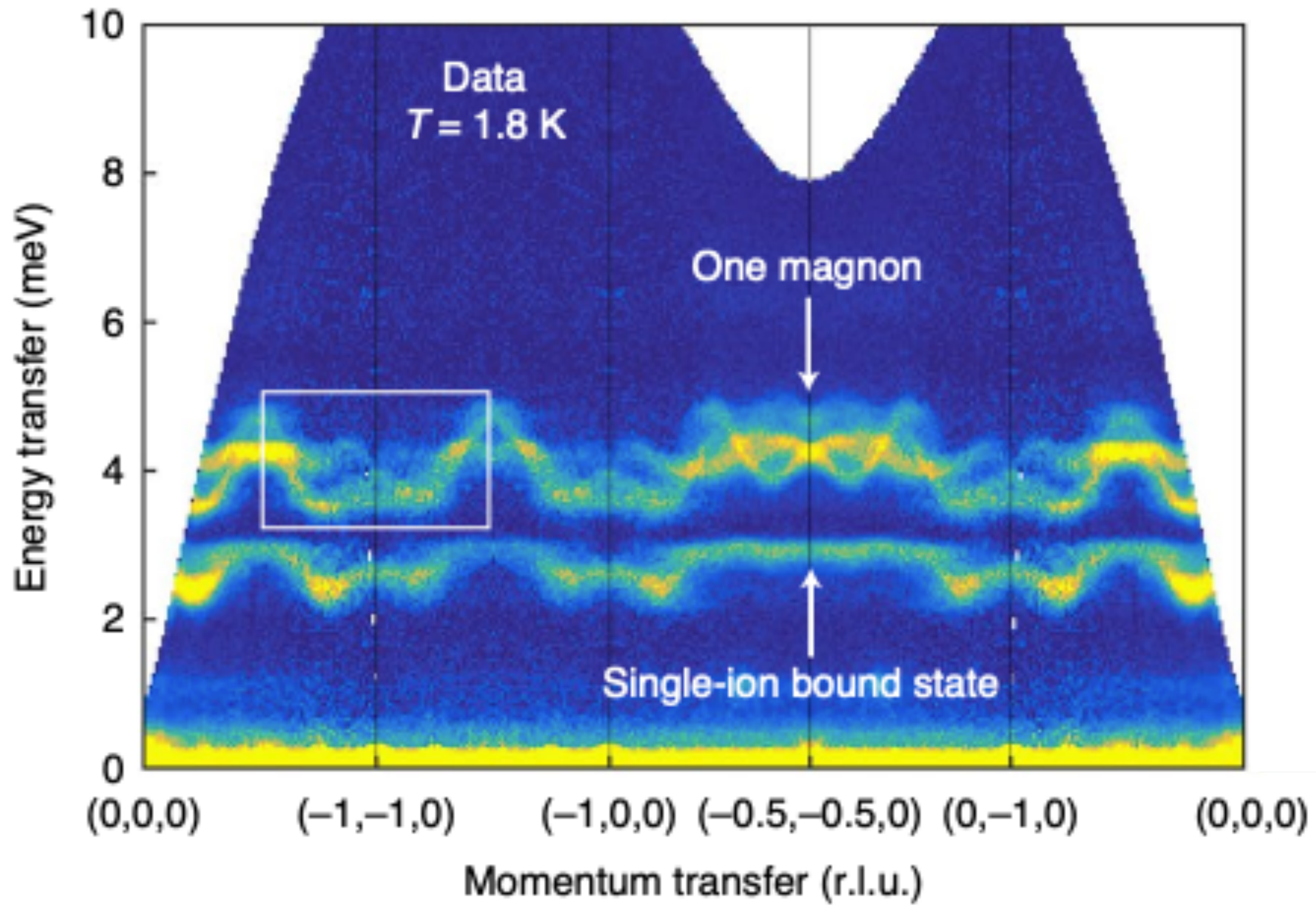
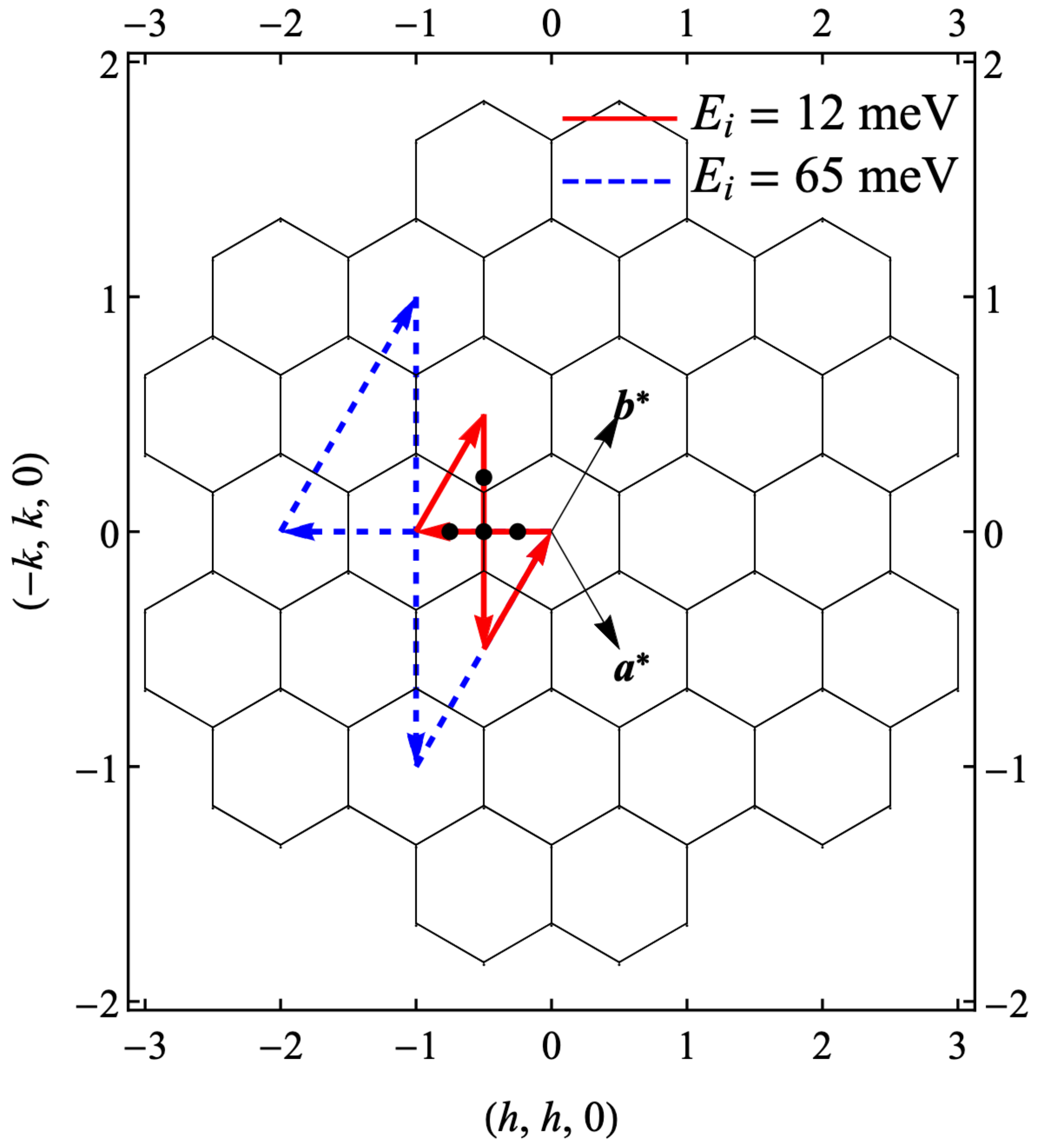
Inelastic Neutron Scattering

Scattering intensities

- $\mathcal{S}^{\alpha\beta}(\mathbf{Q}, \omega)$ is 4 dimensional: 3 momentum (space) dimensions and 1 energy (time) dimension.

- Often look at 2-dimensional slices, e.g., a path in momentum space along on axis, energy transfer along the other.





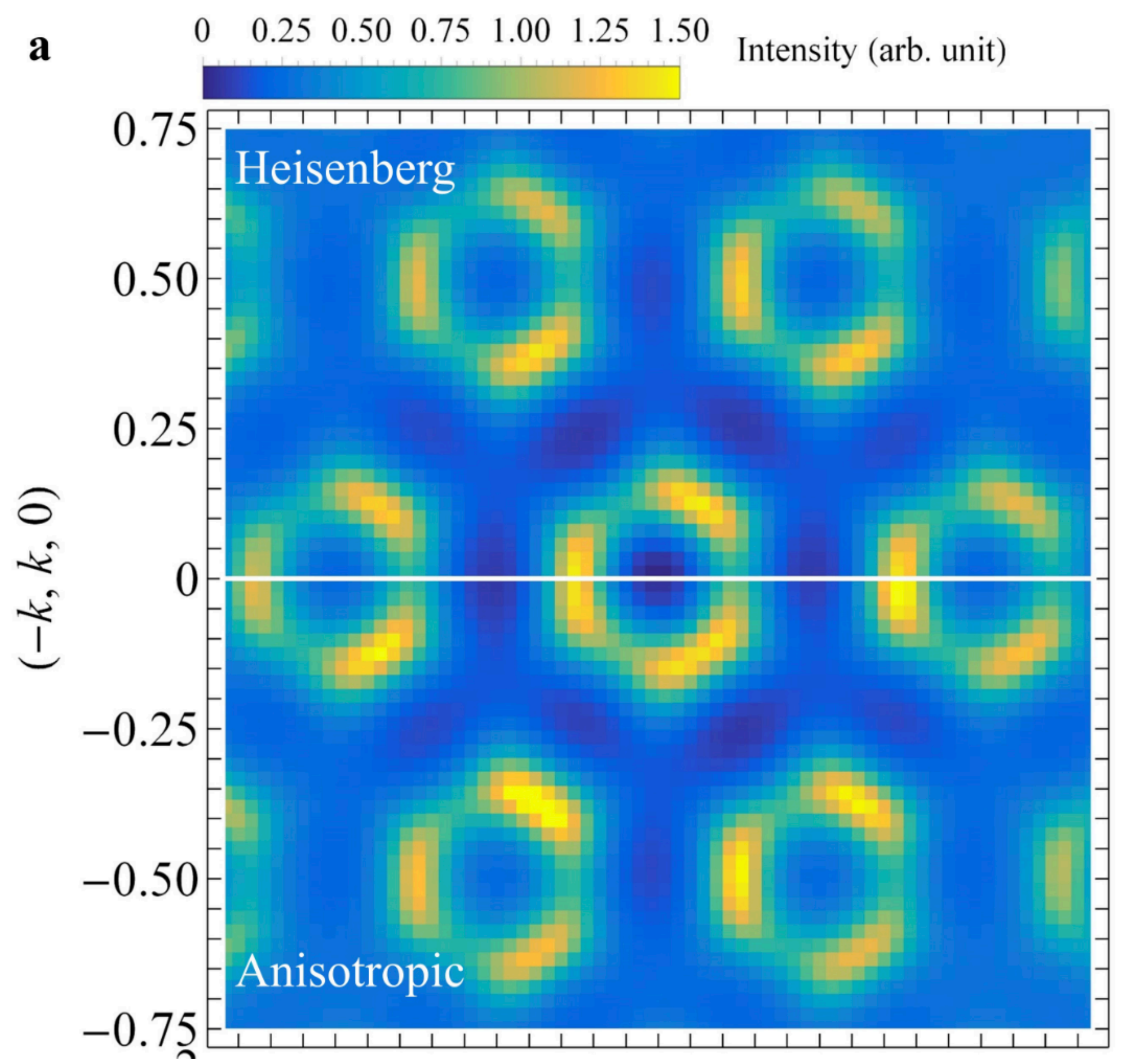
Inelastic Neutron Scattering

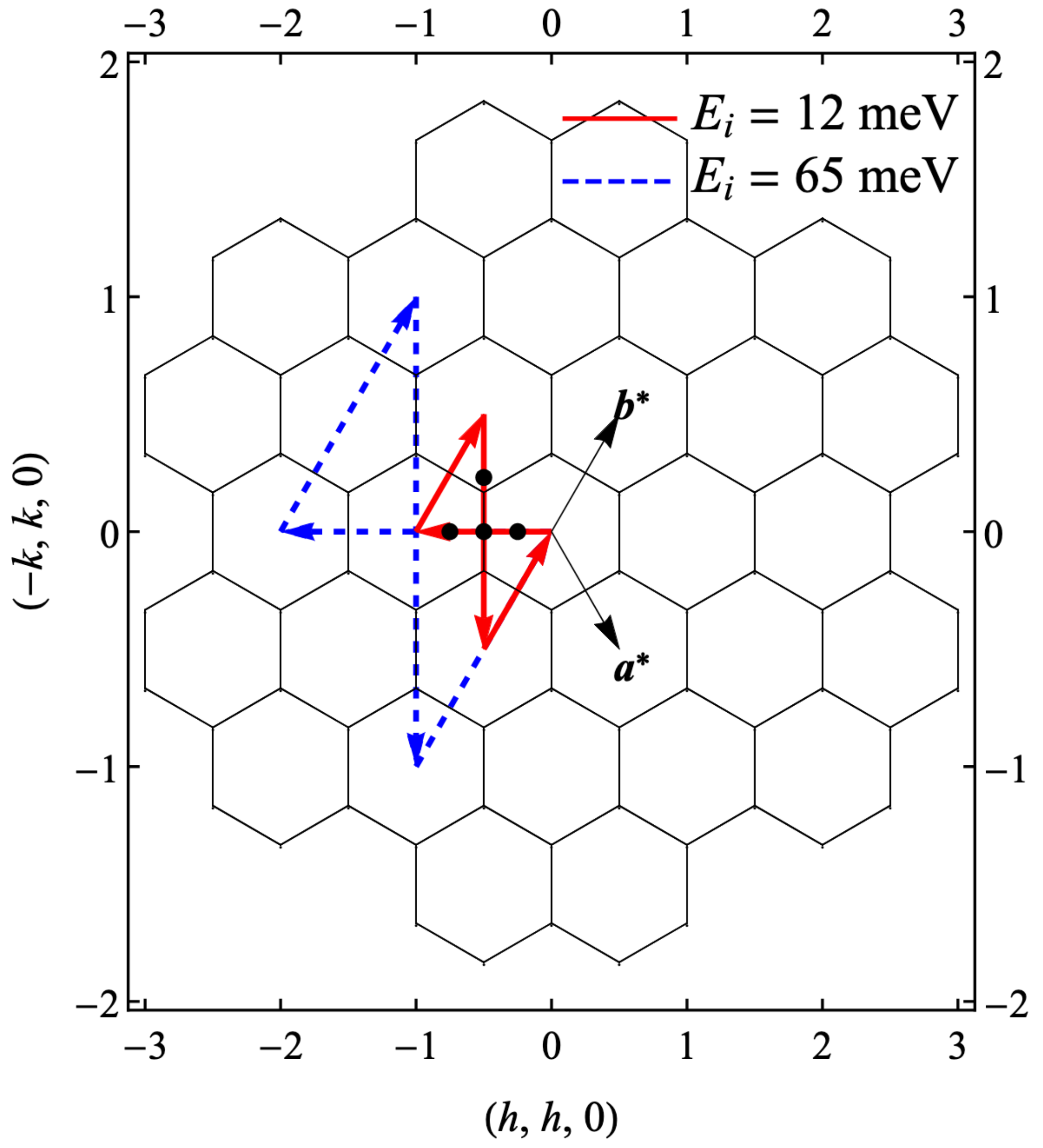
Static (equal-time) correlations

- If we're interested in just the magnetic structure, not the dynamics, we can consider the static structure factor

$$\mathcal{S}^{\alpha\beta}(\mathbf{Q}) = \int d\omega \, \mathcal{S}^{\alpha\beta}(\mathbf{Q},\omega) = \sum_{j,j'} e^{\mathrm{i}\mathbf{Q}\cdot\left(\mathbf{R}_j - \mathbf{R}_{j'}\right)} \left\langle S_j^{\alpha} S_{j'}^{\beta} \right\rangle$$

- This is simply the Fourier transform of a static spin configuration.





Calculating the Structure Factors

Quantum Mechanical Approaches

- Calculating the Dynamical Spin Structure Factor (DSSF) Quantum Mechanically

$$\mathcal{S}^{\alpha\beta}\left(\mathbf{q},\omega\right) = \frac{1}{\mathcal{Z}}\sum_{\mu,\nu} e^{-\epsilon_\nu/k_b T} \left\langle\nu\right| S^{\alpha}_{\mathbf{q}} \left|\mu\right\rangle \left\langle\mu\right| S^{\beta}_{-\mathbf{q}} \left|\nu\right\rangle \delta\left(\epsilon_\mu - \epsilon_\nu - \omega\right)$$

- This is, in general, hard. Most approaches have limitations.

Calculating the Structure Factors

Classical picture

- Consider what happens when we replace the operators with classical variables

$$\mathcal{S}^{\alpha\beta}(\mathbf{Q}) = \sum_{j,j'} e^{\mathrm{i}\mathbf{Q}\cdot\left(\mathbf{R}_j - \mathbf{R}_{j'}\right)} \left\langle S_j^{\alpha} S_{j'}^{\beta} \right\rangle$$

Calculating the Structure Factors

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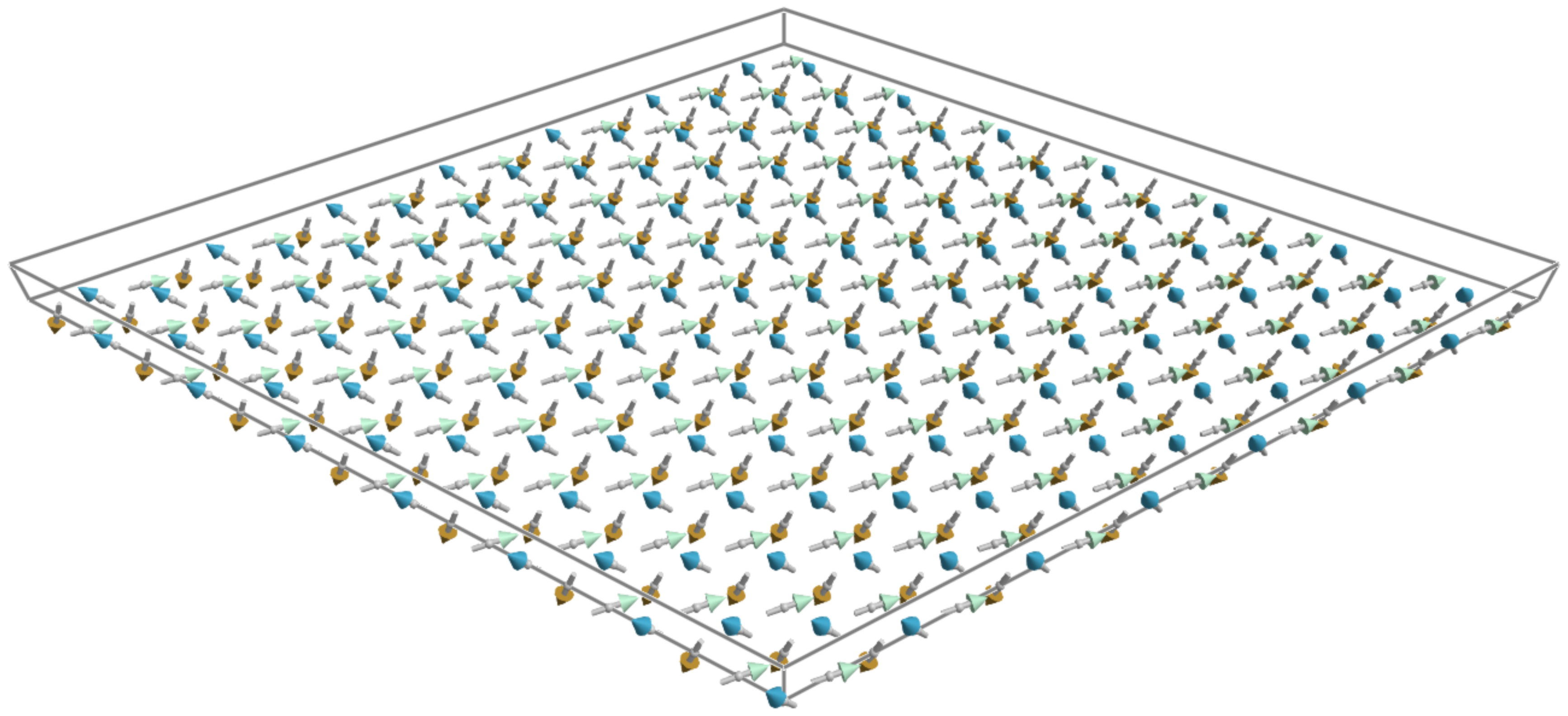
Calculating the Structure Factors

Classical picture

- Becomes a question of having a spin configuration.



S_j^{β}

Calculating the Structure Factors

Classical picture

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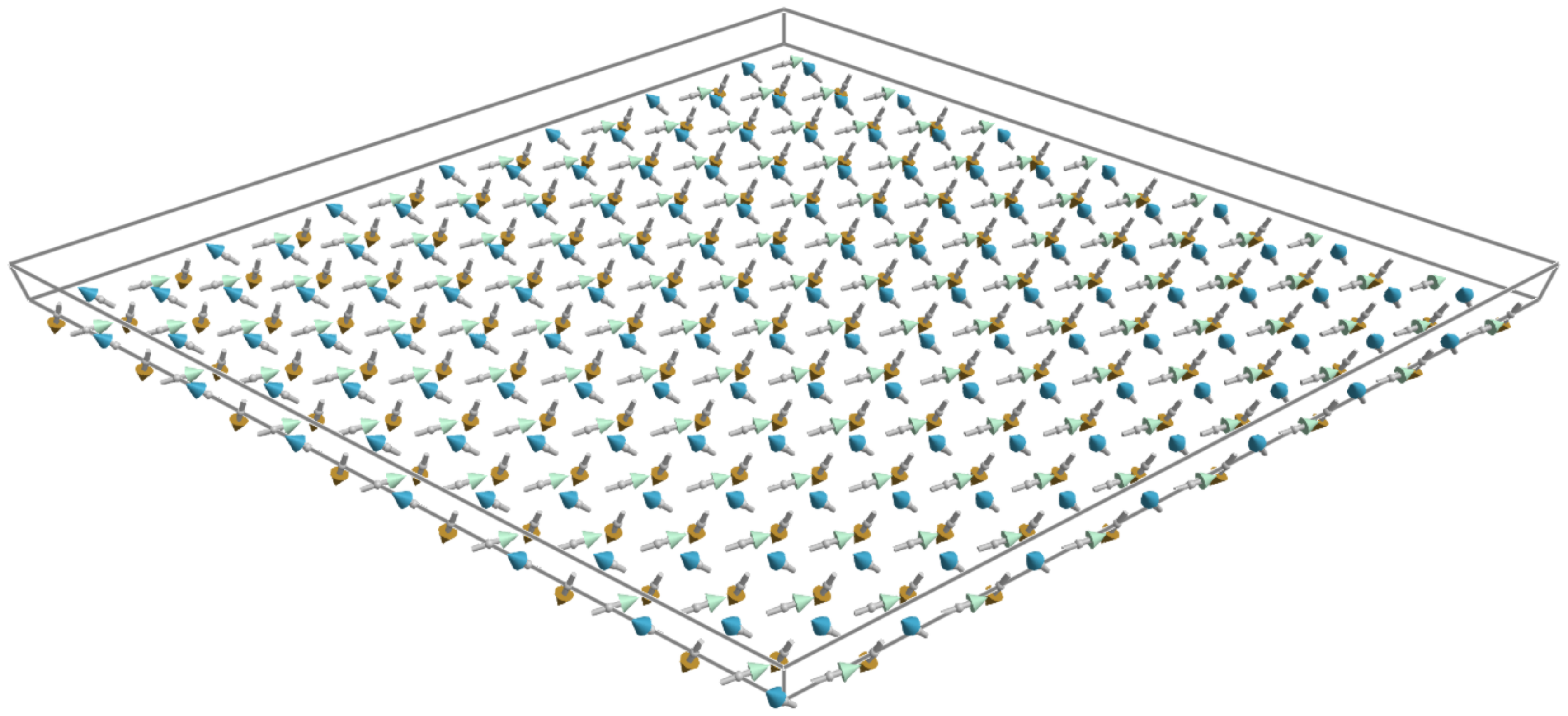
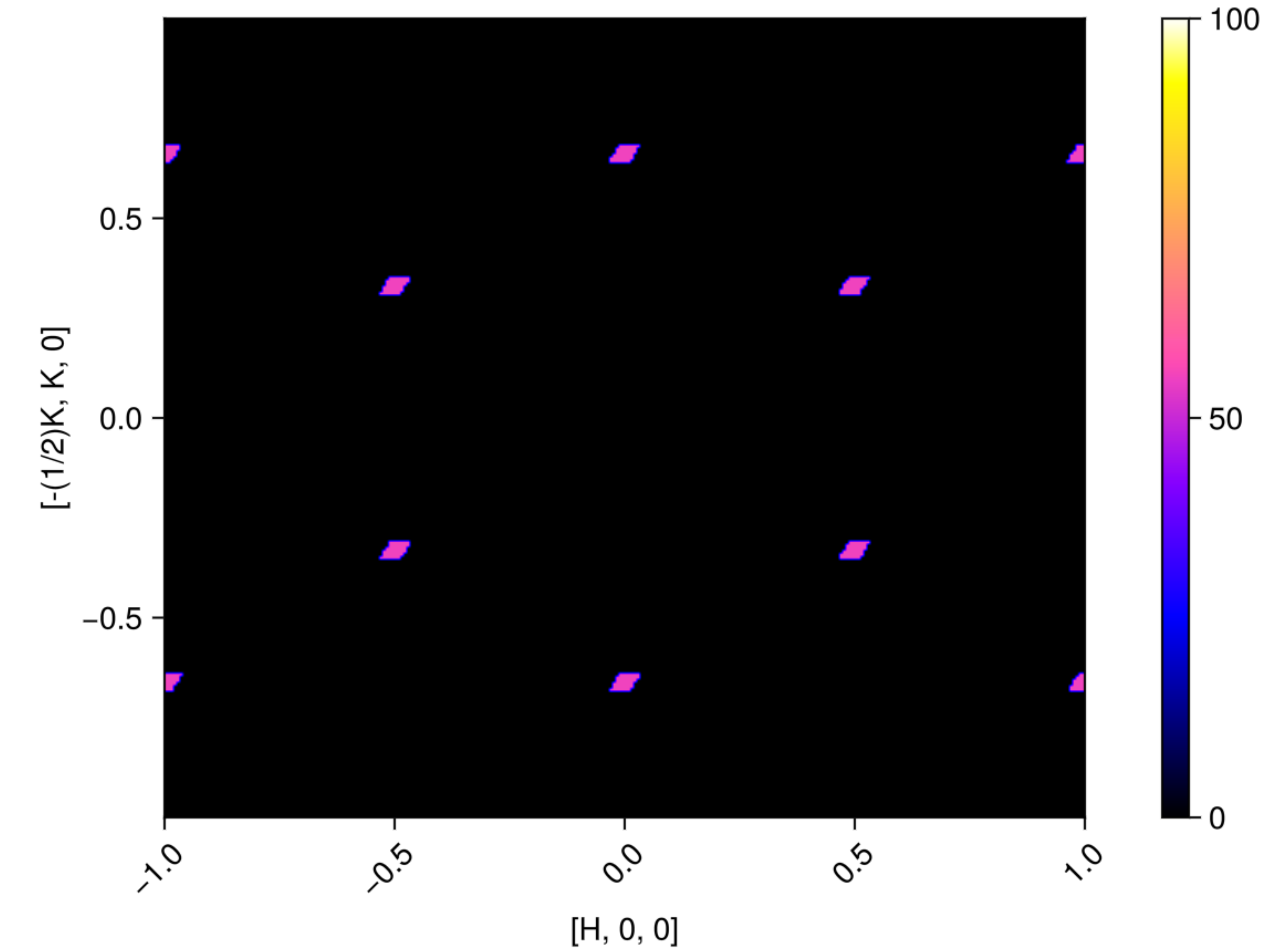


s_j^β

$$\sum_{j,j'} e^{-i\mathbf{q}\cdot(\mathbf{r}_j-\mathbf{r}_{j'})} s_j^\alpha s_{j'}^\beta$$



$\mathcal{S}^{\alpha\alpha}(\mathbf{q})$

Calculating the Structure Factors

Classical picture

- Now do the same for the dynamical structure factor

$$\mathcal{S}^{\alpha\beta}(\mathbf{q},\omega) = \sum_{j,j'} \int_{-\infty}^{\infty} e^{-i\omega t} e^{-i\mathbf{q}\cdot(\mathbf{r_j}-\mathbf{r_{j'}})} \left\langle \hat{S}_j^{\alpha} \hat{S}_{j'}^{\beta}(t) \right\rangle \frac{dt}{2\pi}$$

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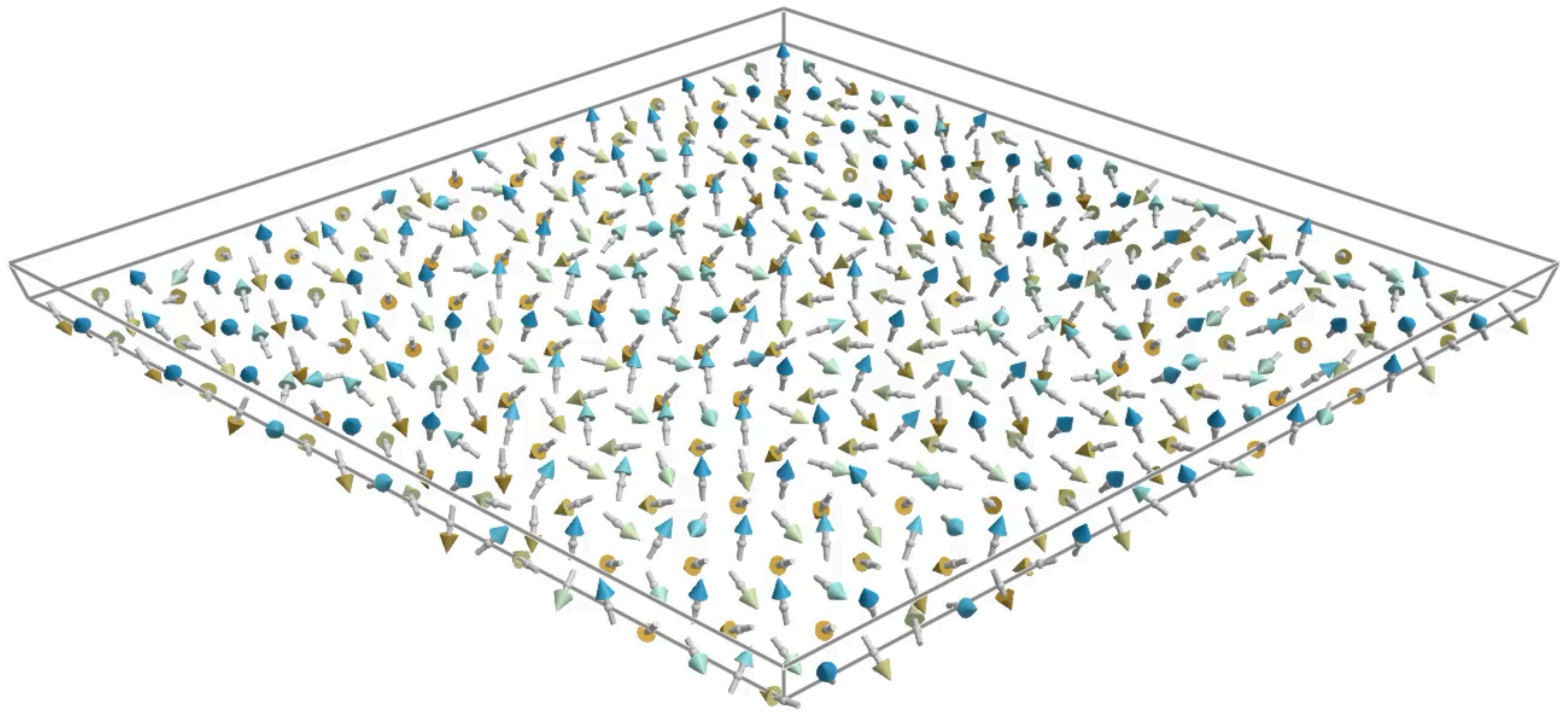
Calculating the Structure Factors

Classical picture

- So this is a question of calculating spin dynamics, most generally, trajectories.



$s_{j'}^{\beta}(t)$

Calculating the Structure Factors

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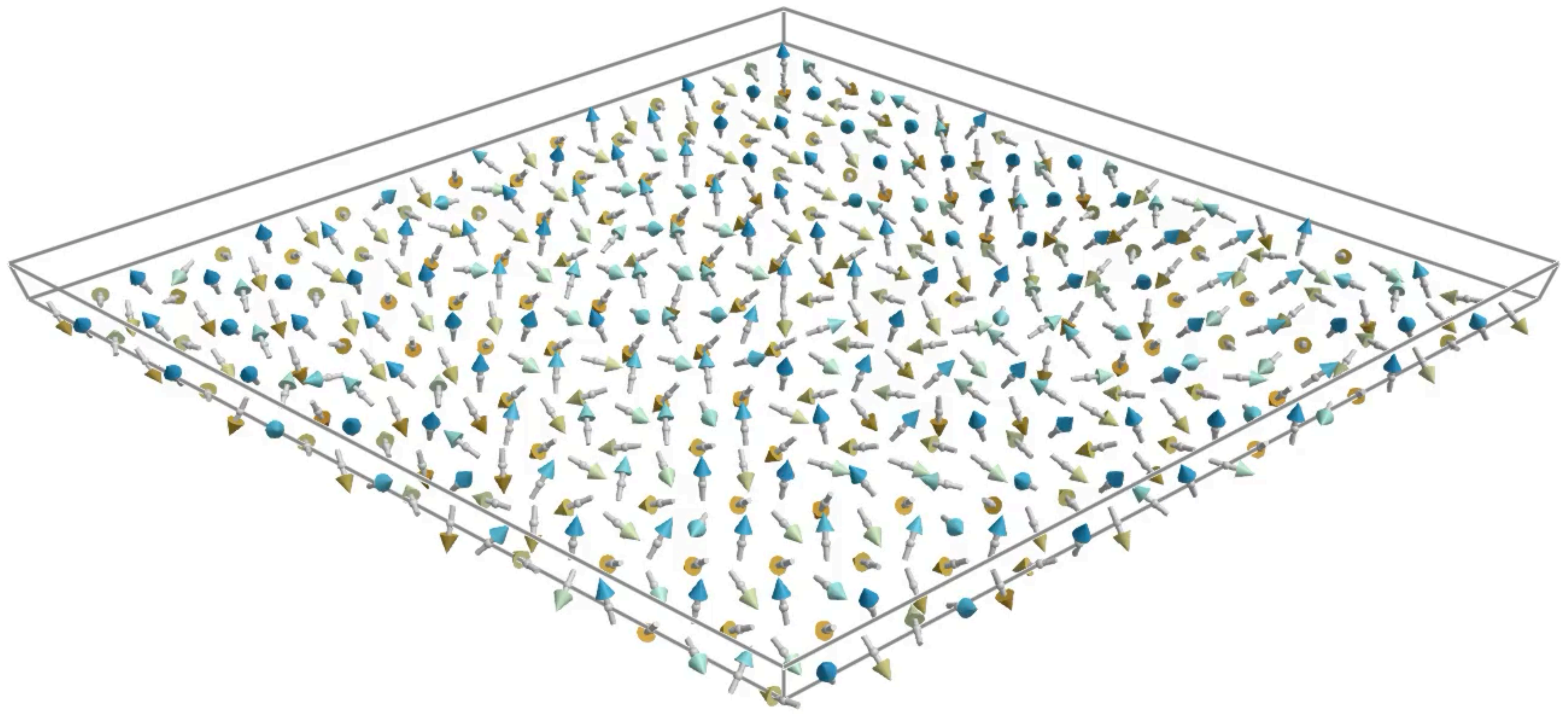

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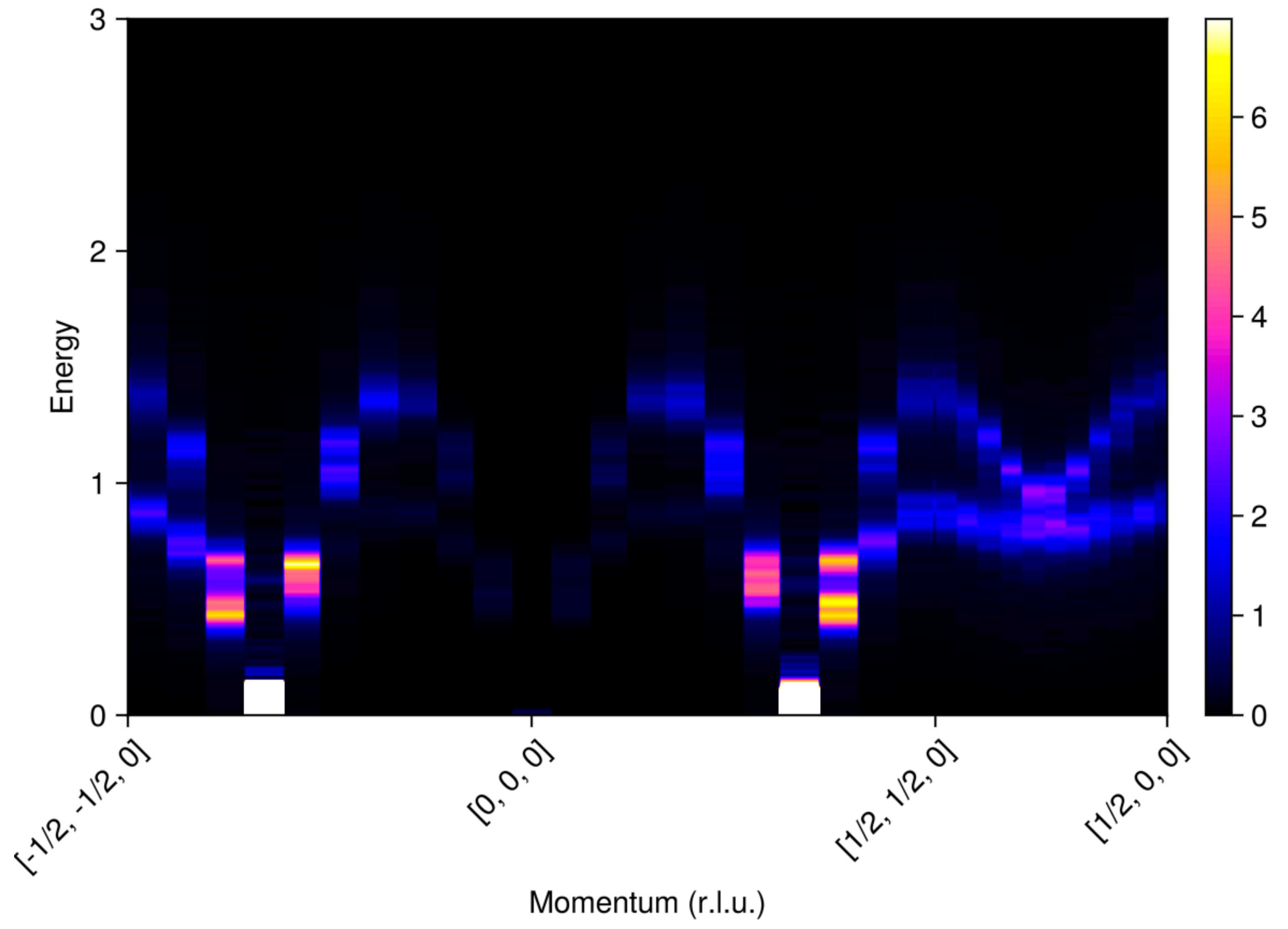


$s_{j'}^{\beta}(t)$

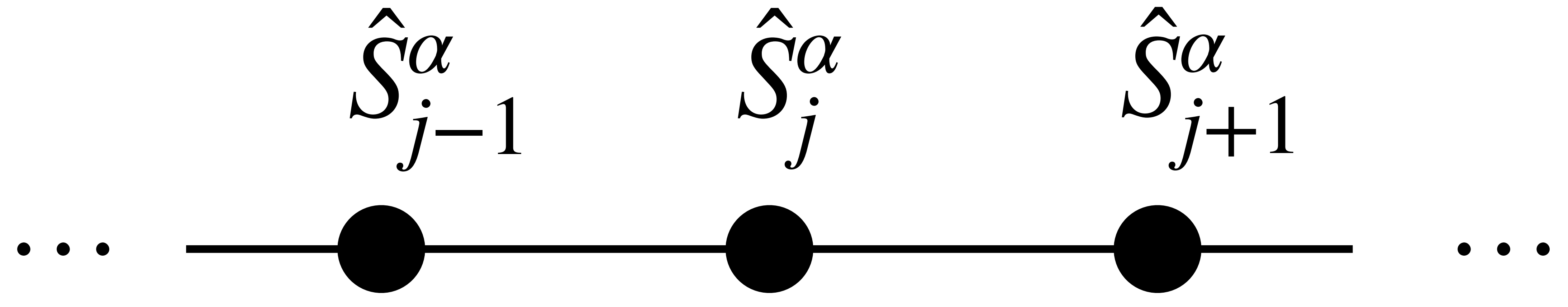
$\mathcal{S}^{\alpha\alpha}(\mathbf{q},\omega)$

Spin Hamiltonians

Starting point for the calculation of dynamics

- The basic formalism for modeling magnetic systems.
- Generally most appropriate when considering insulators (though can be bullied into dealing with some metals)
- Relevant at low temperatures
- Picture involves angular momentum operators of the ion of each site of a lattice
- Operators on different sites commute.

$$\hat{H} = J \sum_{\langle j,k \rangle} \hat{S}_j^\alpha \hat{S}_k^\alpha + \sum_j \left(\hat{S}^z \right)^2 + \mu_b g B \sum_j \hat{S}^z$$



Spin Hamiltonians

Dipoles and Spin Operators

$$|\Omega\rangle = \bigotimes_j |\Omega_j\rangle$$

$$|\Omega\rangle \leftrightarrow \left(\langle\Omega|\,\hat{S}^x\,|\Omega\rangle\,,\langle\Omega|\,\hat{S}^y\,|\Omega\rangle\,,\langle\Omega|\,\hat{S}^z\,|\Omega\rangle\right) \equiv \vec{\mathbf{s}}$$

2-level quantum state ← One-to-one correspondence → Real 3-vector on sphere

$$\hat{S}^x_j = \begin{pmatrix} 0 & \frac{1}{2} \\ \frac{1}{2} & 0 \end{pmatrix} \quad \hat{S}^y_j = \begin{pmatrix} 0 & \frac{-i}{2} \\ \frac{i}{2} & 0 \end{pmatrix} \quad \hat{S}^z_j = \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & -\frac{1}{2} \end{pmatrix}$$

$$|\Omega_j\rangle = \begin{pmatrix} \alpha_1 \\ \alpha_2 \end{pmatrix}$$

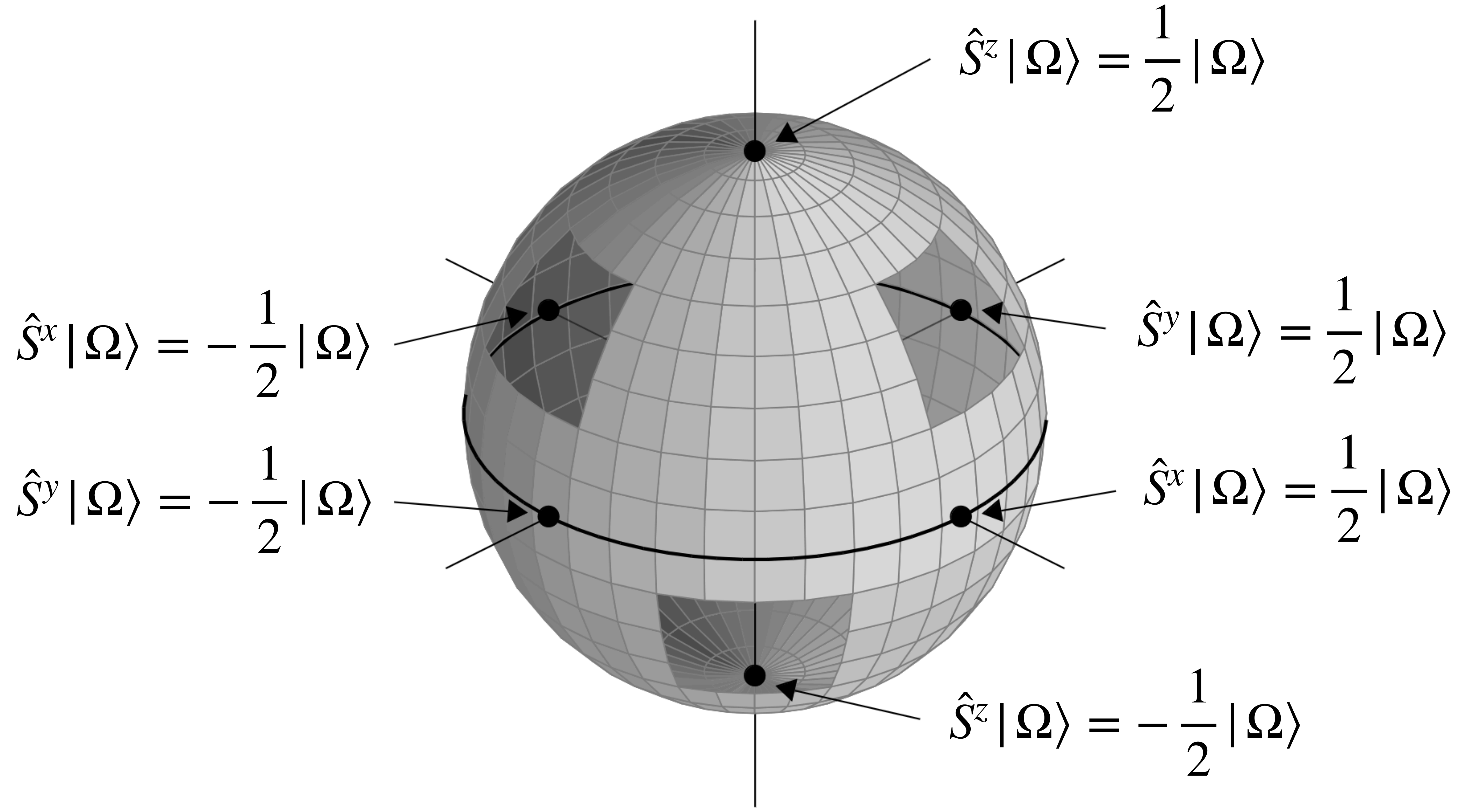


Image from: P. Woit, *Quantum Theory, Groups and Representations (2014)*

Spin Hamiltonians

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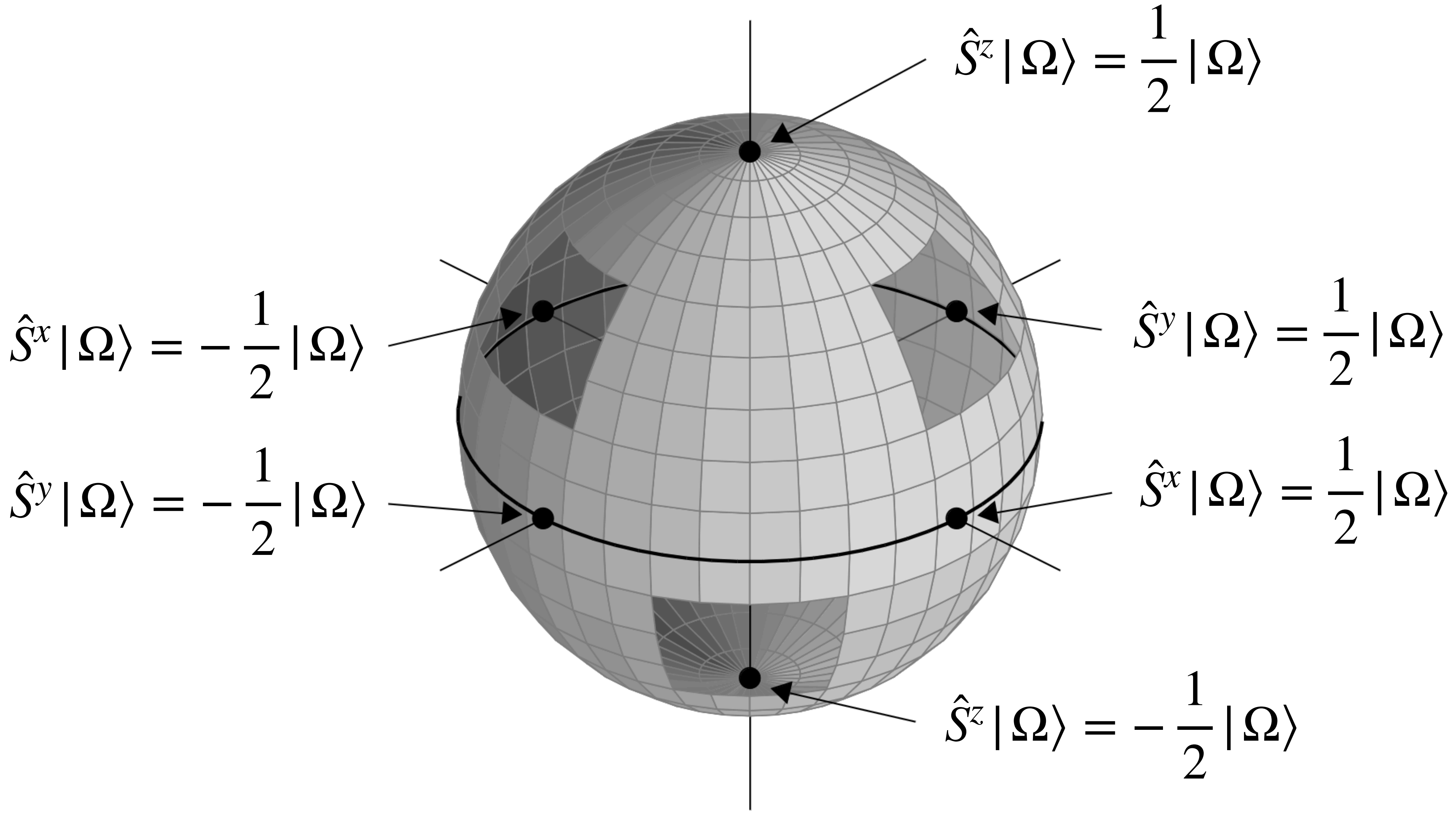
2-level quantum state ⟵ One-to-one correspondence ⟶ Real 3-vector on sphere

$$\Big|\Omega(\theta,\phi)\rangle = e^{i\phi/2}\cos\left(\frac{\theta}{2}\right)|\uparrow\rangle + e^{-i\phi/2}\sin\left(\frac{\theta}{2}\right)|\downarrow\rangle$$



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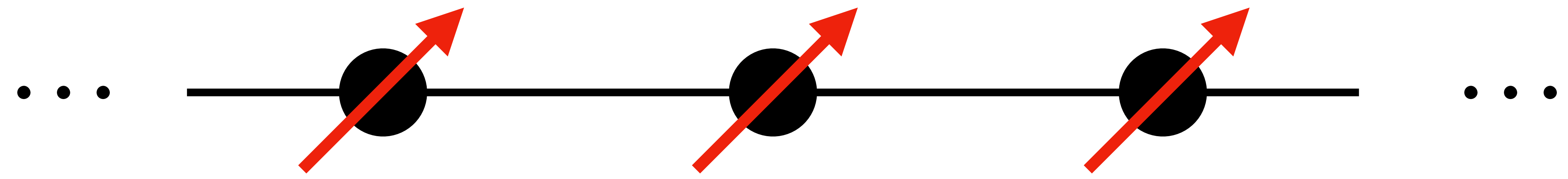
Spin Hamiltonians

Starting point for the calculation of dynamics

- To obtain a classical picture, we can use the Bloch sphere correspondence to put a “dipole” on each site.

- Note that this implicitly involves taking an expectation value with respect to a simple (product state) wave function.

$$\hat{H} = J \sum_{\langle j,k \rangle} \hat{S}_j^\alpha \hat{S}_k^\alpha + \sum_j \left(\hat{S}^z \right)^2 + \mu_b g B \sum_j \hat{S}^z$$



Spin Hamiltonians

Most important interaction terms

$$\hat{H} = J \sum_{\langle j,k \rangle} \hat{S}_j^{\alpha} \hat{S}_k^{\alpha} + D \sum_j \left(\hat{S}^z \right)^2 + \mu_b g B \sum_j \hat{S}^z$$

Exchange

Onsite
Anisotropy

Zeeman

Spin Hamiltonians

$J < 0$ — Ferromagnetic (FM) Exchange

$$\hat{H} = J \sum_{\langle j,k \rangle} \hat{S}_j^\alpha \hat{S}_k^\alpha$$

Exchange

Spin Hamiltonians

$J < 0$ — Ferromagnetic (FM) Exchange

$$\hat{H} = J \sum_{\langle j,k \rangle} \hat{S}_j^\alpha \hat{S}_k^\alpha$$

$$\downarrow$$

$$H = J \sum_{\langle j,k \rangle} s_j^\alpha s_k^\alpha$$

Spin Hamiltonians

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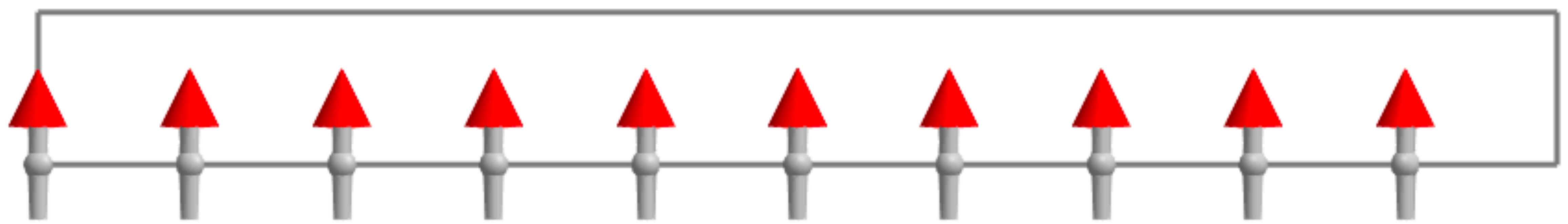

Spin Hamiltonians

$J > 0$ — Anti-ferromagnetic (AFM) Exchange

$$\hat{H} = J \sum_{\langle j,k \rangle} \hat{S}_j^\alpha \hat{S}_k^\alpha$$

$$\downarrow$$

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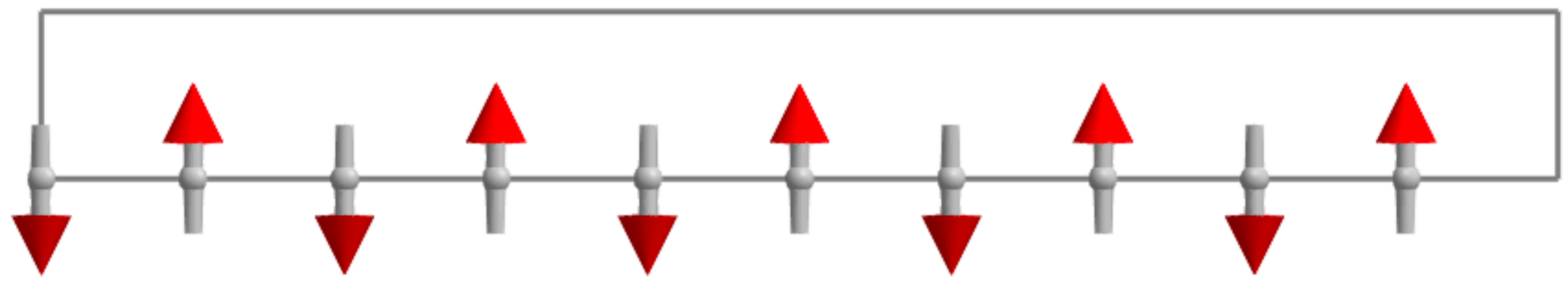

Spin Hamiltonians

Single-ion anisotropy (SIA)

$$\hat{H} = D \sum_{j} \left(\hat{S}^z\right)^2$$

Onsite
Anisotropy

Spin Hamiltonians

Single-ion anisotropy (SIA)

$$\hat{H} = D \sum_j \left(\hat{S}^z \right)^2$$

$$H = D \sum_j (s^z)^2$$

Spin Hamiltonians

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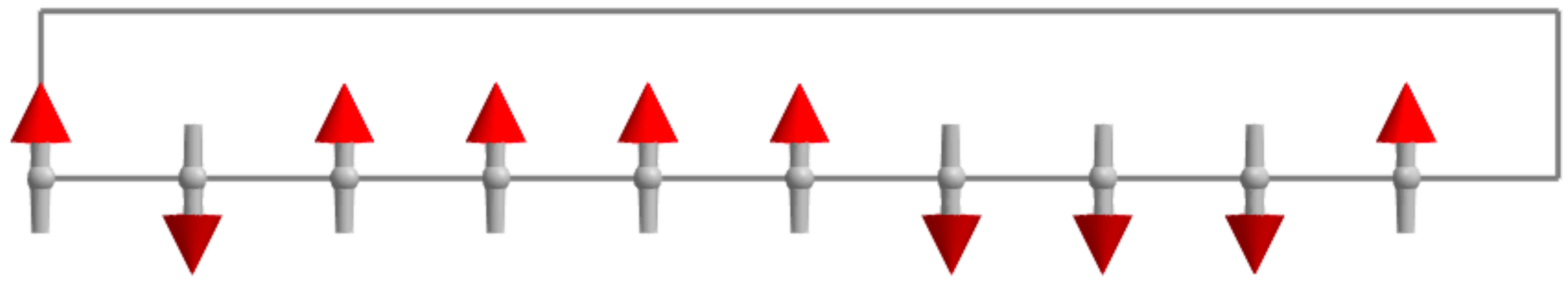
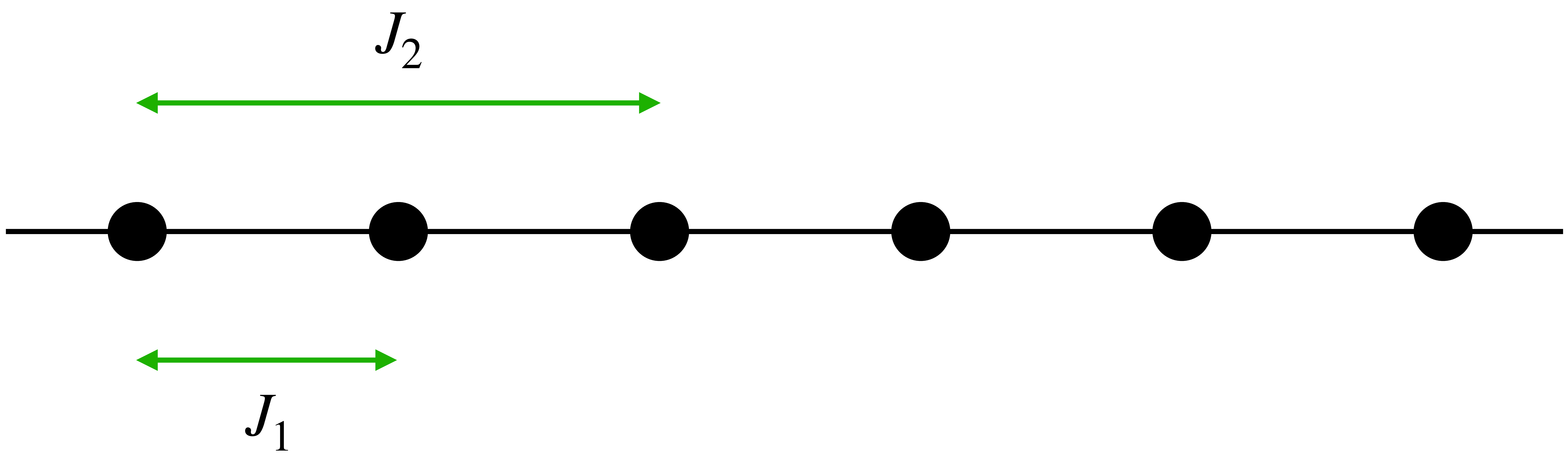


Spin Hamiltonians

Combining Interactions — Frustration

- Simple AFM spin chain with nearest neighbor (NN) and next-nearest neighbor (NNN) interactions

$$\hat{H} = J_1 \sum_{\langle j,k \rangle} s_j^\alpha s_k^\alpha + J_2 \sum_{\langle\langle j,k \rangle\rangle} s_j^\alpha s_k^\alpha, \quad J_1, J_2 > 0$$



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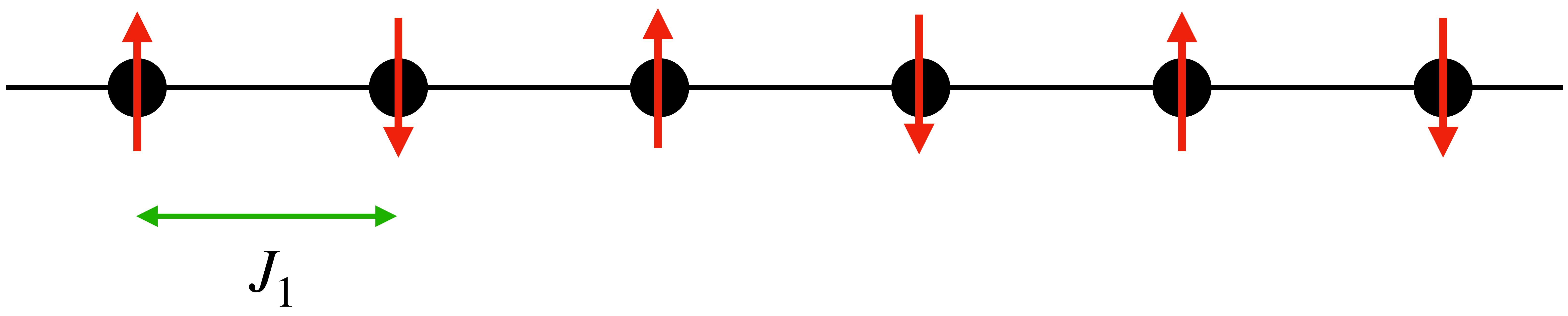

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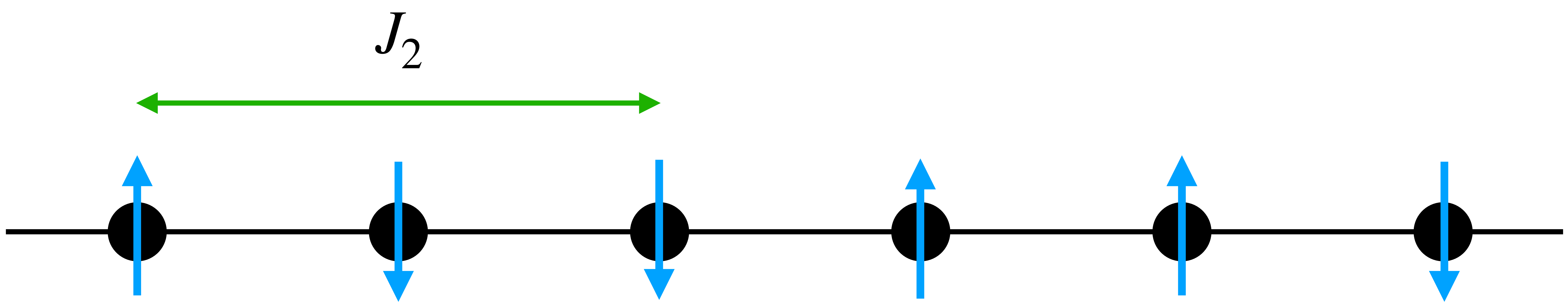

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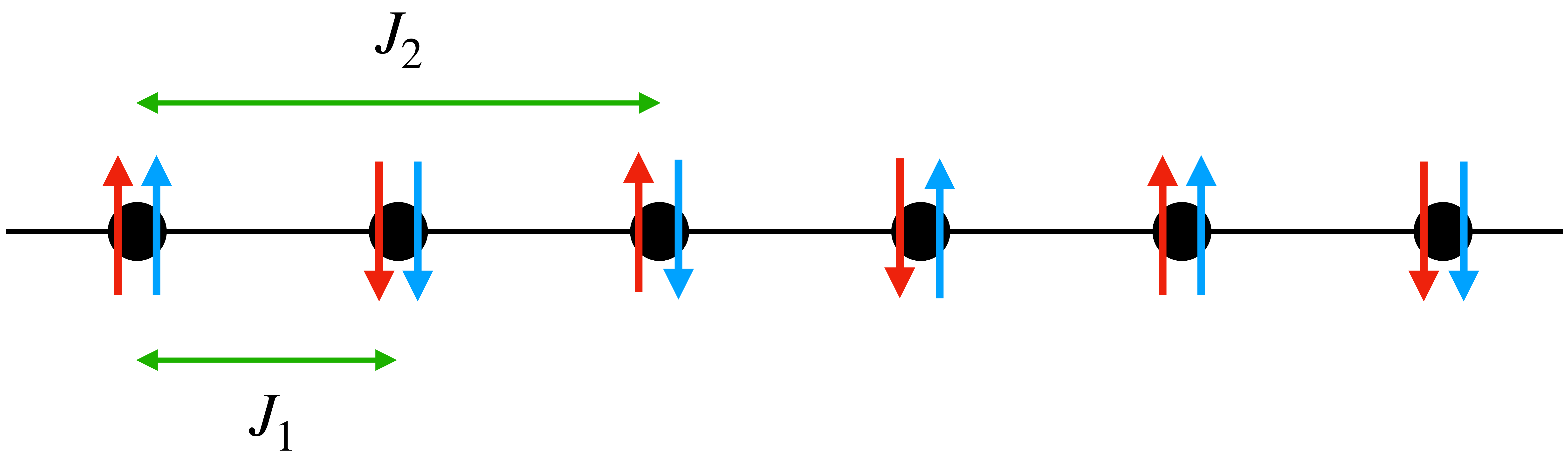
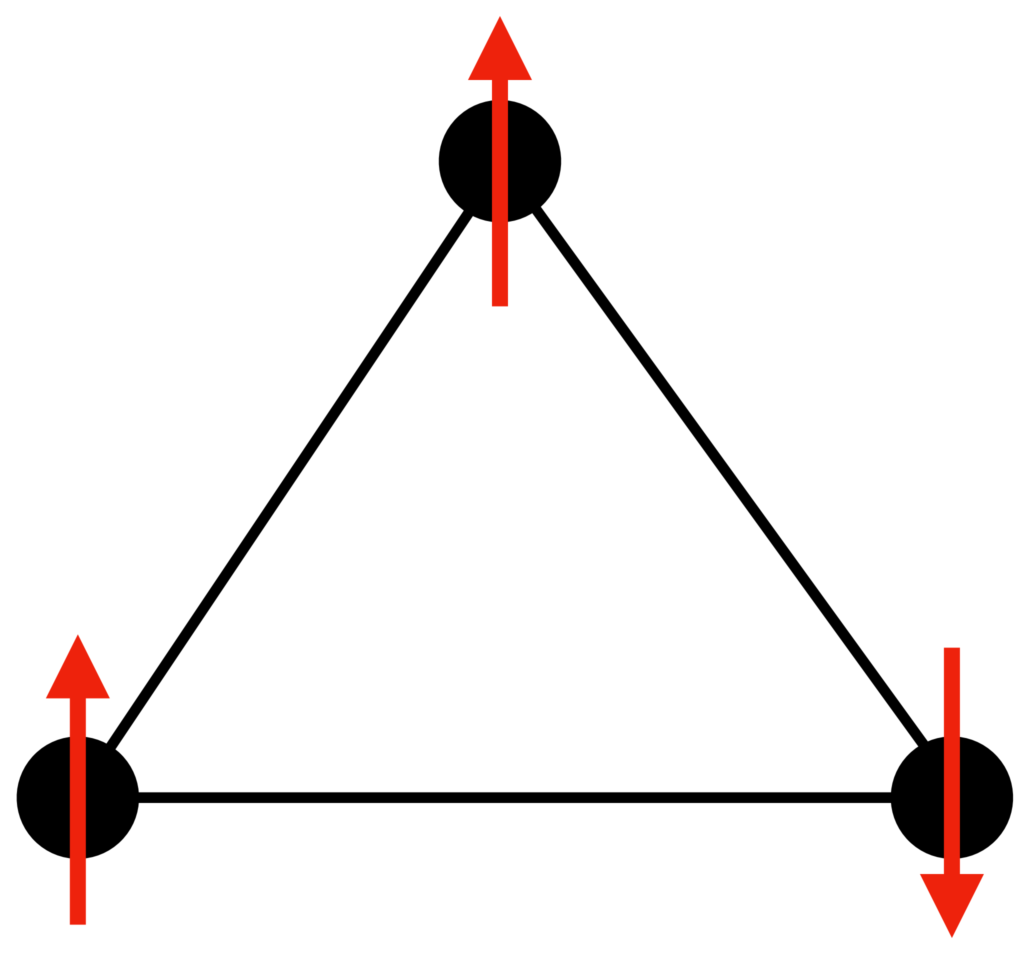


Spin Hamiltonians

Geometric Frustration

- Simple nearest-neighbor AFM interactions on a triangular lattice

$$\hat{H} = J \sum_{\langle j,k \rangle} s_j^{\alpha} s_k^{\alpha}, \quad J > 0$$

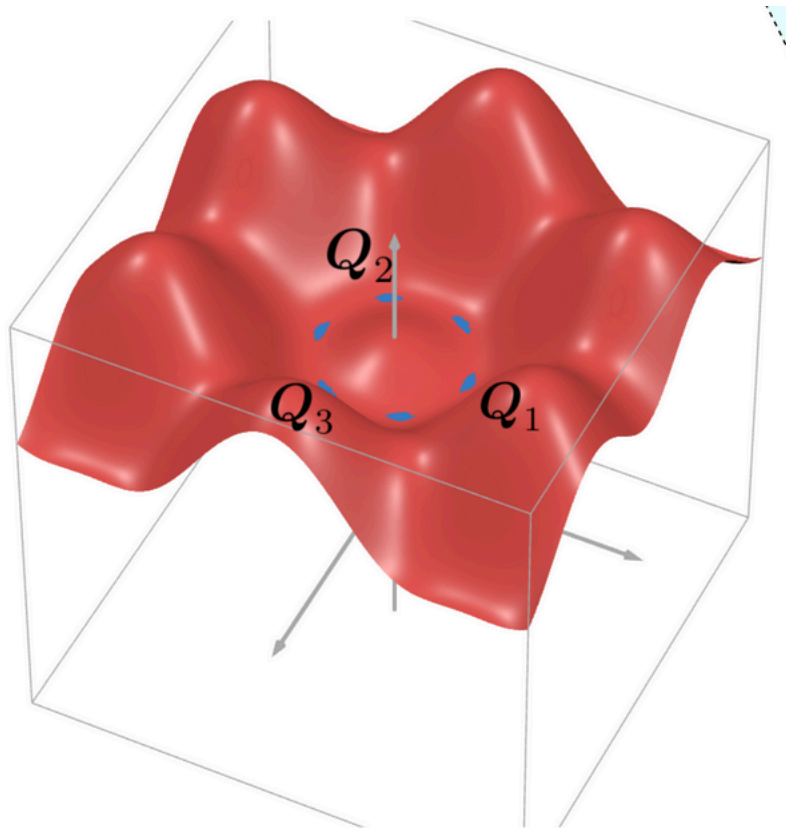


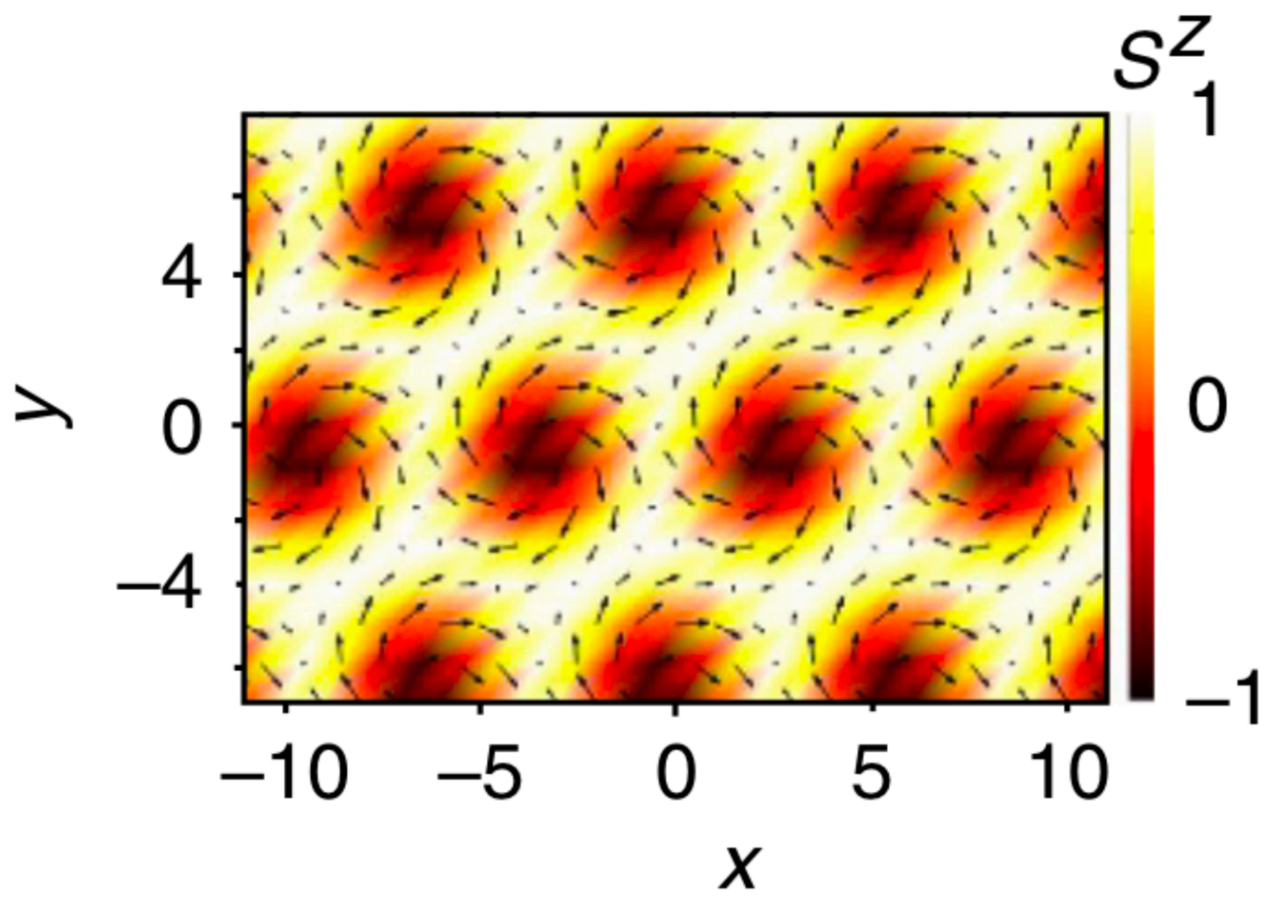
Spin Hamiltonians

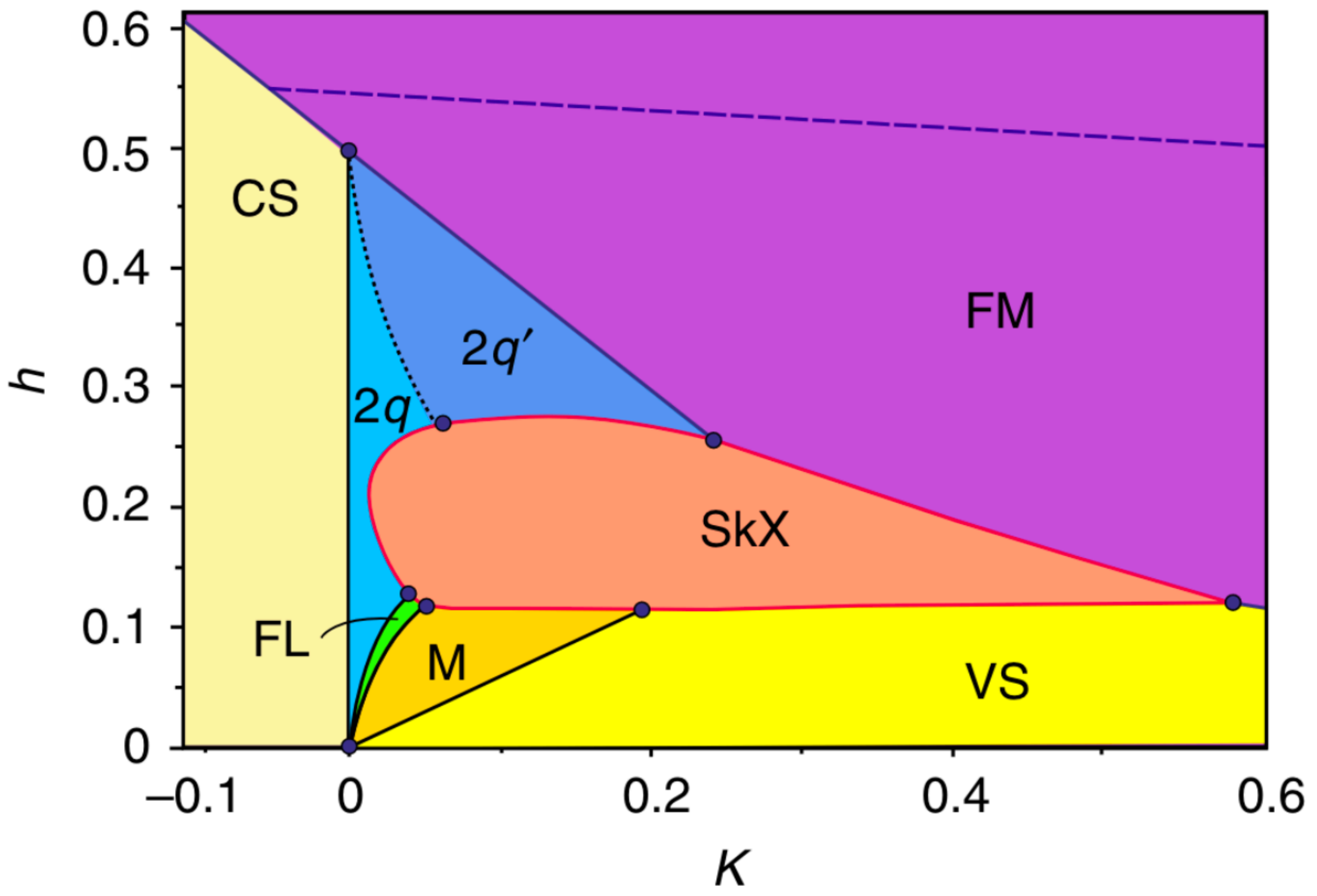
Skyrmions

- Delicate balancing of interactions can lead to interesting magnetic order

$$H = J_1 \sum_{\langle j,k \rangle} s_j^\alpha s_k^\alpha + J_2 \sum_{\langle\langle j,k \rangle\rangle} s_j^\alpha s_k^\alpha - \frac{D}{2} \sum_j \left(s_j^z\right)^2 - h \sum_j s_j^z$$







Leonov and Mostovoy, "Multiply periodic states…," Nature Communications (2015).

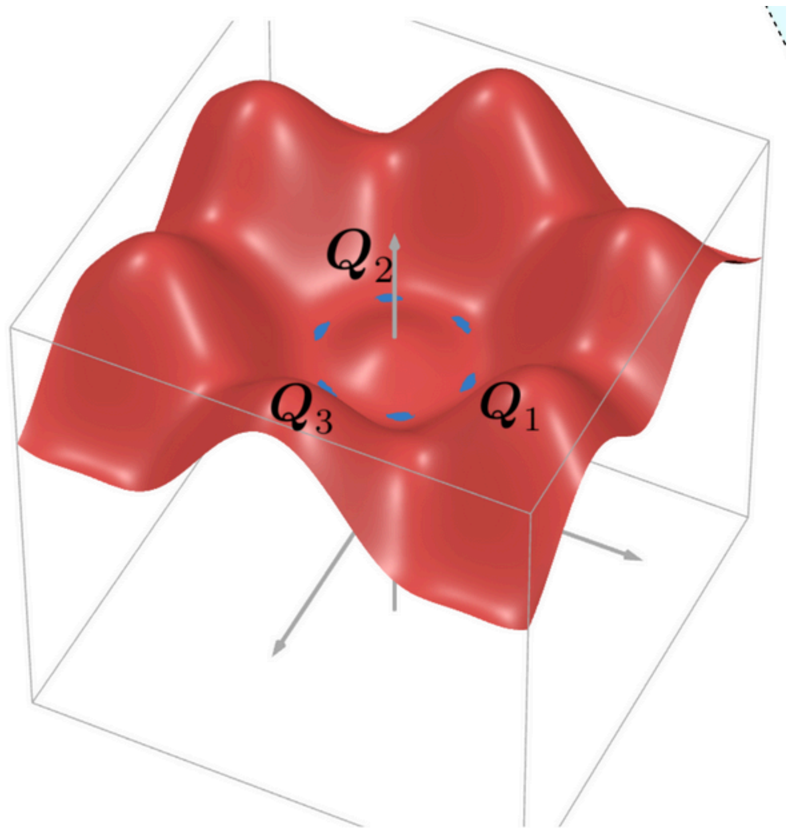
Mühlbauer et al, "Skyrmion lattice…," Science (2009).

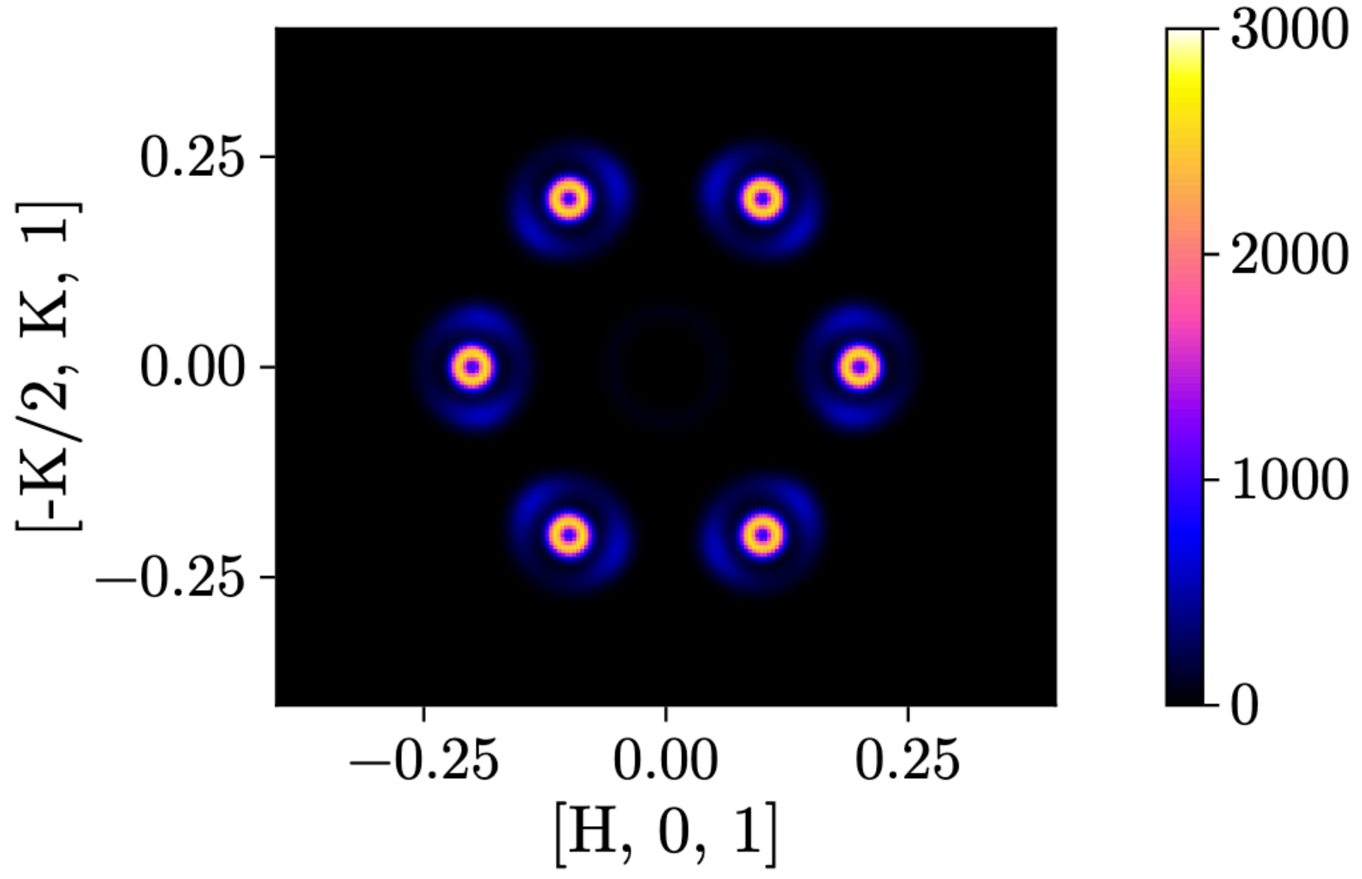
Spin Hamiltonians

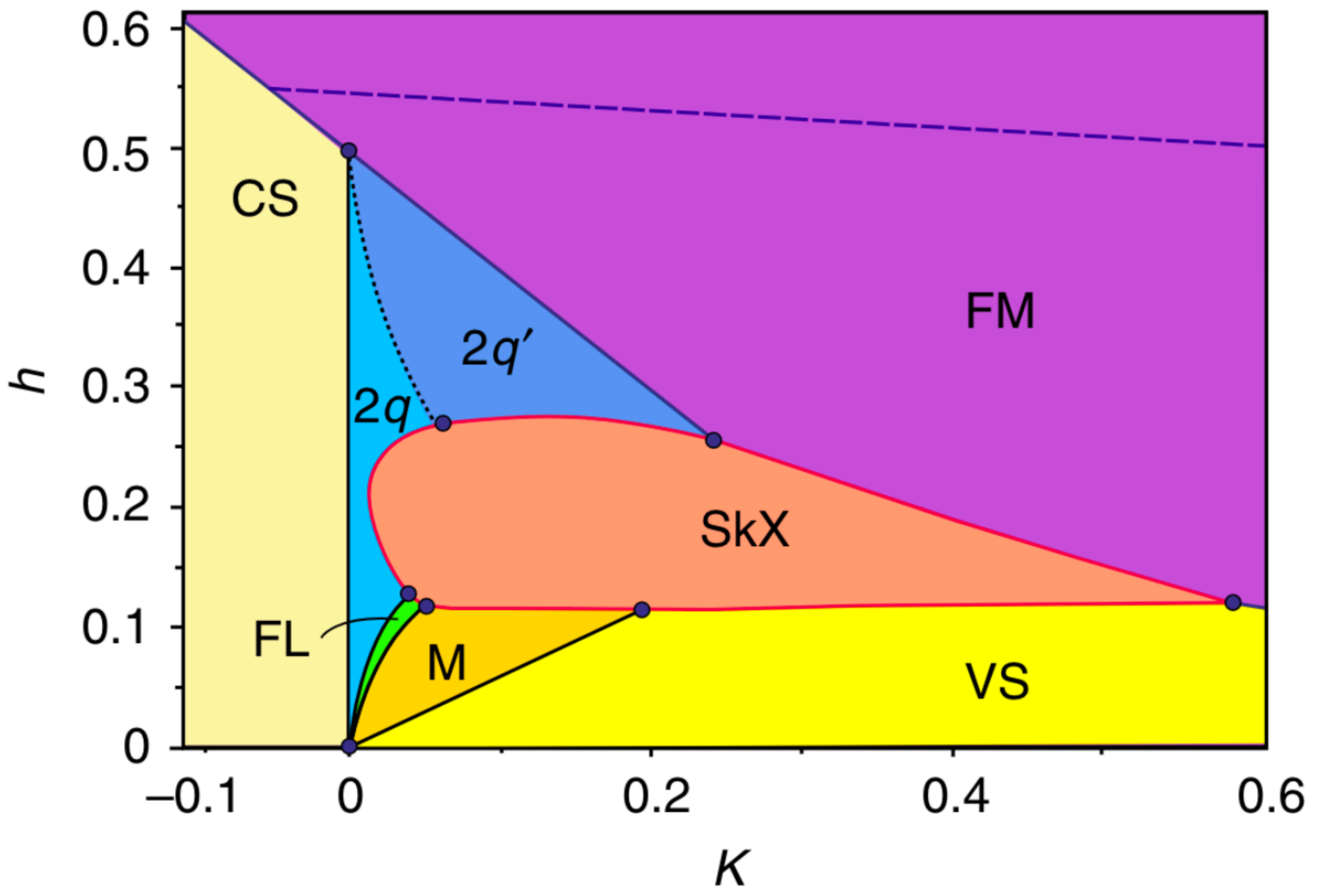
Skyrmions

- Delicate balancing of interactions can lead to interesting magnetic order

$$H = J_1 \sum_{\langle j,k \rangle} s_j^\alpha s_k^\alpha + J_2 \sum_{\langle\langle j,k \rangle\rangle} s_j^\alpha s_k^\alpha - \frac{D}{2} \sum_j \left(s_j^z\right)^2 - h \sum_j s_j^z$$







Leonov and Mostovoy, "Multiply periodic states…," Nature Communications (2015).

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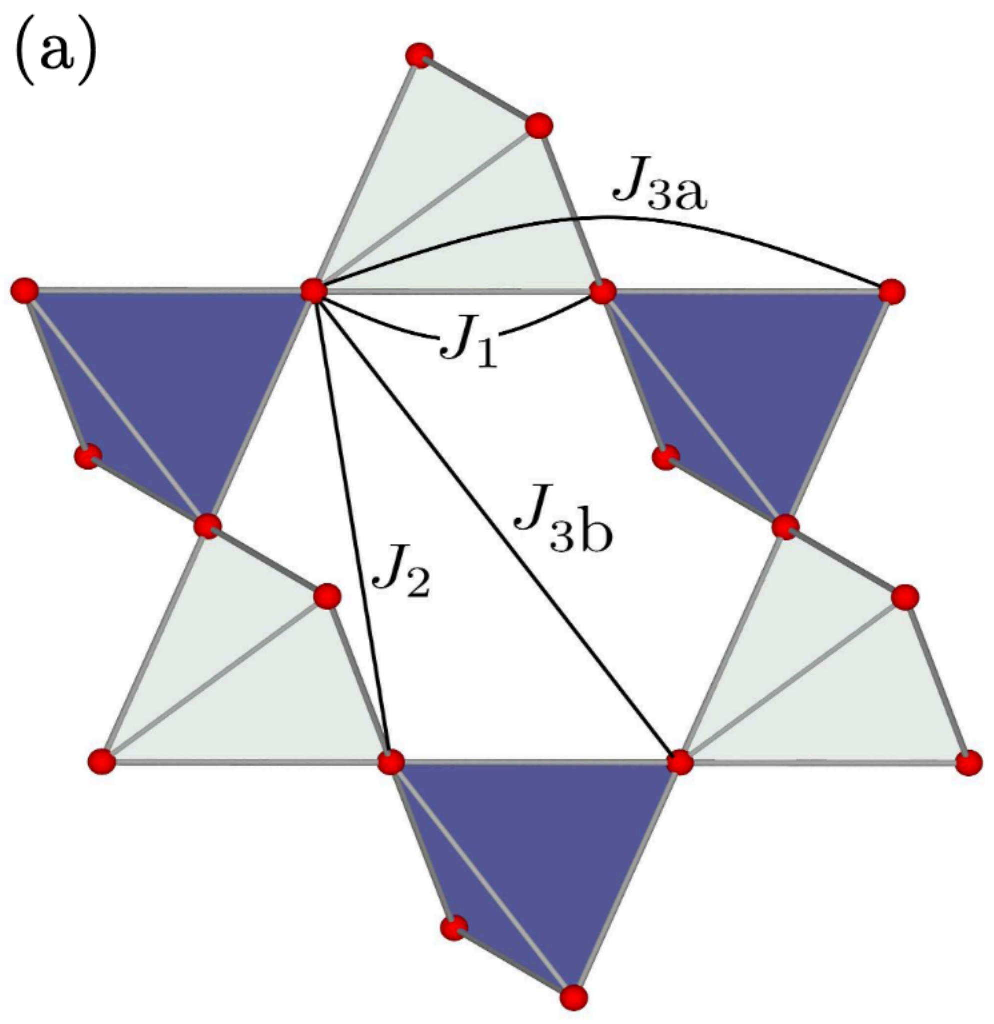
Spin Hamiltonians

Classical Spin Liquids

- In some situations, competing interactions can result in many different ground states with the same (or very similar) energy
- This is the case for the pyrochlore antiferromagnetic $MgCr_2O_4$
- Demo in Sunny

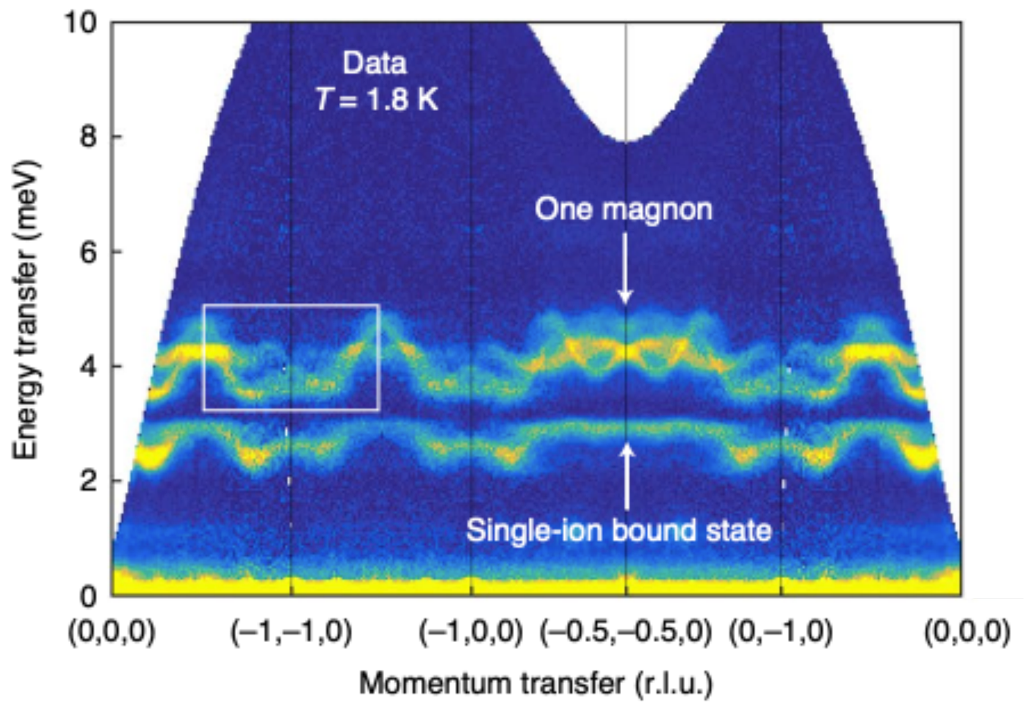


$$\hat{H} = \sum_i J_i \sum_{\langle j,k \rangle} s_j^\alpha s_k^\alpha, \quad J_i > 0$$

Bai et al, "Magnetic excitations of the classical spin liquid…," PRL 122 (2019).

Connecting Theory and Experiment

- At this point, we have seen the basic observables as well as the components for building a theory.
- Often we're in the position of wanting to find a spin Hamiltonian that corresponds to observed data

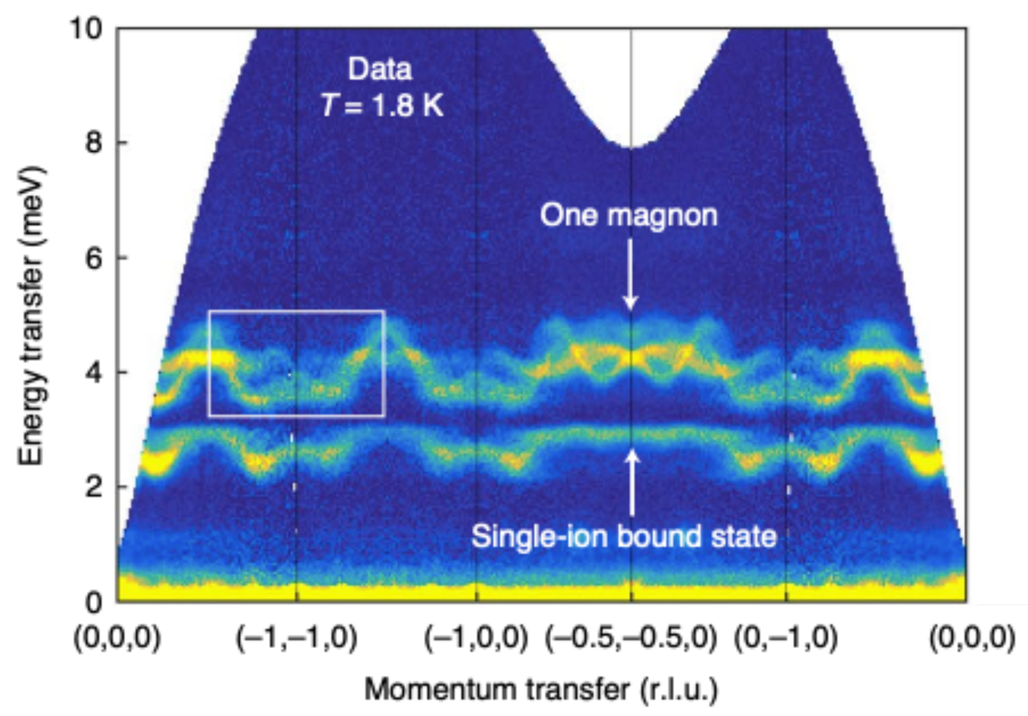


$$\hat{H}$$

Connecting Theory and Experiment

- At this point, we have seen the basic observables as well as the components for building a theory.
- Often we’re in the position of wanting to find a spin Hamiltonian that corresponds to observed data
- To do the inverse problem, we first need an approach to solving the forward problem.

$$\hat{H} \longrightarrow$$



Spin Dynamics
Classical picture

- The dynamics of classical spins are given by the Landau-Lifshitz equations.

- Each spin attempts to precess about a time-varying local magnetic field determined by $\frac{dH}{d\mathbf{s}_j}$.

$$\frac{d\mathbf{s}_j}{dt} = -\,\mathbf{s}_j \times \frac{dH}{d\mathbf{s}_j}$$

Spin Dynamics

Classical picture

- Demo of decoupled spins in magnetic field and its dispersion

- Demo of FM coupled spins in magnetic field and its dispersion.

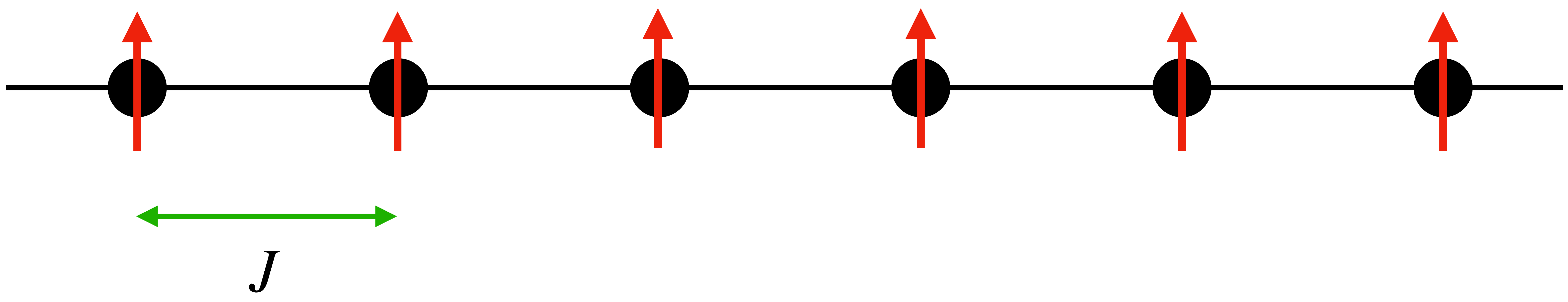
$$\frac{d\mathbf{s}_j}{dt} = -\mathbf{s}_j \times \frac{dH}{d\mathbf{s}_j}$$

Spin Dynamics

Analytical solution — Classical

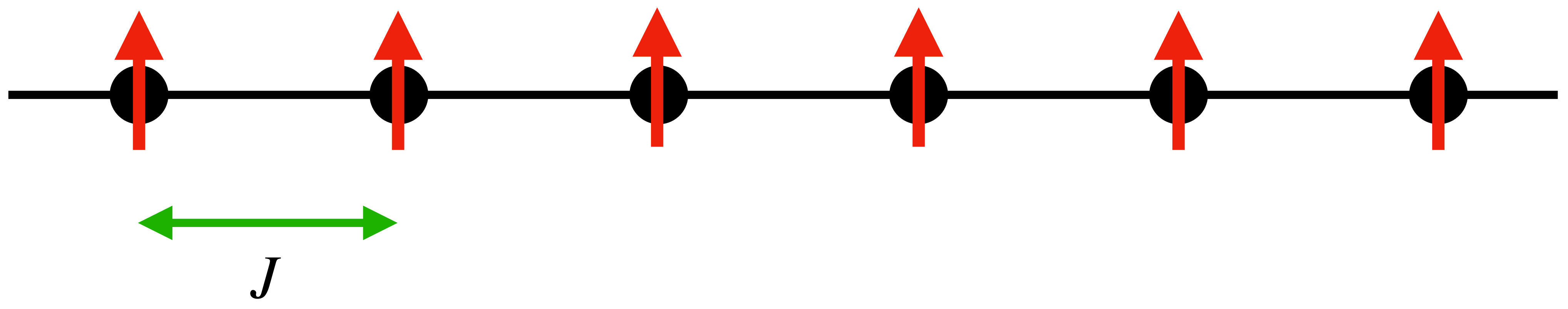
- If we assume the Landau-Lifshitz equations, the classical dynamics of a simple Heisenberg spin chain is easy to solve analytically.

$$H = J \sum_{\langle j,k \rangle} s_j^\alpha s_k^\alpha, \quad J < 0$$



Spin Dynamics

Analytical solution — Classical

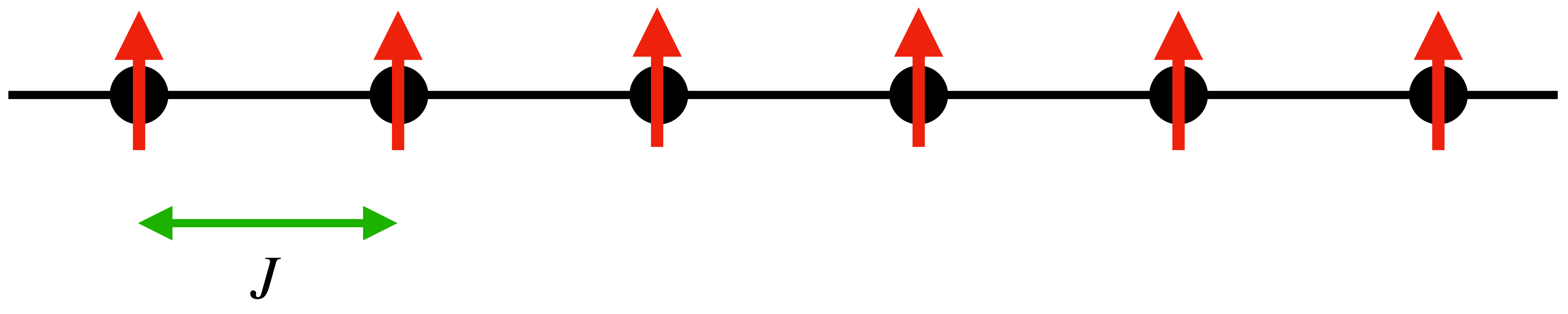


- Rewrite the classical Hamiltonian in ordinary vector notation

$$H = -J \sum_i \boldsymbol{s}_i \cdot \boldsymbol{s}_{i+1}$$

Spin Dynamics

Analytical solution — Classical



- Rewrite the classical Hamiltonian in ordinary vector notation

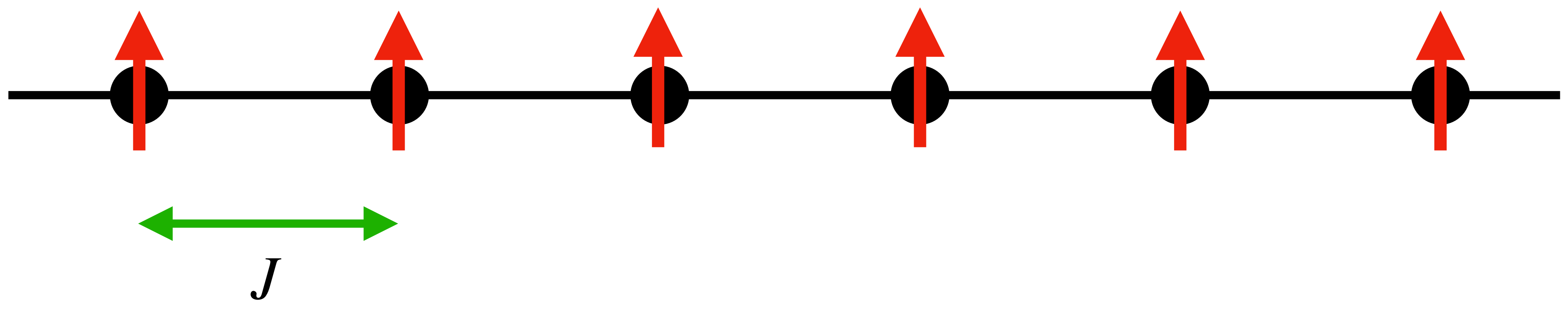
$$H = -J \sum_i \boldsymbol{s}_i \cdot \boldsymbol{s}_{i+1}$$

- Determine its derivative

$$\frac{dH}{d\boldsymbol{s}_j} = \boldsymbol{s}_{j-1} + \boldsymbol{s}_{j+1}$$

Spin Dynamics

Analytical solution — Classical



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$$H = -J \sum_i \boldsymbol{s}_i \cdot \boldsymbol{s}_{i+1}$$

- Determine its derivative

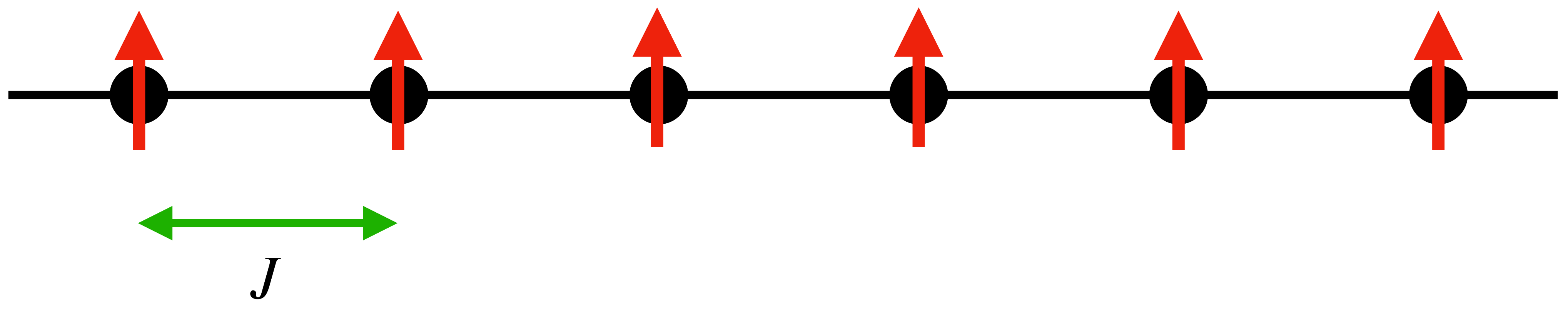
$$\frac{dH}{d\boldsymbol{s}_j} = \boldsymbol{s}_{j-1} + \boldsymbol{s}_{j+1}$$

- Insert into Landau-Lifshitz equation

$$\frac{d\mathbf{s}_j}{dt} = J\boldsymbol{s}_j \times (\boldsymbol{s}_{j-1} + \boldsymbol{s}_{j+1})$$

Spin Dynamics

Analytical solution — Classical



- Assume only have small oscillations about the ground state.

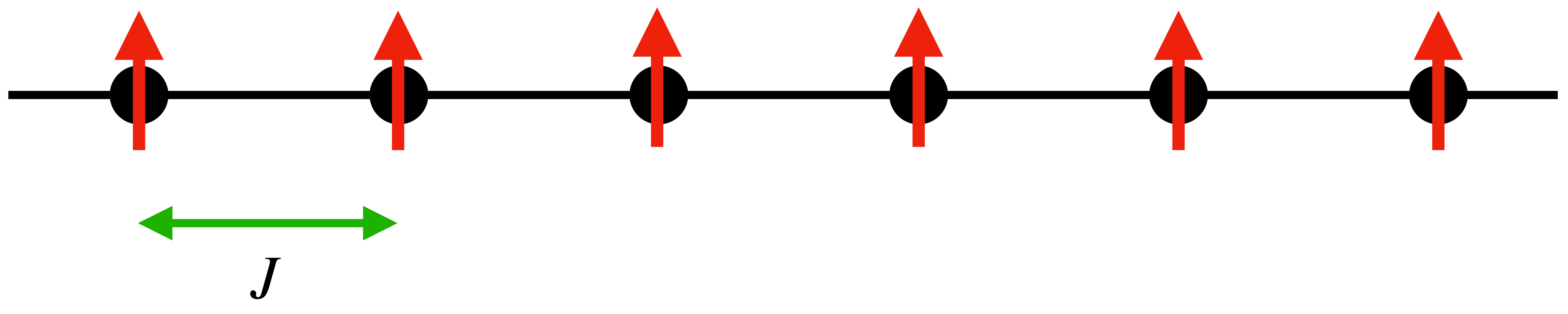
$$\frac{ds_j^x}{dt} \approx JS\left(2s_j^y - s_{j-1}^y - s_{j+1}^y\right)$$

$$\frac{ds_j^y}{dt} \approx -JS\left(2s_j^y - s_{j-1}^y - s_{j+1}^y\right)$$

$$\frac{ds_j^z}{dt} \approx 0$$

Spin Dynamics

Analytical solution — Classical



- Assume only have small oscillations about the ground state and insert ansatz for normal mode.

$$\frac{ds_j^x}{dt} \approx JS\left(2s_j^y - s_{j-1}^y - s_{j+1}^y\right)$$

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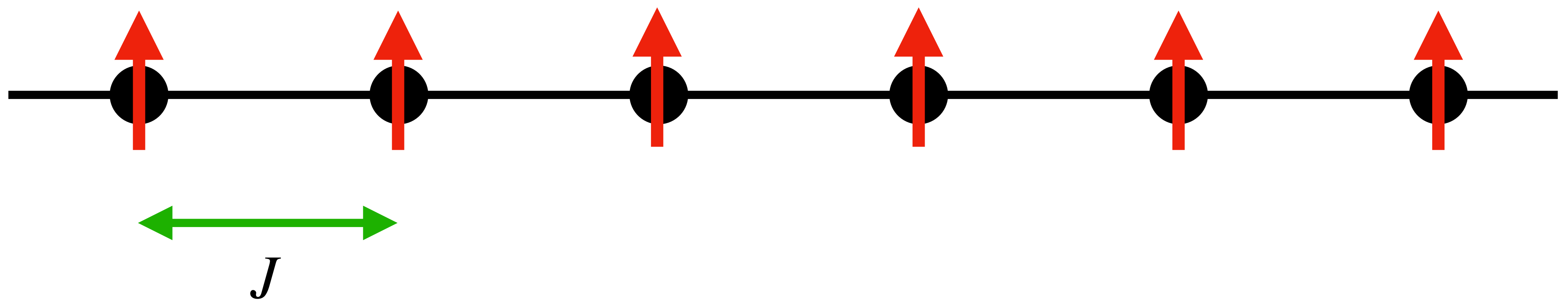
$$s_j^x = Ae^{\mathrm{i}(qja-\omega t)}$$

$$s_j^y = Be^{\mathrm{i}(qja-\omega t)}$$

Spin Dynamics

Analytical solution — Classical



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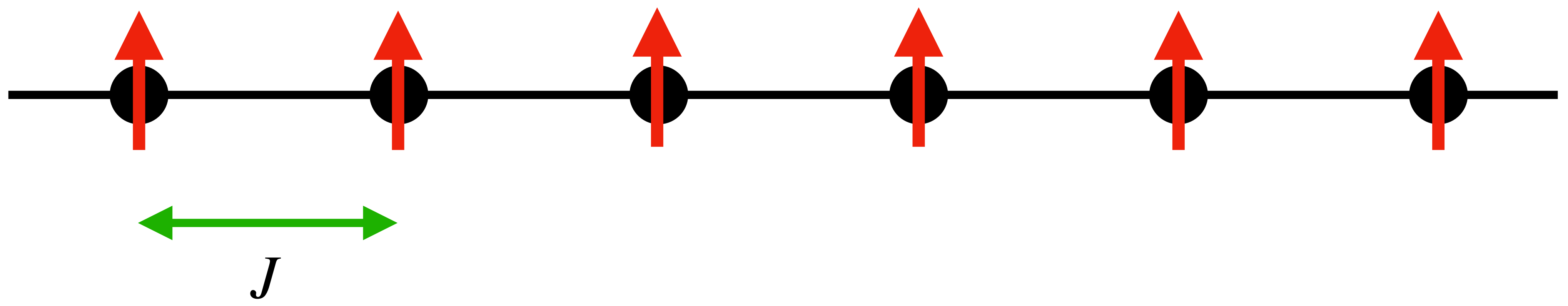
- After algebra, determine

$$A = \mathrm{i}B$$

Spin Dynamics

Analytical solution — Classical



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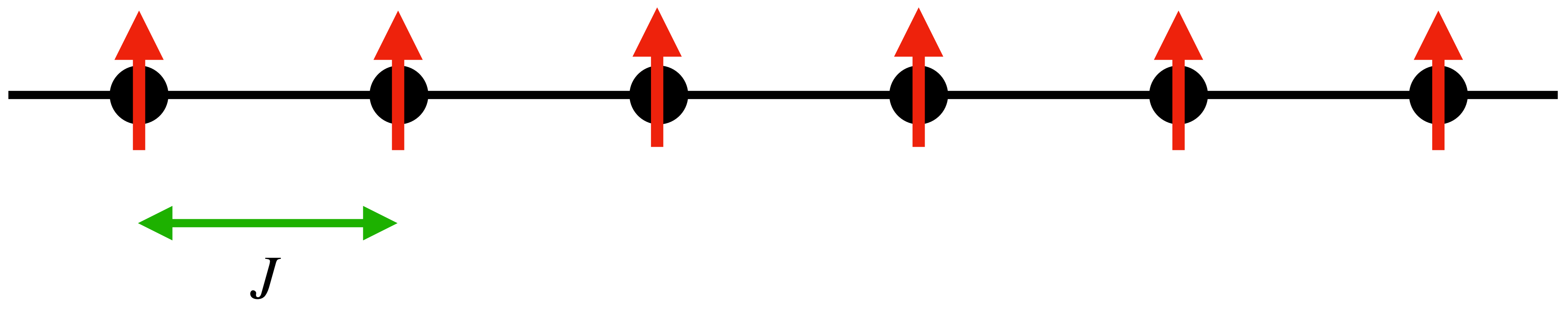
- After algebra, determine

$$A = \mathrm{i}B \quad \Longrightarrow \quad \boxed{\omega = 2JS\left(1 - \cos\left(qa\right)\right)}$$

Spin Dynamics
Analytical solution — Classical



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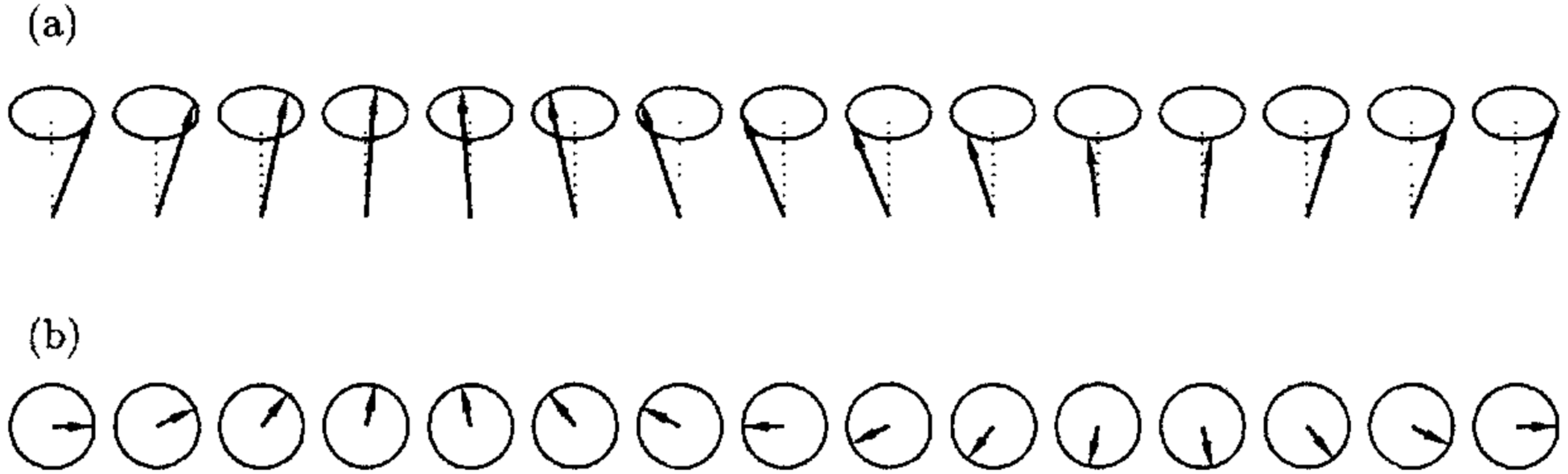


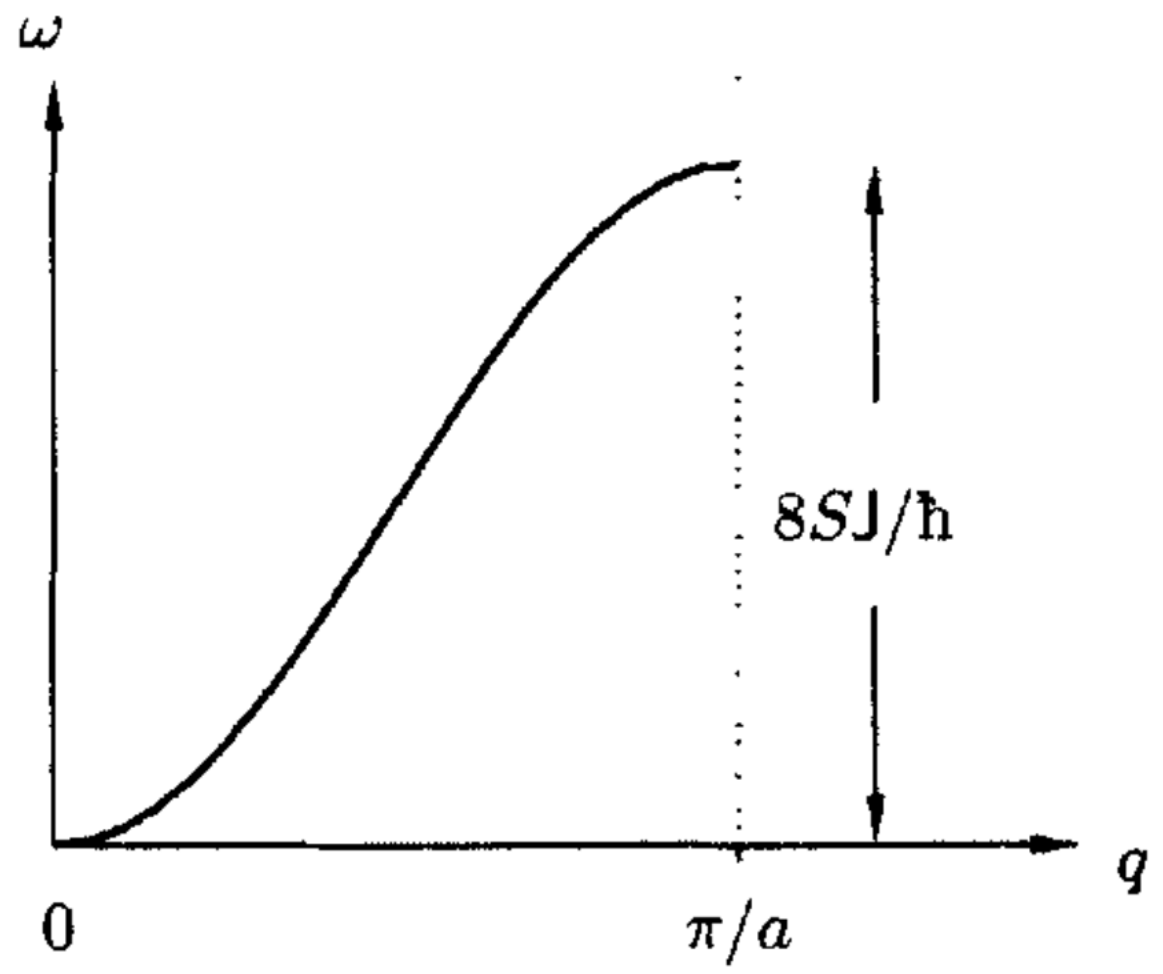
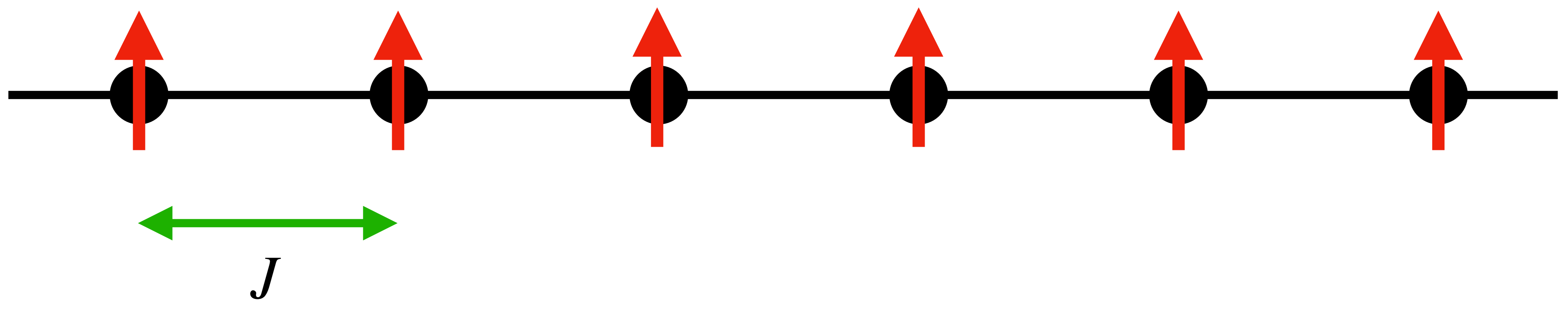


Fig: S. Blundell, *Magnetism in Condensed Matter*, OUP (2001).

Spin Dynamics

Analytical solution — QM Approach

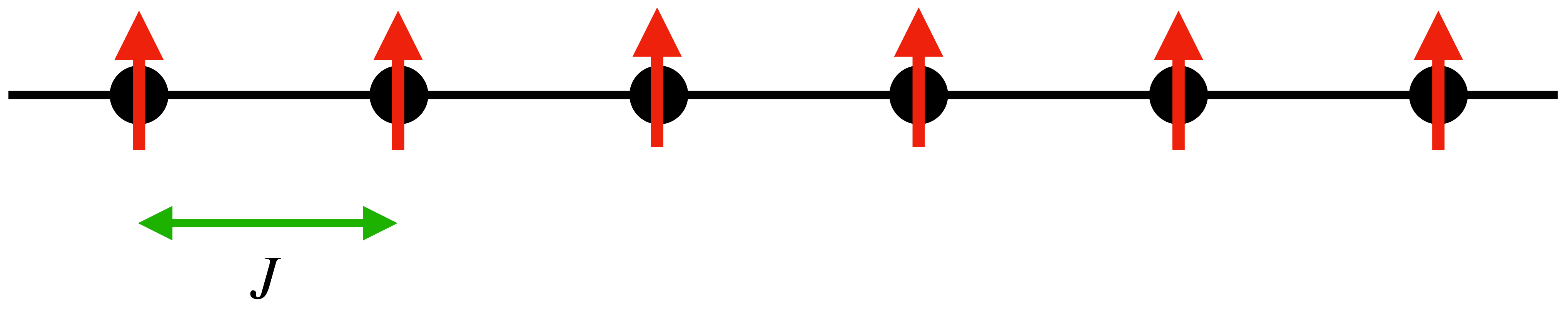


- Write out the Hamiltonian more explicitly.

$$\hat{H} = -J \sum_{\langle i,j \rangle} \hat{S}_i^\alpha \hat{S}_j^\alpha \qquad \hat{H} = -J \sum_i \hat{S}_i^x \hat{S}_{i+1}^x + \hat{S}_i^y \hat{S}_{i+1}^y + \hat{S}_i^z \hat{S}_{i+1}^z$$

Spin Dynamics

Analytical solution — QM Approach



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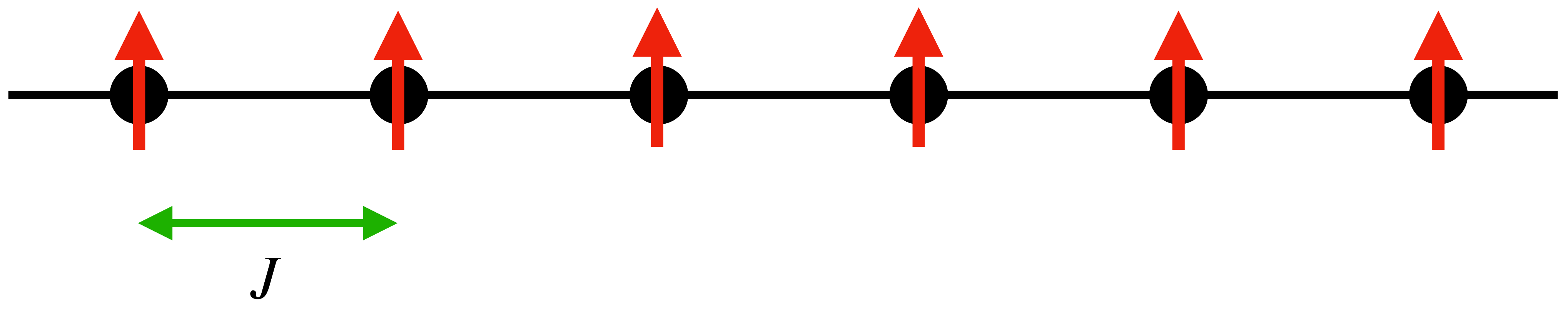
- For convenience, rewrite in terms of raising and lowering operators.

$$\hat{H} = -J \sum_i \hat{S}_i^z \hat{S}_{i+1}^z + \frac{1}{2} \left(\hat{S}_i^+ \hat{S}_{i+1}^- + \hat{S}_i^- \hat{S}_{i+1}^+ \right)$$

Spin Dynamics

Analytical solution — QM Approach



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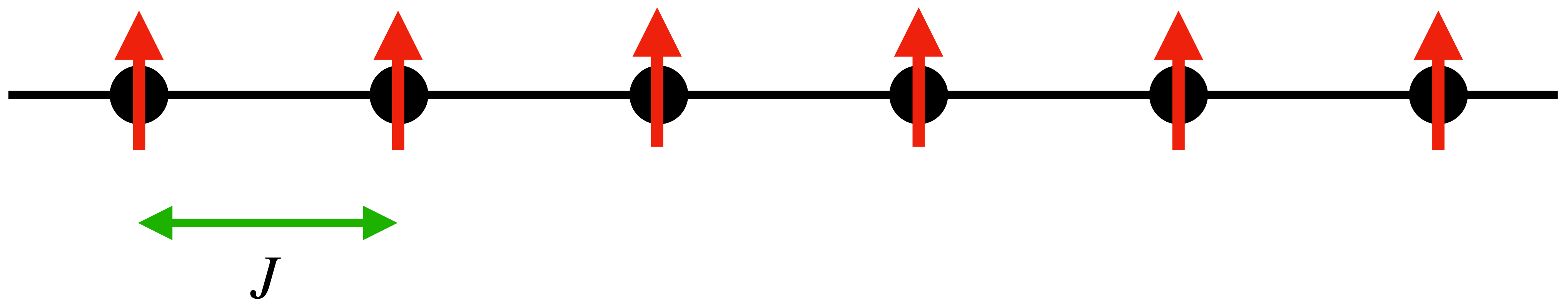
- Examine action of Hamiltonian on expected ground state

$$|\phi\rangle = \bigotimes_i |\uparrow\rangle_i \qquad \hat{H}\,|\phi\rangle = -NS^2 J\,|\phi\rangle$$

Spin Dynamics

Analytical solution — QM Approach

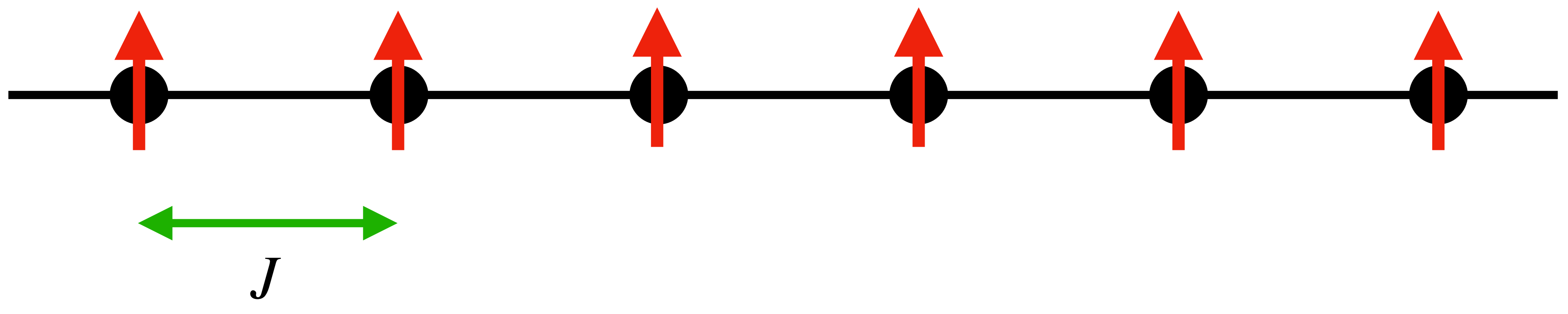


- Now let's consider an excited state — flip one spin.

$$|j\rangle \equiv \hat{S}_j^- |\phi\rangle = |\downarrow\rangle_j \bigotimes_{i \neq j} |\uparrow\rangle_i$$

Spin Dynamics

Analytical solution — QM Approach



- Now let's consider an excited state — flip one spin

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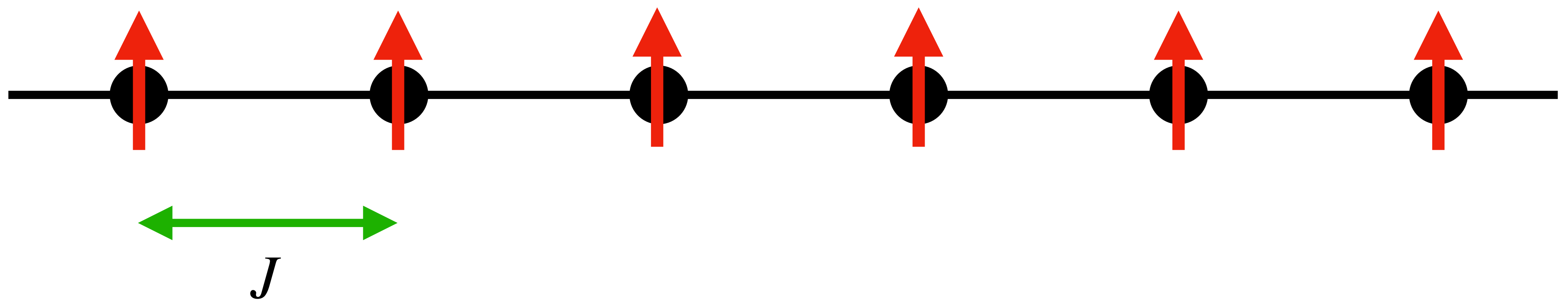
- Consider the action of the Hamiltonian on this state.

$$\hat{H} |j\rangle = \left[\left(-NS^2 J + 2SJ \right) |j\rangle - SJ |j+1\rangle - SJ |j-1\rangle \right]$$

Spin Dynamics

Analytical solution — QM Approach



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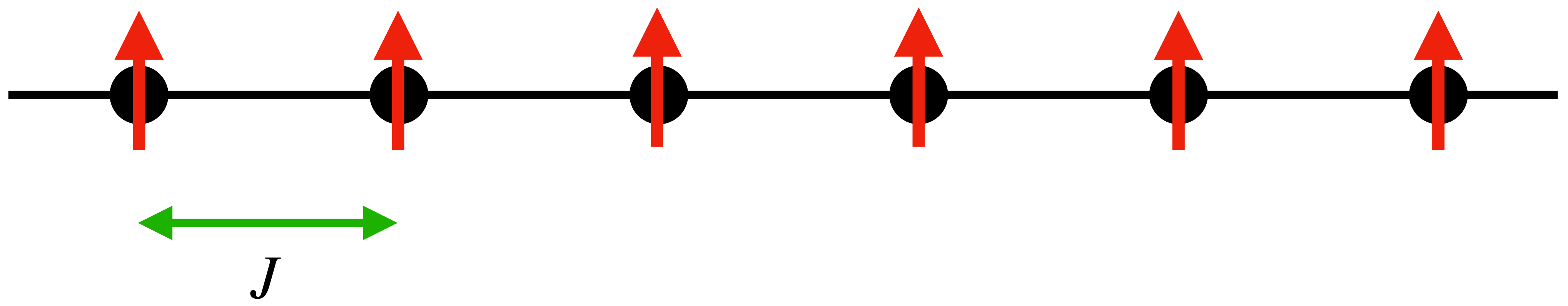
- Consider the action of the Hamiltonian on this state

$$\hat{H}|j\rangle = \left[\left(-NS^2J + 2SJ\right)|j\rangle - SJ|j+1\rangle - SJ|j-1\rangle\right]$$

- Note this is *not* an eigenstate — "spreads out" to neighboring excited states.

Spin Dynamics

Analytical solution — QM Approach

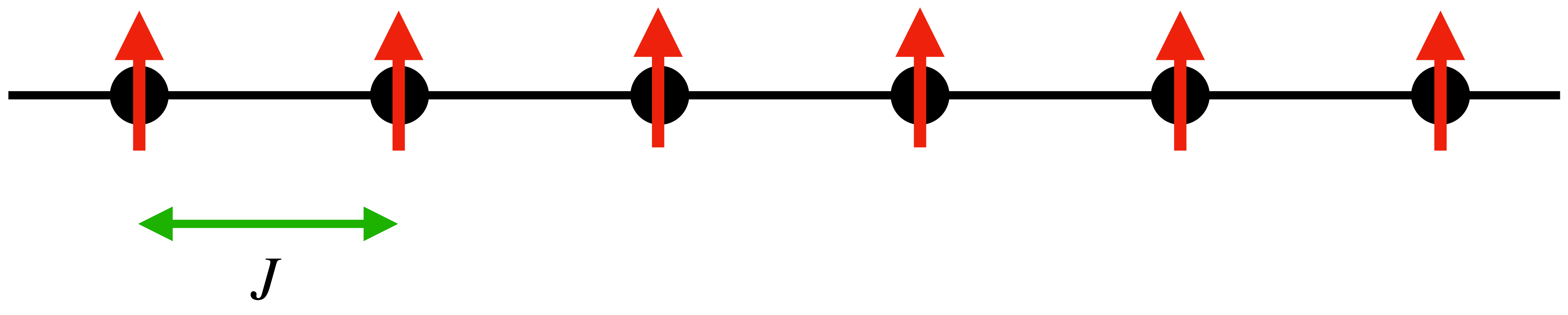


- To find an eigenstate, we apply a Fourier transform to our proposed excitation.

$$|q\rangle = \frac{1}{\sqrt{N}} \sum_j e^{\mathrm{i} q r_j} |j\rangle$$

Spin Dynamics

Analytical solution — QM Approach



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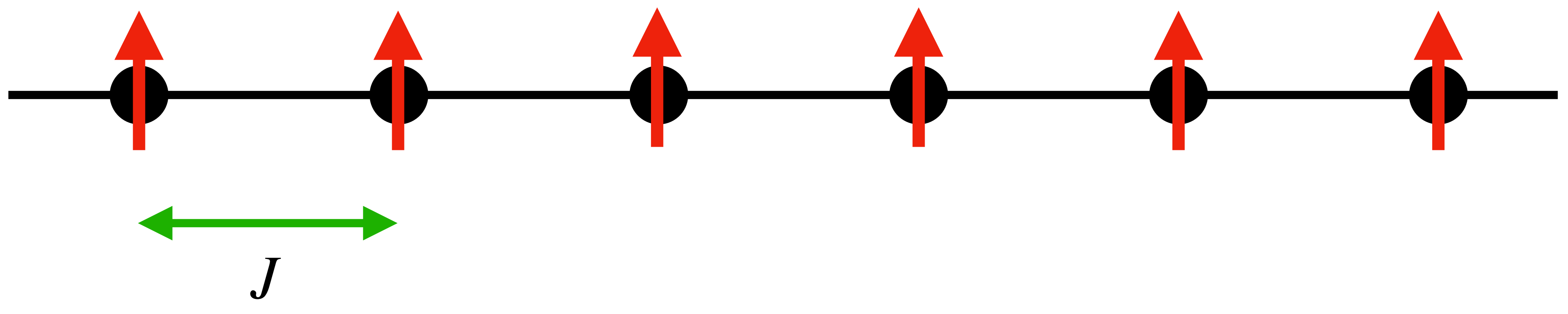
- Applying the Hamiltonian to this state we find

$$\hat{H}|q\rangle = \left[-NS^2J + 2JS\left(1 - \cos qa\right)\right]|q\rangle$$

Spin Dynamics

Analytical solution — QM Approach



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- Applying the Hamiltonian to this state we find

$$\hat{H}|q\rangle = \left[-NS^2J + 2JS(1 - \cos qa)\right]|q\rangle$$

- This is an eigenstate and gives us our dispersion relation

$$\boxed{\hbar\omega = 2JS(1 - \cos qa)}$$

Spin Dynamics
Discussion of results

- For this simple problem, the “small oscillations” of the classical formulation yield an identical dispersion relation to the exact solution.
- This is not a general property, but close to true more often than not in realistic magnets.
- In general, we cannot solve the quantum mechanical problem exactly.
- But we can always “linearize” the quantum mechanical problem and solve that.

Spin Dynamics

Background to Linear Spin Wave Theory (LSWT)

- Recall that the spin algebra:

$$\left\{ \hat{S}^x, \hat{S}^y, \hat{S}^z \right\} \qquad \left[\hat{S}^\alpha, \hat{S}^\beta \right] = i\hbar \epsilon_{\alpha\beta\gamma} \hat{S}^\gamma$$

- We can rewrite this algebra in terms of raising and lowering operators

$$\left\{ \hat{S}^z, \hat{S}^+, \hat{S}^- \right\} \quad \text{where} \quad \begin{aligned} \hat{S}^+ &= \hat{S}^x + i\hat{S}^y \\ \hat{S}^- &= \hat{S}^x - i\hat{S}^y \end{aligned}$$

$$\left[\hat{S}^+, \hat{S}^- \right] = 2\hat{S}^z$$

$$\left[\hat{S}^z, \hat{S}^+ \right] = \hat{S}^+$$

$$\left[\hat{S}^z, \hat{S}^- \right] = -\hat{S}^-$$

Spin Dynamics

Background to Linear Spin Wave Theory (LSWT)

- We can instantiate this same algebra using two flavors of boson, b_0, b_1

$$n_0 = b_0^\dagger b_0$$

$$n_1 = b_1^\dagger b_1$$

$$n_0 + n_1 = 2S$$

$$S^+ = b_0^\dagger b_1$$

$$S^- = b_1^\dagger b_0$$

$$\hat{S}^z = \frac{1}{2}\left(b_0^\dagger b_0 - b_1^\dagger b_1\right)$$

$$\left[\hat{S}^+, \hat{S}^-\right] = 2\hat{S}^z$$

$$\left[\hat{S}^z, \hat{S}^+\right] = \hat{S}^+$$

$$\left[\hat{S}^z, \hat{S}^-\right] = -\hat{S}^-$$

Spin Dynamics

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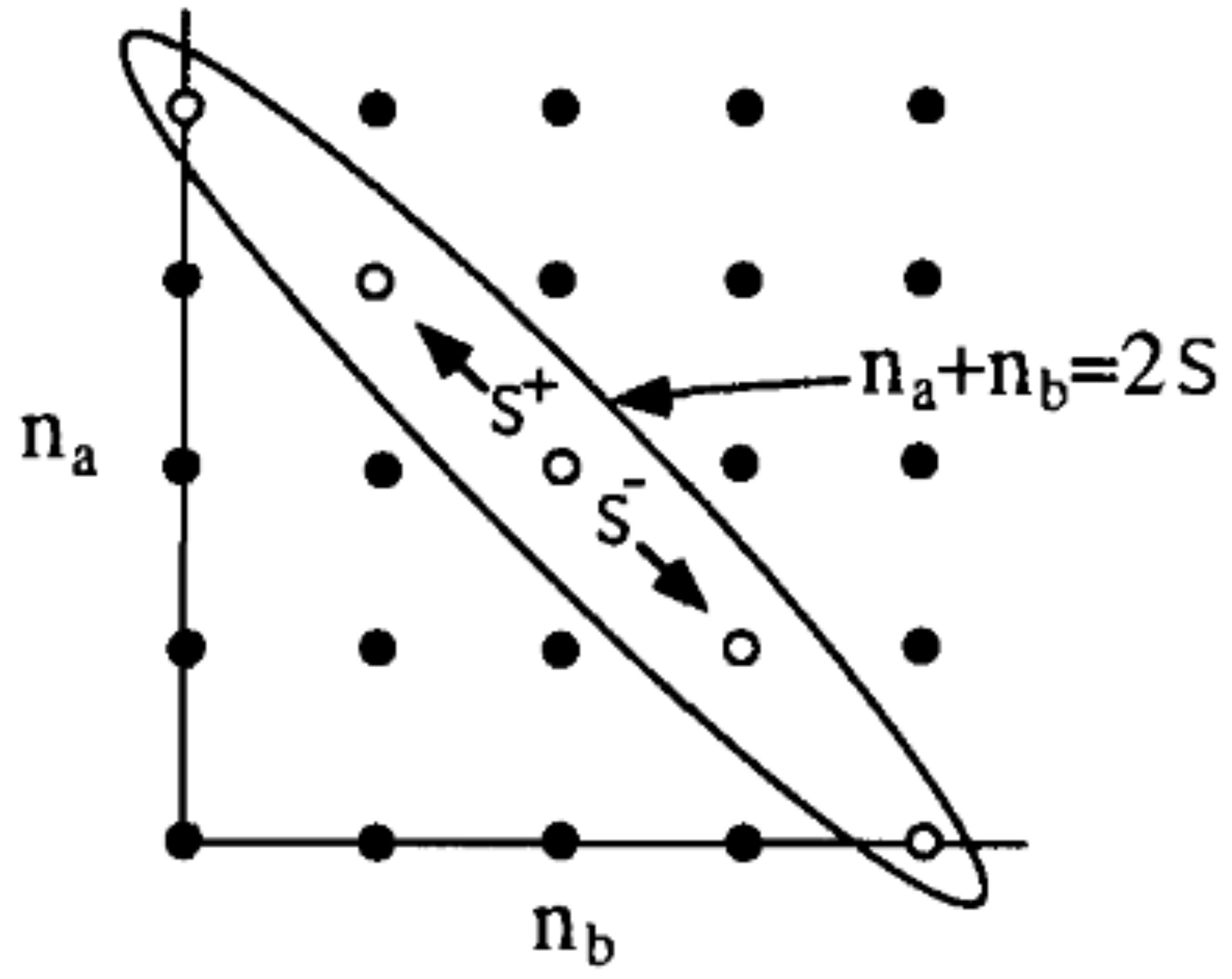

A. Auerbach. *Interacting Electrons and Quantum Magnetism*. (1994)

Spin Dynamics

Background to Linear Spin Wave Theory (LSWT)

- The boson algebra allows us rewrite a spin Hamiltonian in terms of harmonic oscillators, two per site.

- If we can remove one of these harmonic oscillators, we find a single mode per site — exactly as was the case for the linearized classical equations.

- The “elimination” (i.e. condensation) of one of these harmonic oscillators is the quantum analog of linearization.

Spin Dynamics

Recipe for LSWT

1. Find a product state ground state (this will be "condensed" and the expansion builds off this starting point).

2. Rewrite the spin operators in your Hamiltonian in terms of Schwinger bosons, one of which "creates" this ground state.

3. Condense out the ground state boson with a Holstein-Primakoff transformation.

4. Fourier transform on the lattice

5. Para-diagonalize if necessary (Bogoliubov transformation)

Spin Dynamics

Recipe for LSWT

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4. Fourier transform on the lattice
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Spin Dynamics

Transformations associated with ground state

- The ground state is an SU(2) coherent state, i.e., a dipole. It is thus uniquely specified by either by SU(2) rotation (on a ket) or an SO(3) rotation (on a vector).

$$\hat{S}_j^\alpha \rightarrow U_j^\dagger\left(\theta,\phi\right)\hat{S}_j^\alpha U_j\left(\theta,\phi\right) \qquad \hat{S}_j^\alpha \rightarrow \sum_\beta R_{j,\alpha\beta}\left(\theta,\phi\right)\hat{S}_j^\beta$$

Spin Dynamics
Bosonize

- After rotating into these local reference frames, substitute in Schwinger boson representation of spin operators.

$$\hat{S}_j^+ \rightarrow b_{j,0}^\dagger b_{j,1} \qquad \hat{S}_j^- \rightarrow b_{j,1}^\dagger b_{j,0} \qquad \hat{S}_j^z \rightarrow \frac{1}{2}\left(b_{j,0}^\dagger b_{j,0} - b_{j,1}^\dagger b_{j,1}\right)$$

- Then “condense” the ground state boson.

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

Spin Dynamics
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- Then “condense” the ground state boson.

$$b_{j,0}^\dagger = b_{j,0} = \sqrt{2S}\sqrt{1 - \frac{b_{j,1}^\dagger b_{j,1}}{2S}} \longleftarrow \sum_j \left\langle b_{j,1}^\dagger b_{j,1} \right\rangle$$

Use as criterion to evaluated validity of any expansion.

Spin Dynamics

Collect terms in orders of S

- Expand the Holstein-Primakoff Boson in powers of S and collect terms of like order

$$\hat{H} = \hat{H}^{(0)} + \hat{H}^{(2)} + \hat{H}^{(4)} + \mathcal{O}\left(\frac{1}{S}\right)$$

$\mathcal{O}\left(S^2\right)$ — Classical energy

$\mathcal{O}\left(S\right)$ — Quadratic in bosons; LSWT Hamiltonian

$\mathcal{O}\left(1\right)$ — Quartic in bosons; Magnon-magnon interactions

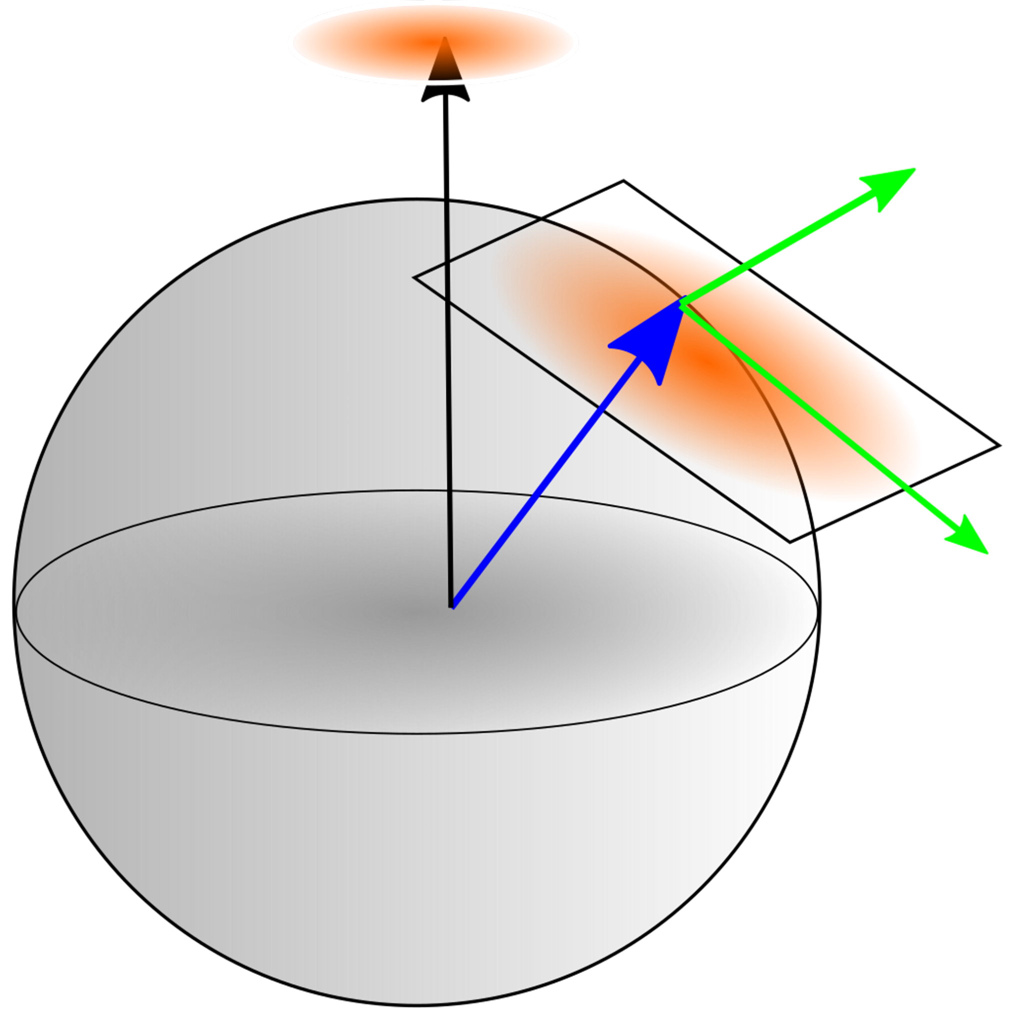
Spin Dynamics
LSWT Summary

- These steps are essentially the quantum analog of the linearization procedure for the classical dynamics.

  1. We start with the ground state (rotation of spin operators, definition of bosons).

  2. When condensing, we "expand" about the ground state.

  3. The condensation leaves us with one mode, $b^\dagger_{j,1} = \hat{X}_j + i\hat{P}_j$, per site



Spin Dynamics
Remarks on LSWT

- LSWT solution for the ferromagnetic spin chain results in the same dispersion as the fully classical approach and the exact solution.

$$\hbar\omega = 2JS\left(1 - \cos qa\right)$$

- Correspondence between between the classical result and the LSWT result *always* holds.
- The correspondence between these results and the *exact* result is special

Spin Dynamics

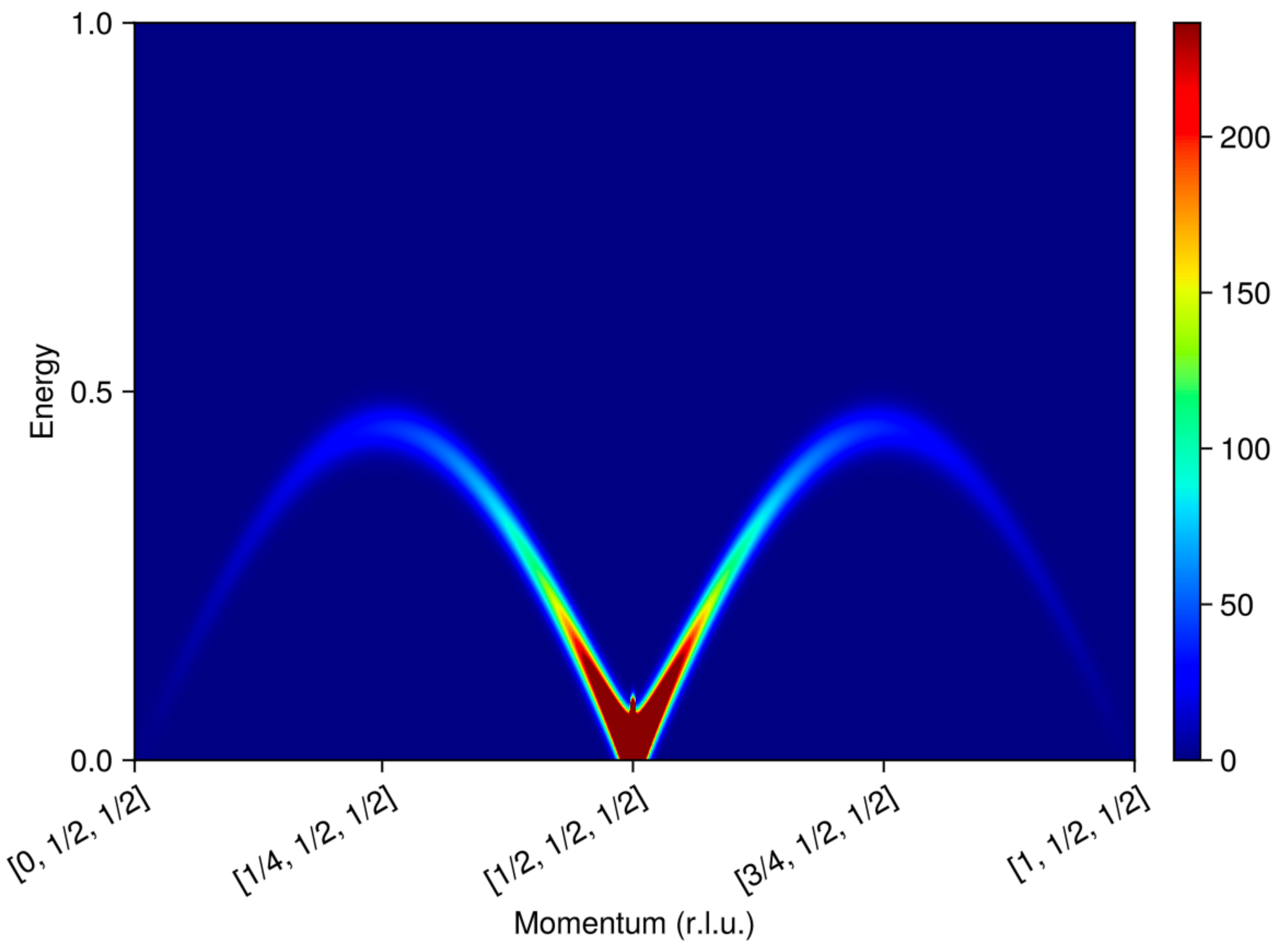
LSWT vs "real" solution for antiferromagnet ($CuSO_4 \cdot 5D_2O$)

- The LSWT solution to the antiferromagnetic spin chain is

$$\hbar\omega = 2SJ\sqrt{1 - \cos^2(qa)}$$

- The actual result is known analytically (Bethe ansatz) and has been studied in material realizations

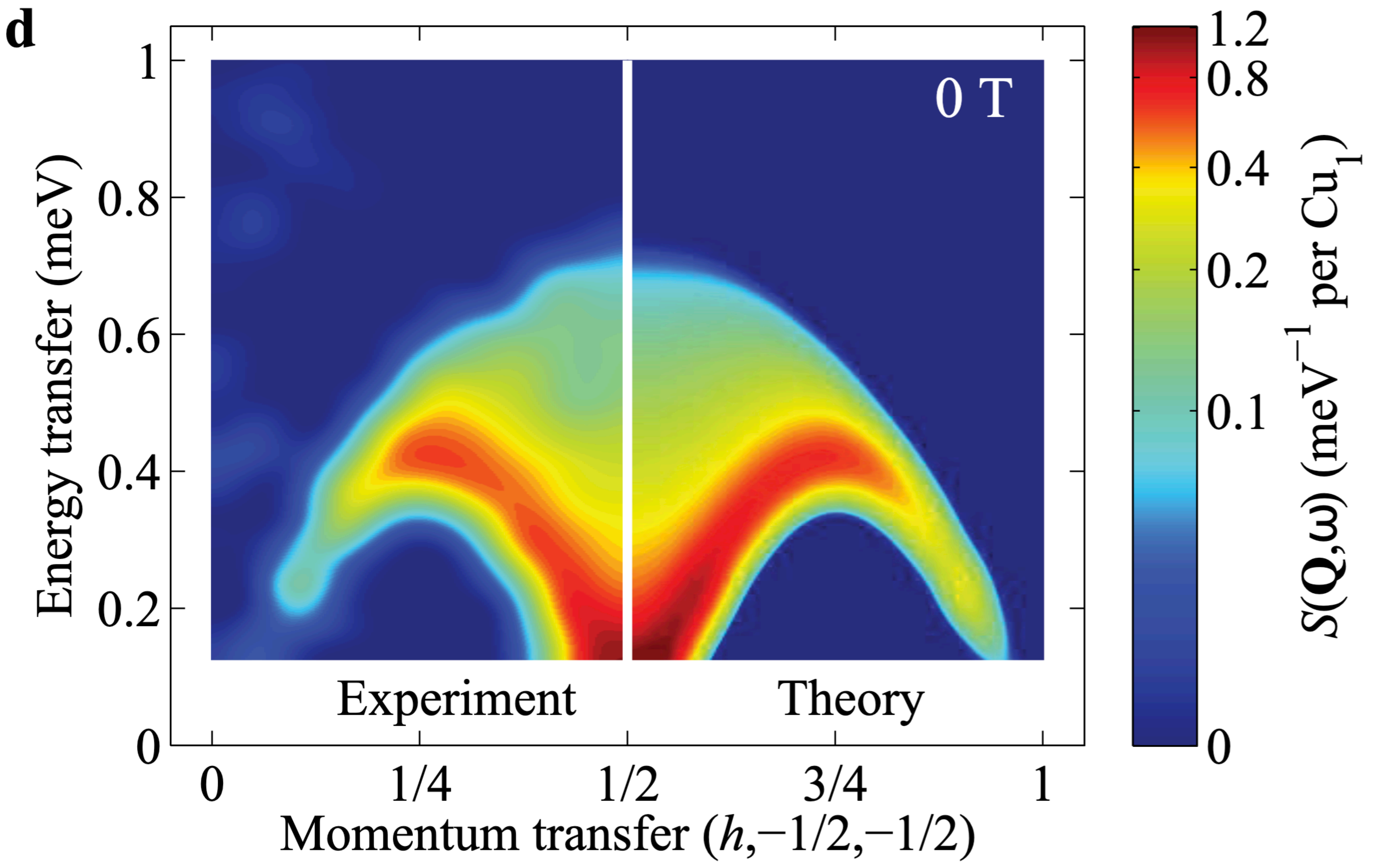
LSWT



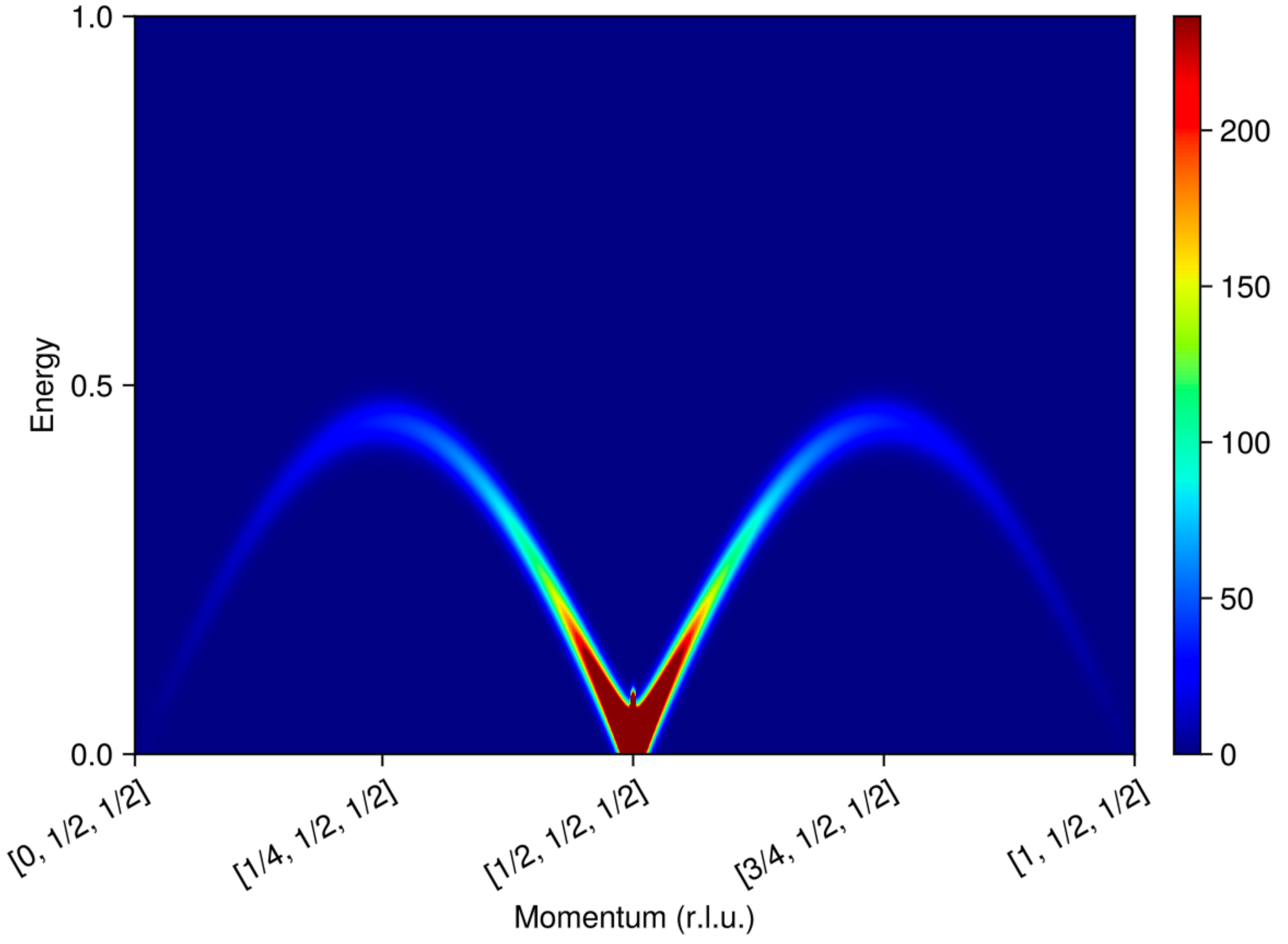
Spin Dynamics

LSWT vs “real” solution for antiferromagnet ($CuSO_4 \cdot 5D_2O$)

Real Solution



LSWT

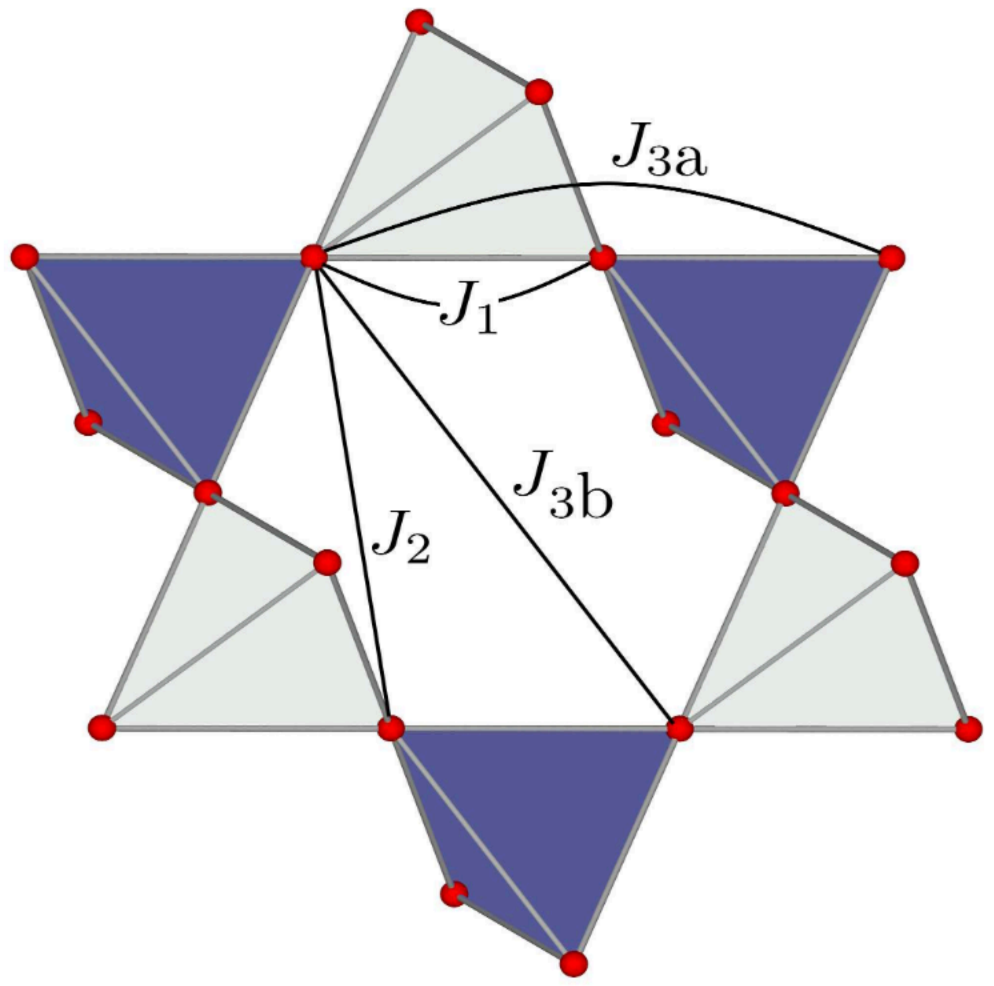


M. Mourigal et al., “Fractional spinon excitations…,” Nature Physics 9 (2013).

Spin Hamiltonians

Classical Spin Liquids

- Recall this model supported many different ground states with the same (or very similar) energy
- If we calculate small oscillations around a range of these ground states and average the results, what does this look like?



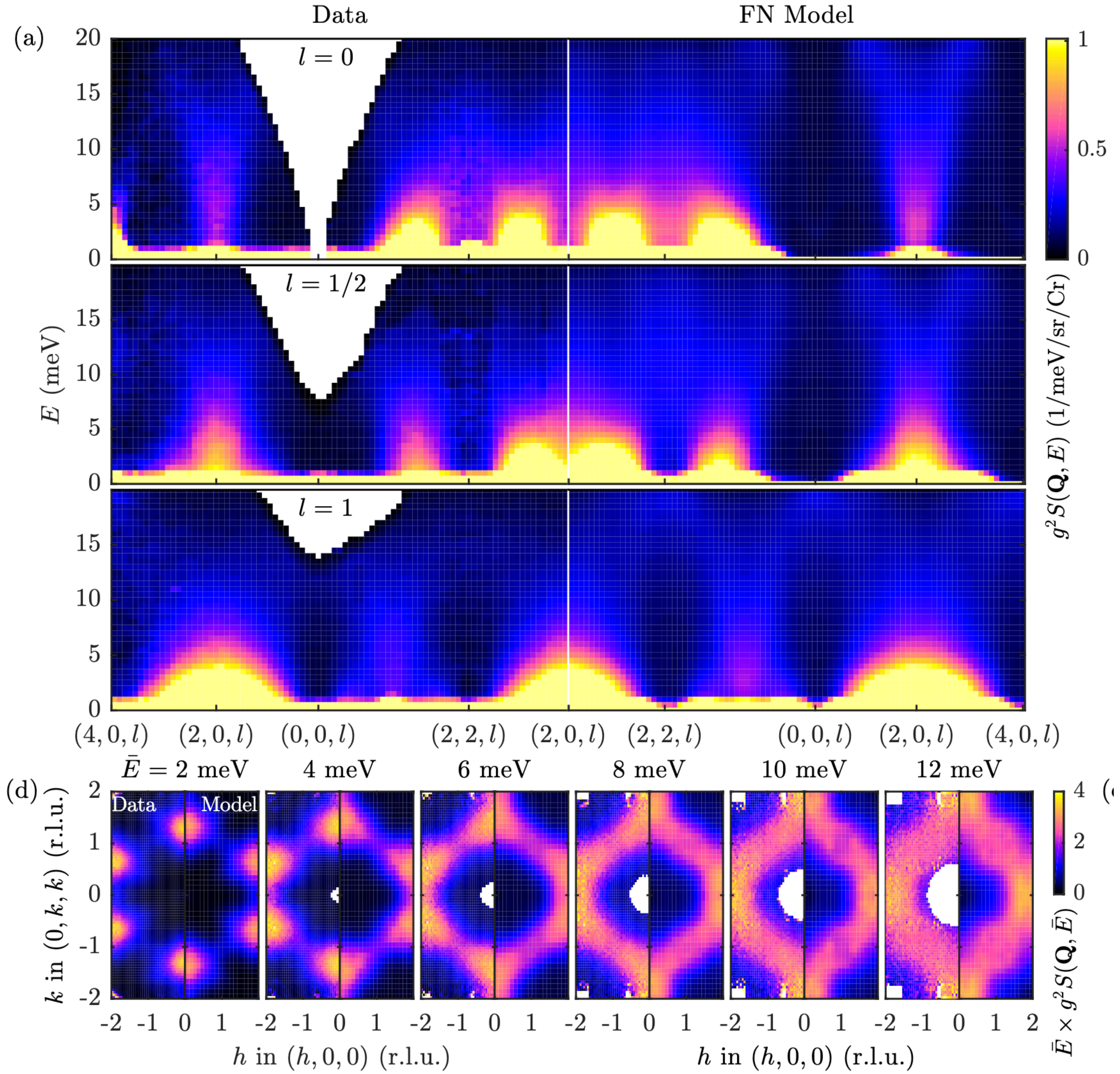
$$\hat{H} = \sum_i J_i \sum_{\langle j,k \rangle} s_j^\alpha s_k^\alpha, \quad J_i > 0$$

Bai et al, "Magnetic excitations of the classical spin liquid…," PRL 122 (2019).

Spin Hamiltonians

Classical Spin Liquids

- Note the broadening — a central point of concern in contemporary magnetism research.
- “Normal mode” picture breaks down or is obscured



Bai et al, “Magnetic excitations of the classical spin liquid…,” PRL 122 (2019).

Recap

- Neutron scattering experiments give us a fairly detailed account of the dynamics of a quantum magnet.
- In classical and semiclassical approaches, we start from a picture of clearly separated spin operators on each site, or equivalently, a dipole on each site
- The interactions determine a ground state, which can sometimes be very complicated
- Linear dynamics are just small oscillations on top of this ground state
- Despite being very classical, these methods remain very important to magnetism research

Part II

Generalizing classical and semiclassical methods

- We’ve attempted to convince you that there is strong value in thinking about a magnetic dynamics classically.
- We’ve also shown that the classical picture sometimes fails.
- Here we’ll show a systematic procedure for extending classical methods to encompass a somewhat wider range of cases.

I. SU(N) Semiclassics

Conceptual motivation

$$\hat{H} = J \sum_{\langle i,j \rangle} \hat{S}_i^\alpha \hat{S}_j^\alpha + D \sum_i \left(\hat{S}_i^z \right)^2 + h \sum_i \hat{S}^z \longrightarrow i\hbar \frac{d}{dt} | \psi \rangle = \hat{H} | \psi \rangle$$

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I. SU(*N*) Semiclassics

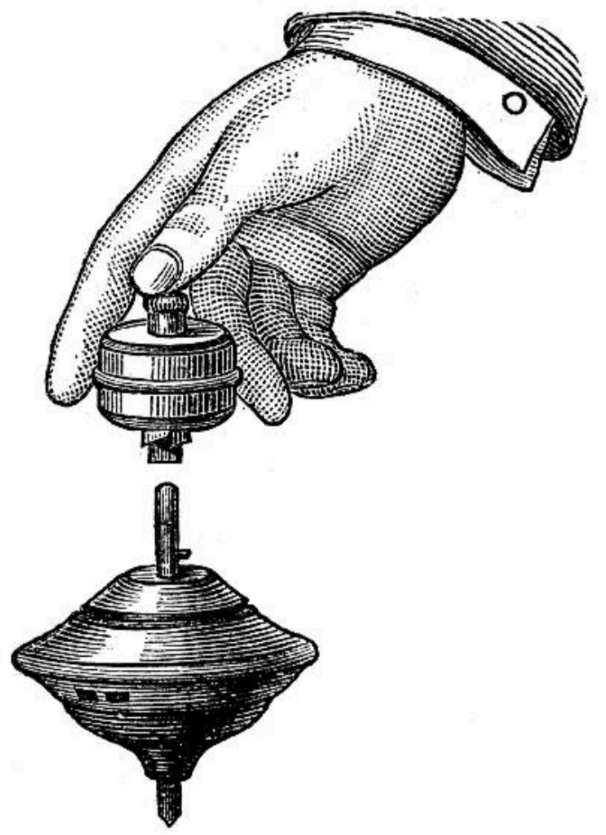
Conceptual motivation

$$\hat{H} = J \sum_{\langle i,j \rangle} \hat{S}_i^\alpha \hat{S}_j^\alpha + D \sum_i \left(\hat{S}_i^z\right)^2 + h \sum_i \hat{S}^z$$

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

$$H_{\text{cl}} = J \sum_{\langle i,j \rangle} \mathbf{s}_i \cdot \mathbf{s}_j + D \sum_i \left(s_i^z\right)^2 + h \sum_i s_i^z$$

$$\frac{d\mathbf{s}_i}{dt} = \nabla_{\mathbf{s}_i} H_{\text{cl}} \times \mathbf{s}_i$$



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I. SU(N) Semiclassics

Conceptual motivation

$$H_{\mathrm{cl}} = J \sum_{\langle i,j \rangle} \mathbf{s}_i \cdot \mathbf{s}_j + D \sum_i \left(s_i^z \right)^2 + h \sum_i s_i^z$$

$$\frac{d\mathbf{s}_i}{dt} = J \left(\mathbf{s}_{i-1} + \mathbf{s}_{i+1} \right) \times \mathbf{s}_i$$

I. SU(N) Semiclassics

Conceptual motivation

$$H_{\mathrm{cl}} = J \sum_{\langle i,j \rangle} \mathbf{s}_i \cdot \mathbf{s}_j + D \sum_i \left(s_i^z\right)^2 + h \sum_i s_i^z$$

$$\frac{d\mathbf{s}_i}{dt} = \begin{pmatrix} 0 \\ 0 \\ 2Ds_i^z \end{pmatrix} \times \mathbf{s}_i$$

I. SU(N) Semiclassics

Conceptual motivation

$$H_{\mathrm{cl}} = J \sum_{\langle i,j \rangle} \mathbf{s}_i \cdot \mathbf{s}_j + D \sum_i \left(s_i^z \right)^2 + h \sum_i s_i^z$$

$$\frac{d\mathbf{s}_i}{dt} = \begin{pmatrix} 0 \\ 0 \\ h \end{pmatrix} \times \mathbf{s}_i$$

I. SU(N) Semiclassics

Conceptual motivation

$$H_{\mathrm{cl}} = J \sum_{\langle i,j \rangle} \mathbf{s}_i \cdot \mathbf{s}_j + D \sum_i \left(s_i^z\right)^2 + h \sum_i s_i^z$$

$$\frac{d\mathbf{s}_i}{dt} = \begin{pmatrix} 0 \\ 0 \\ h \end{pmatrix} \times \mathbf{s}_i$$

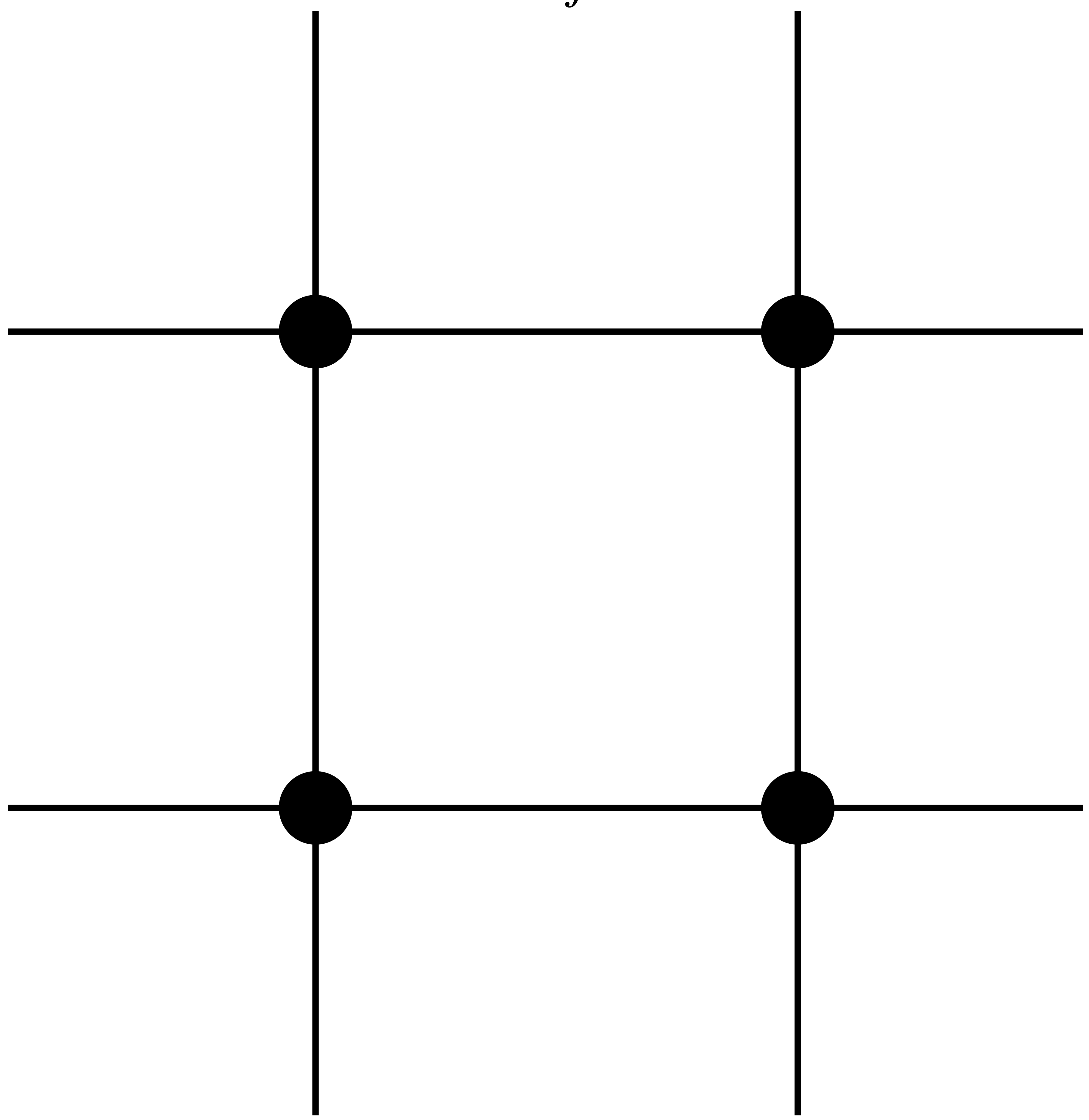
$$\frac{d}{dt} |\psi\rangle = h\hat{S}^z |\psi\rangle$$

I. SU(*N*) Semiclassics

Structure of SU(2) (large-S) methods

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

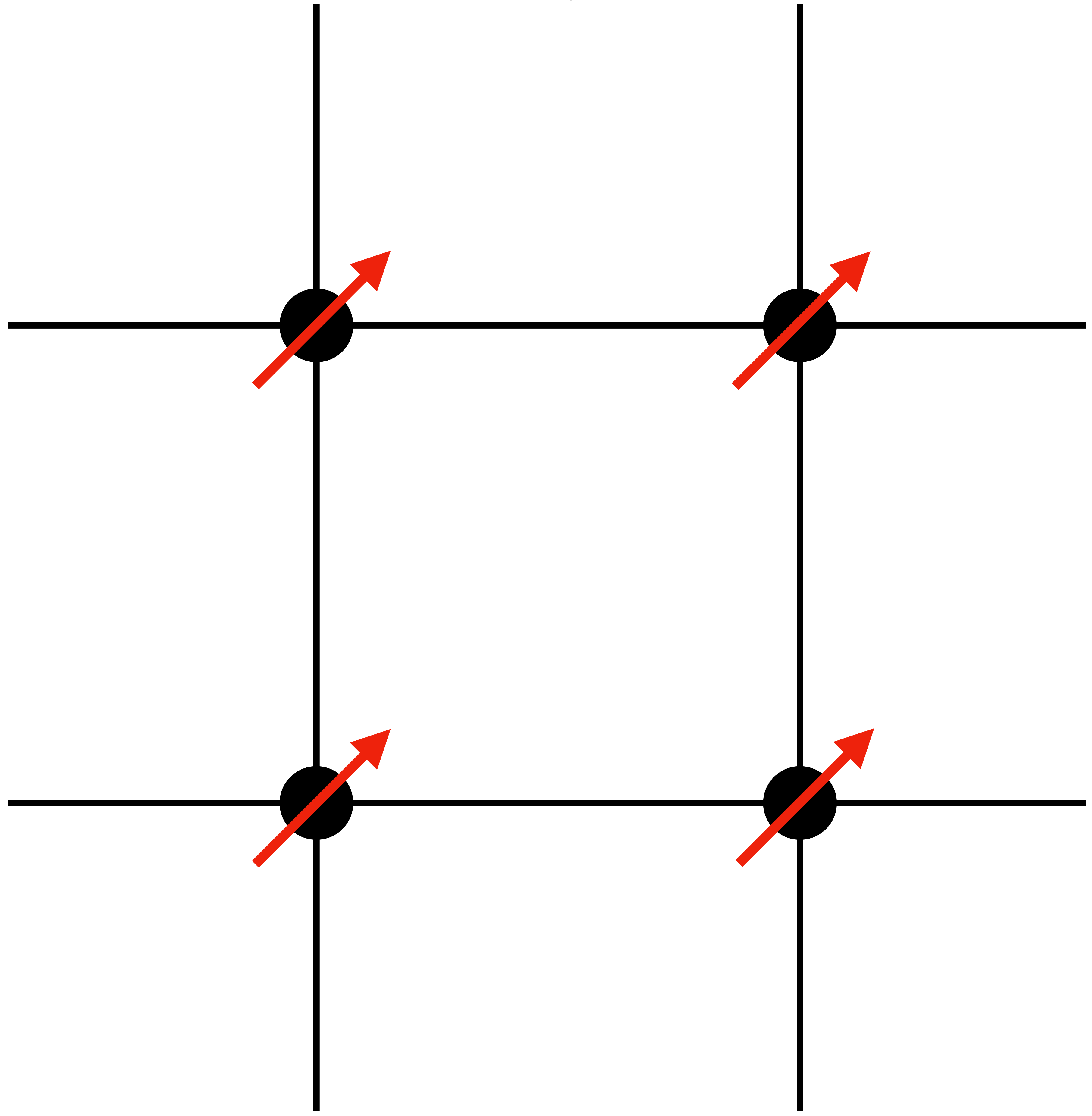
$$|\Psi\rangle = \bigotimes_j |\Psi_j\rangle$$



I. SU(*N*) Semiclassics

Structure of SU(2) (large-S) methods

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



- 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

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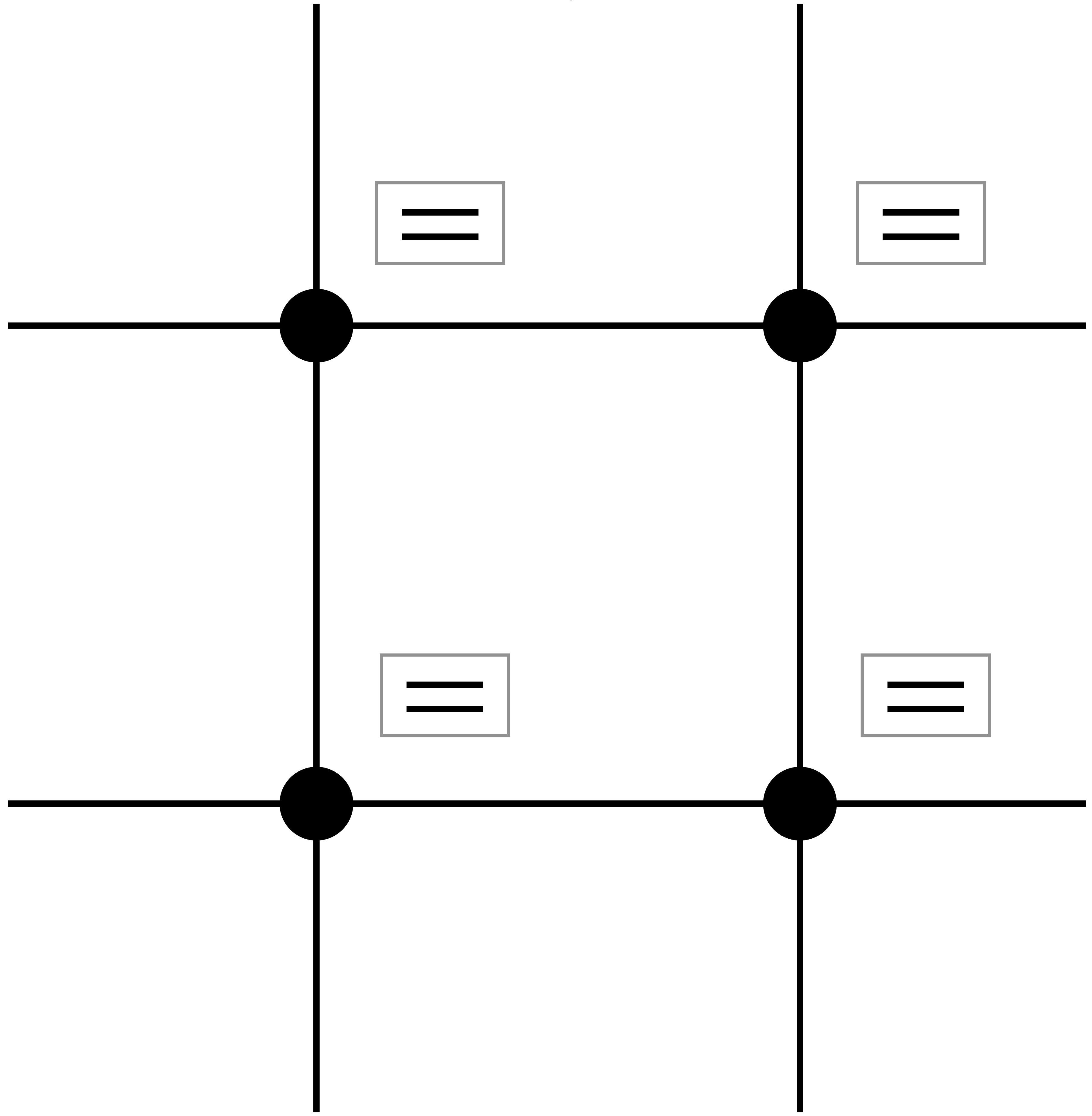
I. SU(*N*) Semiclassics

Structure of SU(2) (large-S) methods

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

- 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



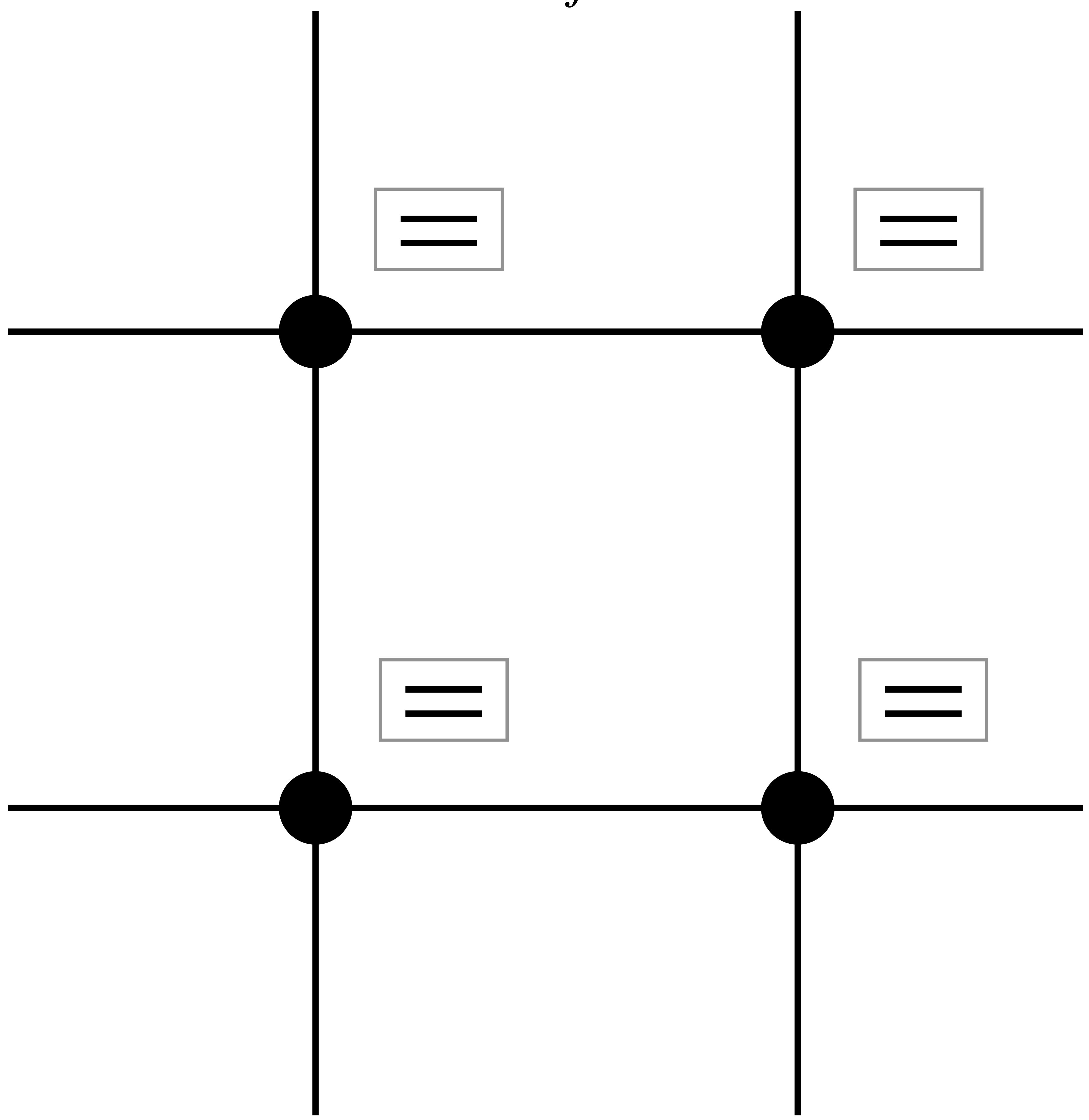
I. SU(*N*) Semiclassics

Structure of SU(2) (large-S) methods

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

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

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



I. SU(*N*) Semiclassics

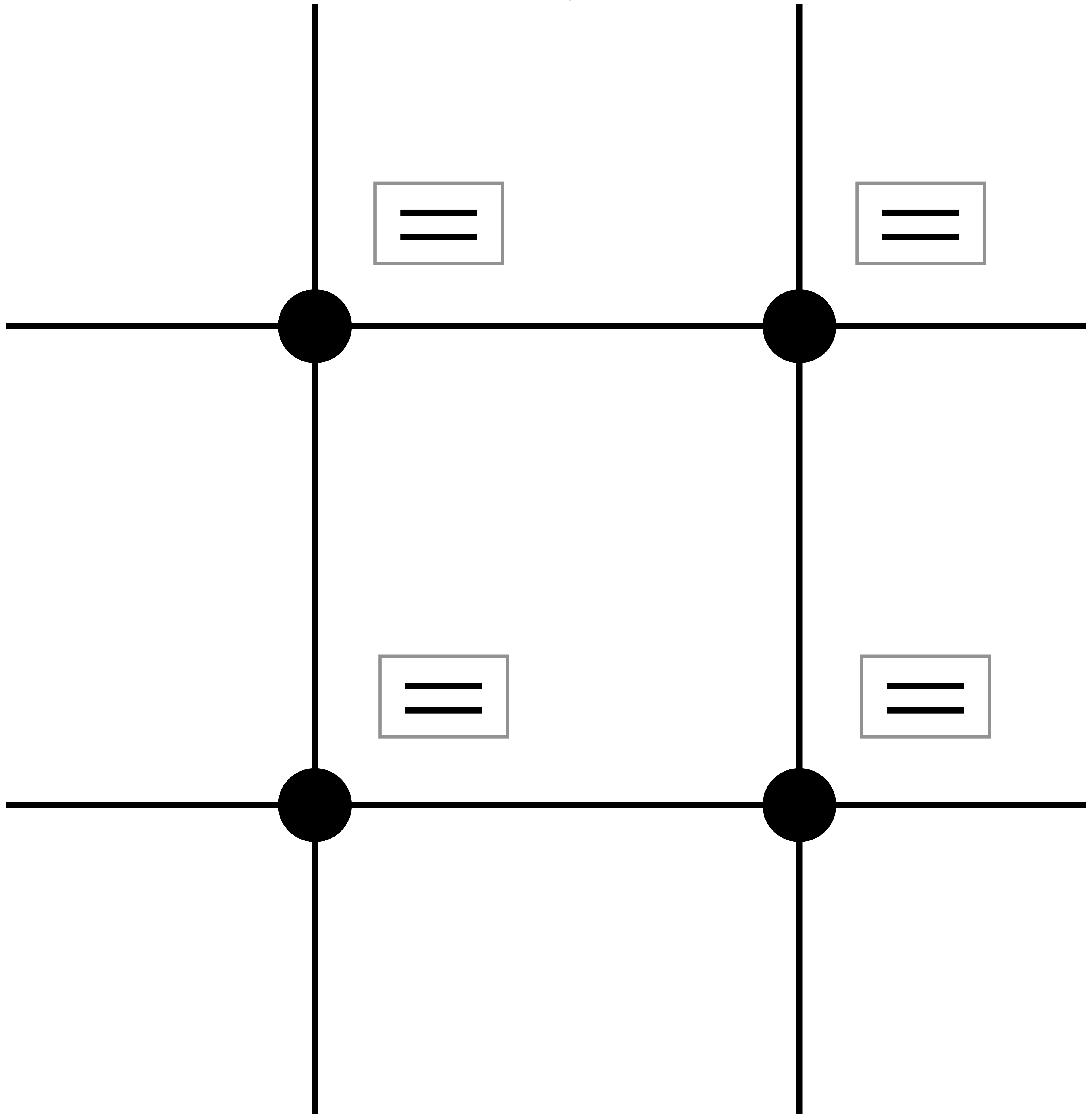
Structure of SU(2) (large-S) methods

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

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

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

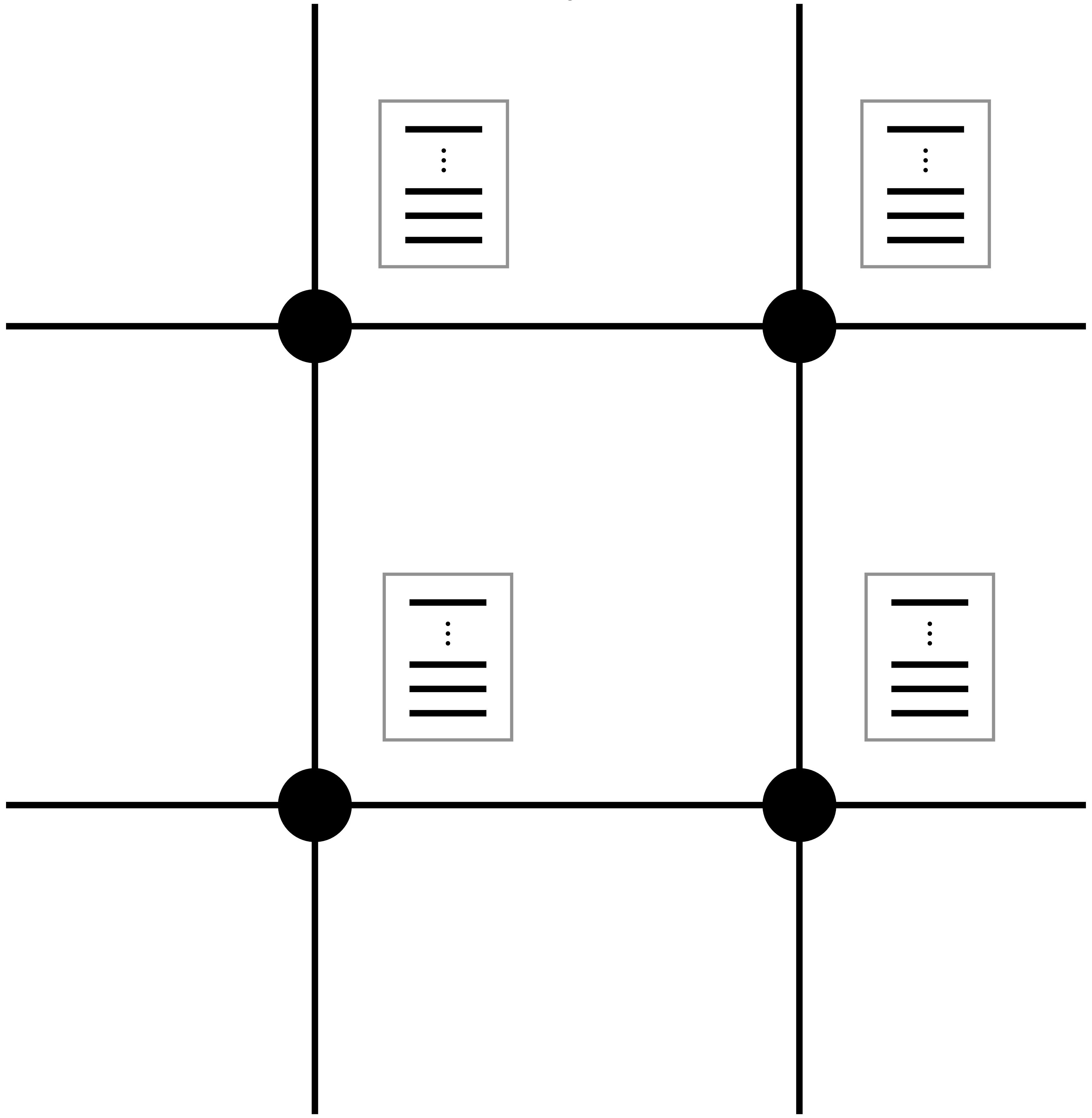
$$|\Psi\rangle = \bigotimes_j |\Psi_j\rangle$$



I. SU(*N*) Semiclassics

Structure of SU(*N*) (large-M) methods

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



- 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.

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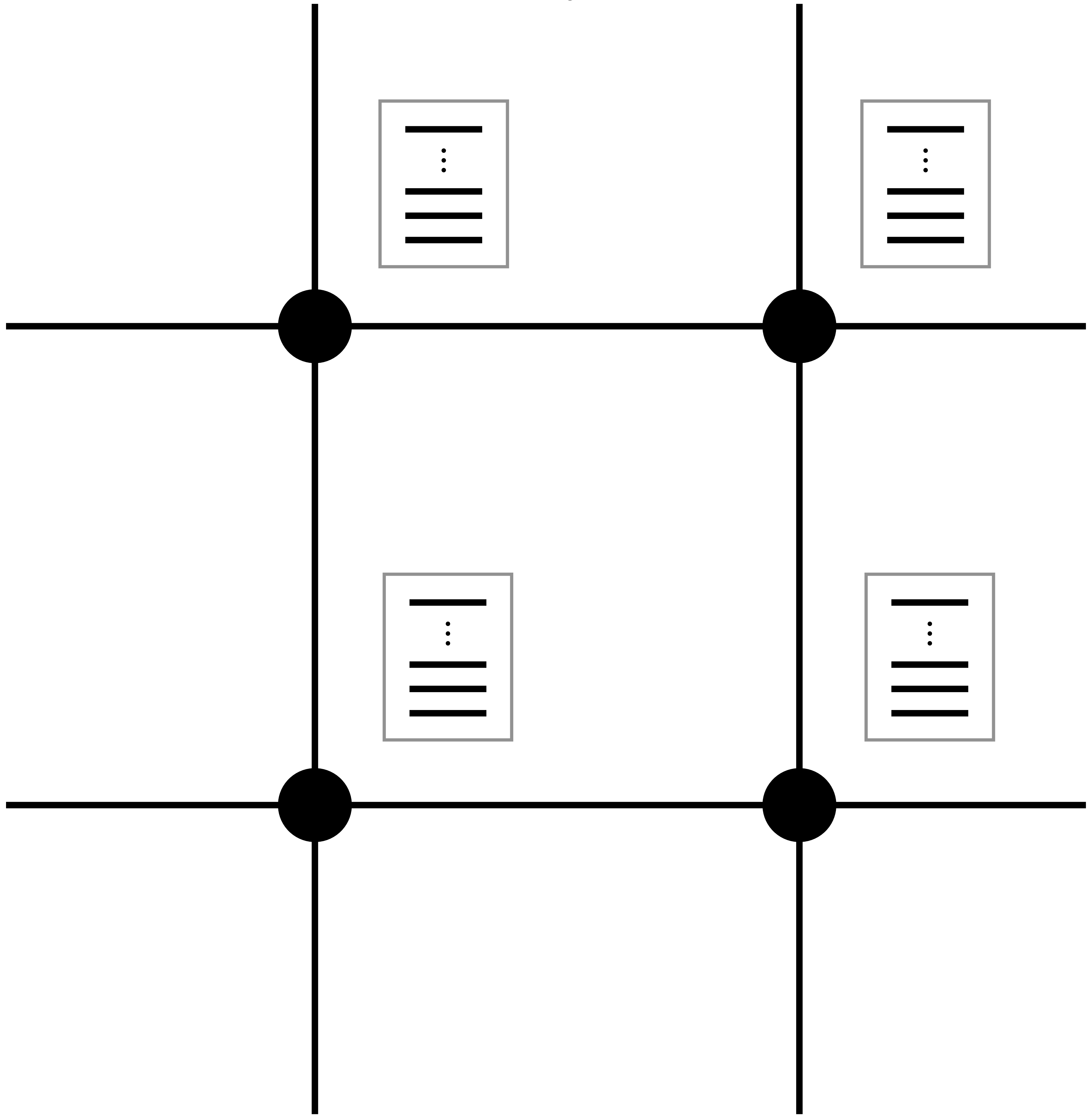
I. SU(*N*) Semiclassics

Structure of SU(*N*) (large-M) methods

- Well defined procedure for defining a classical dynamics.

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

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

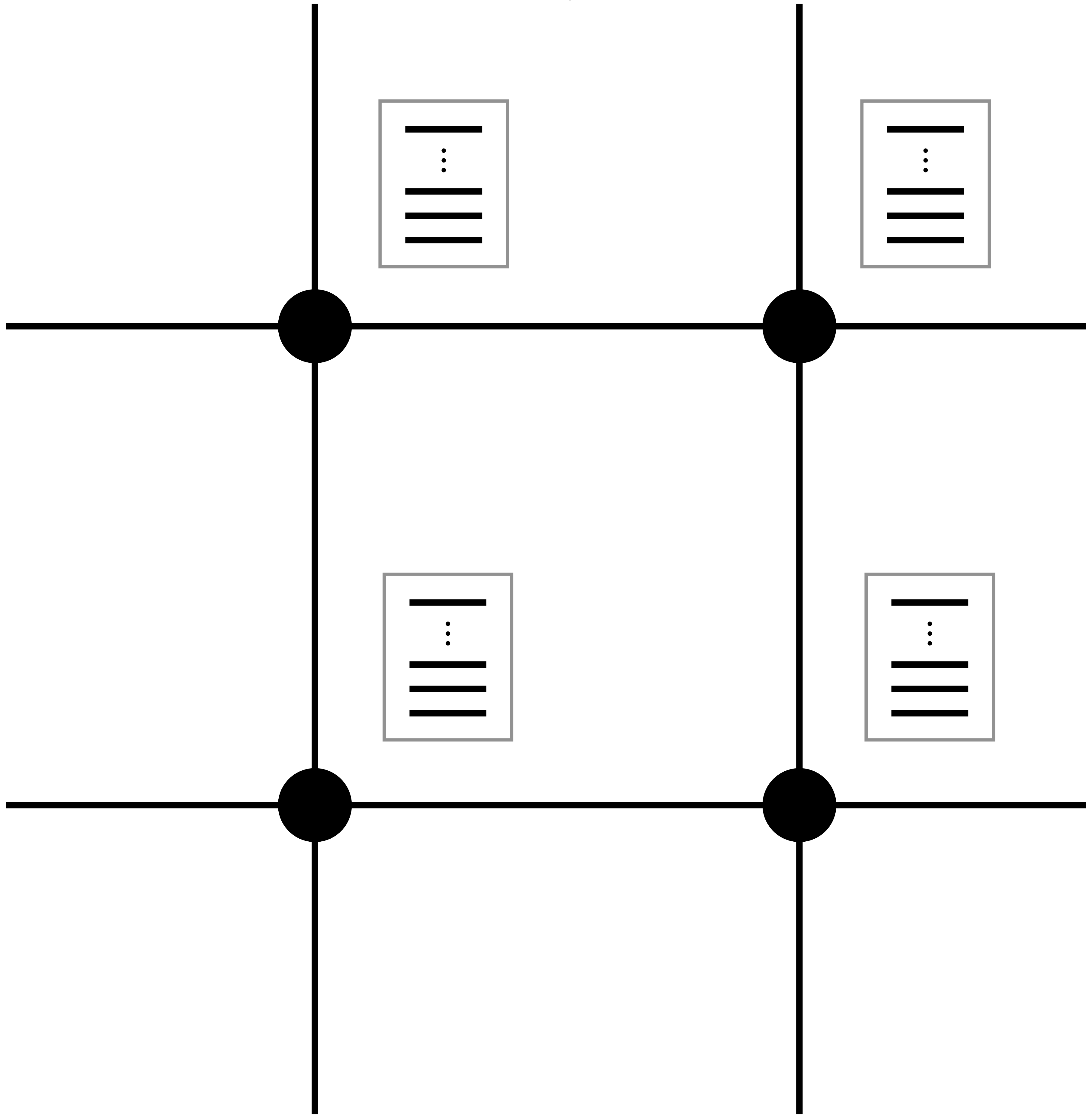


H. Zhang and C. Batista, “Classical spin dynamics based on SU(*N*) coherent states,” PRB **96** (2022).

I. SU(*N*) Semiclassics

Structure of SU(*N*) (large-M) methods

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



- 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).

I. SU(*N*) Semiclassics

SU(2) theory: coherent states

- Actions generated by exponentiating **linear combinations of generators**

$$U(c_\alpha) = e^{i\sum_\alpha c_\alpha \hat{S}^\alpha}$$

- Generate coherent states by applying to a **reference state**

$$|\Omega(c_\alpha)\rangle = U(c_\alpha)|\uparrow\rangle = e^{i\sum_\alpha c_\alpha \hat{S}^\alpha}|\uparrow\rangle$$

- The result of this process will become the **classical phase space**

$$CP^1 \simeq S^2$$

I. SU(*N*) Semiclassics

SU(2) theory: coherent states

- There is a correspondence between all these states (and any 2-level state) with points on a sphere: Bloch sphere construction.

$$|\Omega\rangle \leftrightarrow \left(\langle\Omega|\,\hat{S}^x\,|\Omega\rangle\,,\langle\Omega|\,\hat{S}^y\,|\Omega\rangle\,,\langle\Omega|\,\hat{S}^z\,|\Omega\rangle\right) \equiv \vec{\mathbf{s}}$$

SU(2) coherent state

⟵ One-to-one ⟶ correspondence

Real 3-vector on sphere

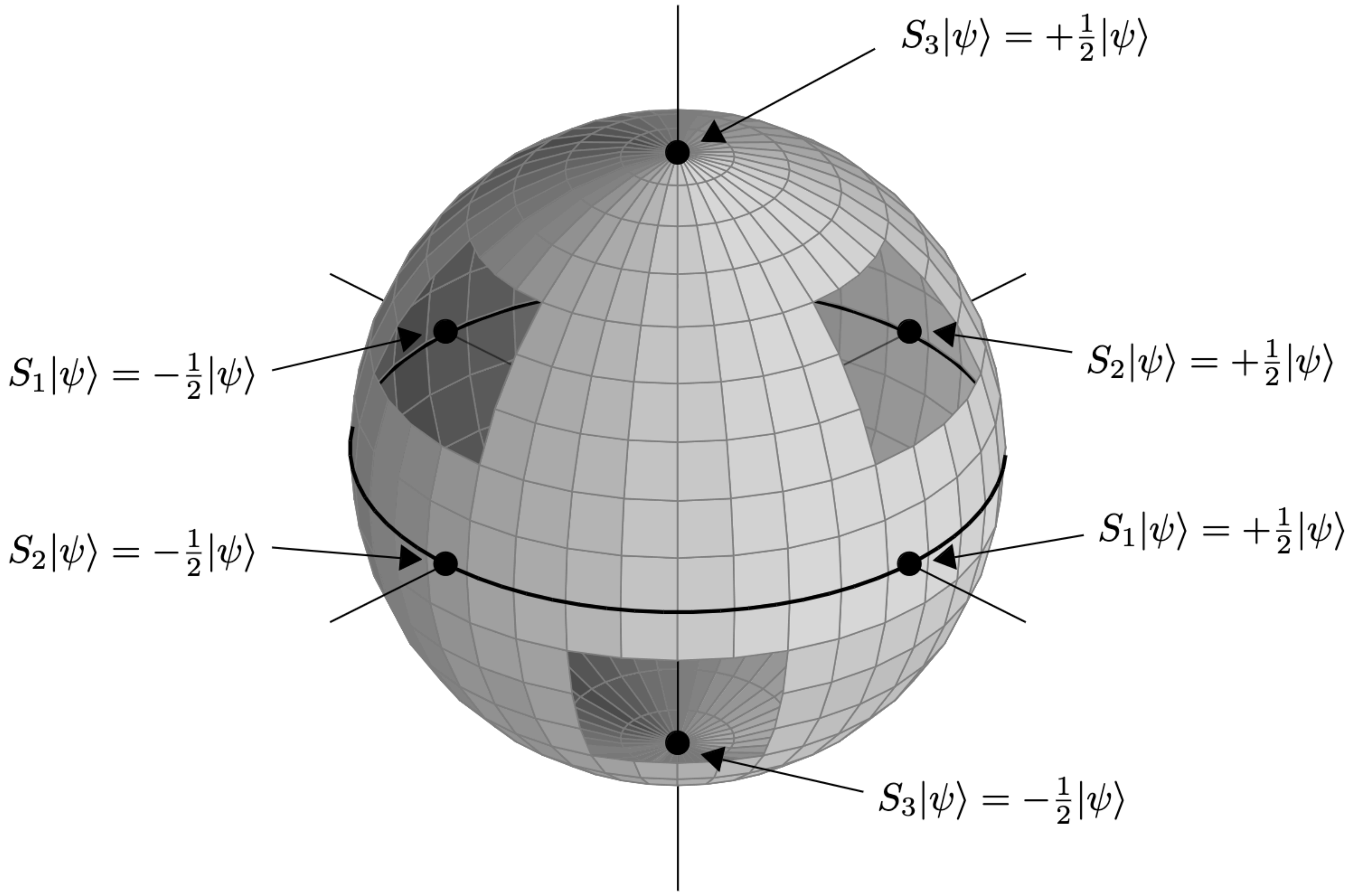


Image from: P. Woit, *Quantum Theory, Groups and Representations (2014)*

I. SU(*N*) Semiclassics

SU(2) theory: classical limit

- $S \to \infty$ while sending $\hbar \to 0$ (while holding $S\hbar$ constant)

$$S^z = \begin{bmatrix} S & & & \\ & S-1 & & \\ & & \ddots & \\ & & & -S \end{bmatrix}$$

Spectrum becomes "more continuous"

$$\left[\hat{S}^\alpha, \hat{S}^\beta\right] = i\epsilon_{\alpha\beta\gamma} S^\gamma$$
$$\implies \hat{S}^\alpha \hat{S}^\beta = \hat{S}^\beta \hat{S}^\alpha + i\epsilon_{\alpha\beta\gamma} \hat{S}^\gamma$$
$$\implies \lim_{S\to\infty} \hat{S}^\alpha \hat{S}^\beta = \hat{S}^\beta \hat{S}^\alpha$$

Operators become "more commutative"

$$\hat{S}^\alpha \hat{S}^\beta \to \lim_{S\to\infty} \langle \Omega | \hat{S}^\alpha \hat{S}^\beta | \Omega \rangle = \langle \Omega | \hat{S}^\alpha | \Omega \rangle \langle \Omega | \hat{S}^\beta | \Omega \rangle = s^\alpha s^\beta$$

Operators "factorize"

I. SU(*N*) Semiclassics

Landau-Lifshitz Equations

- Begin by assuming a product state of SU(2) coherent states.

$$|\Omega\rangle = \bigotimes_j |\Omega_j\rangle$$

- Derive equations of motion in the Heisenberg picture.

$$i\hbar \frac{d\hat{S}^{\alpha}}{dt} = \left[\hat{S}_j^{\alpha}, \hat{H}\left(\mathbf{S}\right)\right]$$

$$= i\hbar \epsilon_{\alpha\beta\gamma} \frac{\partial \hat{H}\left(\mathbf{S}\right)}{\partial \hat{S}_j^{\beta}} S_j^{\gamma}$$

I. SU(N) Semiclassics

Landau-Lifshitz Equations

- Next take the expectation value in a product of coherent states and evaluate in $S \to \infty$ limit.

$$\frac{d\langle\Omega_j|\hat{S}_j^\alpha|\Omega_j\rangle}{dt} = \epsilon_{\alpha\beta\gamma}\frac{\partial\langle\Omega|\hat{H}(\mathbf{S})|\Omega\rangle}{\partial\langle\Omega_j|\hat{S}_j^\beta|\Omega_j\rangle}\langle\Omega_j|\hat{S}_j^\gamma|\Omega_j\rangle$$

- After some notational adjustments, this becomes the Landau-Lifshitz equations.

$$\frac{d\mathbf{s}_j}{dt} = -\mathbf{s}_j \times \frac{dH_{\mathrm{cl}}(\mathbf{s})}{d\mathbf{s}_j}$$

I. SU(N) Semiclassics

Landau-Lifshitz Equations

- Next take the expectation value in a product of coherent states and evaluate in $S \to \infty$ limit.

$$\frac{d\langle\Omega_j|\hat{S}_j^\alpha|\Omega_j\rangle}{dt} = \boxed{\epsilon_{\alpha\beta\gamma}} \frac{\partial\langle\Omega|\hat{H}(\mathbf{S})|\Omega\rangle}{\partial\langle\Omega_j|\hat{S}_j^\beta|\Omega_j\rangle} \langle\Omega_j|\hat{S}_j^\gamma|\Omega_j\rangle$$

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$$\frac{d\mathbf{s}_j}{dt} = -\mathbf{s}_j \boxed{\times} \frac{dH_{\mathrm{cl}}(\mathbf{s})}{d\mathbf{s}_j}$$

I. SU(*N*) Semiclassics

- We can identify vector of expectation values with an operator.

$$\mathbf{s}_j \longrightarrow \mathfrak{n}_j = \sum_\alpha s_j^\alpha \hat{S}^\alpha \longrightarrow \rho_j = 2\mathfrak{n}_j + I/2$$

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$$\mathbf{s}_j \longrightarrow \mathfrak{n}_j = \sum_\alpha s_j^\alpha \hat{S}^\alpha \longrightarrow \rho_j = 2\mathfrak{n}_j + I/2$$

- We can similarly associate the gradient of the classical Hamiltonian with an operator.

$$\frac{dH_{\mathrm{cl}}(\mathbf{s})}{d\mathbf{s}_j} \longrightarrow \mathfrak{H}_j = \sum_\alpha \frac{dH_{\mathrm{cl}}}{ds_j^\alpha} \hat{S}^\alpha$$

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- We can similarly associate the gradient of the classical Hamiltonian with an operator.

$$\frac{dH_{\mathrm{cl}}(\mathbf{s})}{d\mathbf{s}_j} \longrightarrow \mathfrak{H}_j = \sum_\alpha \frac{dH_{\mathrm{cl}}}{ds_j^\alpha}\hat{S}^\alpha$$

- We can then consider time evolution *in the Schrödinger picture* via the Liouville-von Neumann equation

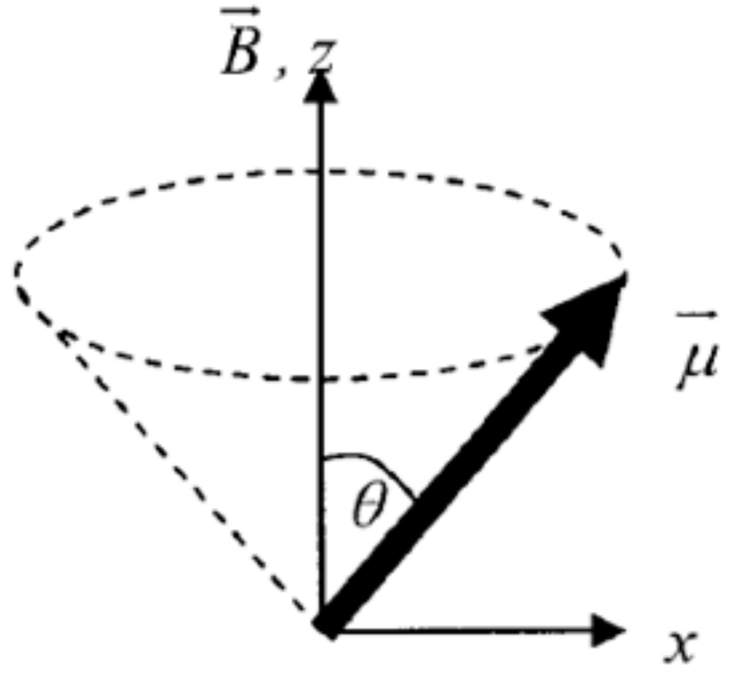
$$\frac{d\rho_j}{dt} = \mathrm{i}\left[\rho_j, \mathfrak{H}_j\right]$$

I. SU(*N*) Semiclassics

Landau-Lifshitz Equations in Schrödinger Picture

- Since evolving a pure state, reduces to an ordinary Schrödinger equation

$$\frac{d|\Omega_j\rangle}{dt} = -\mathrm{i}\mathfrak{H}_j|\Omega_j\rangle \qquad \mathfrak{H}_j = \sum_\alpha \frac{dH_{\mathrm{cl}}}{ds_j^\alpha}\hat{S}^\alpha$$



I. SU(N) Semiclassics

Landau-Lifshitz Equations in Schrödinger Picture

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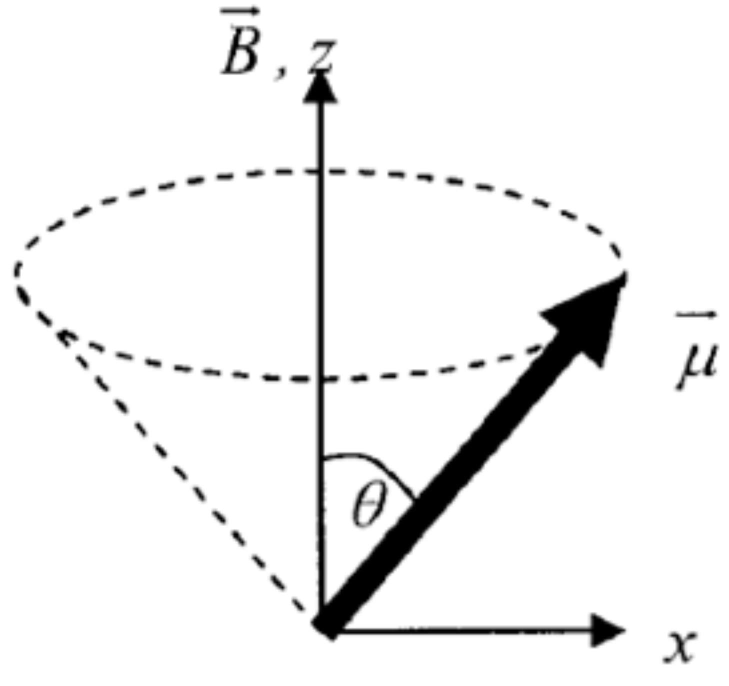
$$\frac{d|\Omega_j\rangle}{dt} = -\,\mathrm{i}\mathfrak{H}_j|\Omega_j\rangle \qquad \mathfrak{H}_j = \sum_\alpha \frac{dH_{\mathrm{cl}}}{ds_j^\alpha}\hat{S}^\alpha$$



$$\frac{d\mathbf{s}_j}{dt} = \frac{dH_{\mathrm{cl}}(\mathbf{s})}{d\mathbf{s}_j} \times \mathbf{s}_j$$

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DD, C. Miles, H. Zhang, C.D.Batista, K. Barros, "Langevin dynamics of generalized spins as SU(N) coherent states," PRB 106 (2022).

I. SU(*N*) Semiclassics

SU(*N*) Theory: coherent states

- Actions generated by exponentiating **linear combinations of generators**

$$U(c_\alpha) = e^{i\sum_\alpha c_\alpha \hat{T}^\alpha}$$

- Generate coherent states by applying to a **reference state**

$$|\Psi(c_\alpha)\rangle = U(c_\alpha)|\uparrow\rangle = e^{i\sum_\alpha c_\alpha \hat{T}^\alpha}|\uparrow\rangle$$

- The result of this process will become the **classical phase space**

$$CP^{N-1}$$

I. SU(*N*) semiclassics

SU(*N*) Theory: coherent states

- For large spins, very often will want to construct multipole operators.
- For example, a physical basis of generators of $SU(3)$ is given on the right.

Dipoles

$$\hat{T}^1 = \hat{S}^x$$
$$\hat{T}^2 = \hat{S}^y$$
$$\hat{T}^3 = \hat{S}^z$$

Quadrupoles

$$\hat{T}^4 = -\left(\hat{S}^x\hat{S}^z + \hat{S}^z\hat{S}^x\right)$$
$$\hat{T}^5 = -\left(\hat{S}^y\hat{S}^z + \hat{S}^z\hat{S}^y\right)$$
$$\hat{T}^6 = \left(\hat{S}^x\right)^2 - \left(\hat{S}^y\right)^2$$
$$\hat{T}^7 = \hat{S}^x\hat{S}^y + \hat{S}^y\hat{S}^x$$
$$\hat{T}^8 = \sqrt{3}\left(\hat{S}^z\right)^2 - \frac{2}{\sqrt{3}}$$

SU(*N*) coherent states

Sources of SU(*N*) generators (observables)

- There also exist many canonical bases, such as the Stevens operators.

Table 1: Extended Stevens operators $\hat{O}_k^q$.

k	q	O_k^q
2	0	$3S_z^2 - s\mathbb{I}$
	±1	$c_\pm[S_z, S_+ \pm S_-]_+$
	±2	$c_\pm(S_+^2 \pm S_-^2)$
4	0	$35S_z^4 - (30s-25)S_z^2 + (3s^2-6s)\mathbb{I}$
	±1	$c_\pm[7S_z^3 - (3s+1)S_z, S_+ \pm S_-]_+$
	±2	$c_\pm[7S_z^2 - (s+5)\mathbb{I}, S_+^2 \pm S_-^2]_+$
	±3	$c_\pm[S_z, S_+^3 \pm S_-^3]_+$
	±4	$c_\pm(S_+^4 \pm S_-^4)$
6	0	$231S_z^6 - (315s-735)S_z^4 + (105s^2 - 525s + 294)S_z^2 - (5s^3 - 40s^2 + 60s)\mathbb{I}$
	±1	$c_\pm[33S_z^5 - (30s-15)S_z^3 + (5s^2 - 10s + 12)S_z, S_+ \pm S_-]_+$
	±2	$c_\pm[33S_z^4 - (18s+123)S_z^2 + (s^2 + 10s + 102)\mathbb{I}, S_+^2 \pm S_-^2]_+$
	±3	$c_\pm[11S_z^3 - (3s+59)S_z, S_+^3 \pm S_-^3]_+$
	±4	$c_\pm[11S_z^2 - (s+38)\mathbb{I}, S_+^4 \pm S_-^4]_+$
	±5	$c_\pm[S_z, S_+^5 \pm S_-^5]_+$
	±6	$c_\pm(S_+^6 \pm S_-^6)$

$[A, B]_+$ indicates the symmetrized product $(AB + BA)/2$, and $s = S(S+1)$, $c_+ = 1/2$, $c_- = 1/2\mathrm{i}$.

Source: https://easyspin.org/documentation/stevensoperators.html

I. SU(*N*) semiclassics

Sources of SU(*N*) generators (observables)

- There also exist many canonical bases, such as the Stevens operators.

- For our purposes, generally not necessary to pick any specific operator basis.

Table 1: Extended Stevens operators $\hat{O}_k^q$.

k	q	O_k^q
2	0	$3S_z^2 - s\mathbb{I}$
	±1	$c_\pm\left[S_z, S_+ \pm S_-\right]_+$
	±2	$c_\pm(S_+^2 \pm S_-^2)$
4	0	$35S_z^4 - (30s-25)S_z^2 + (3s^2-6s)\mathbb{I}$
	±1	$c_\pm\left[7S_z^3 - (3s+1)S_z, S_+ \pm S_-\right]_+$
	±2	$c_\pm\left[7S_z^2 - (s+5)\mathbb{I}, S_+^2 \pm S_-^2\right]_+$
	±3	$c_\pm\left[S_z, S_+^3 \pm S_-^3\right]_+$
	±4	$c_\pm(S_+^4 \pm S_-^4)$
6	0	$231S_z^6 - (315s-735)S_z^4 + (105s^2-525s+294)S_z^2 - (5s^3-40s^2+60s)\mathbb{I}$
	±1	$c_\pm\left[33S_z^5 - (30s-15)S_z^3 + (5s^2-10s+12)S_z, S_+ \pm S_-\right]_+$
	±2	$c_\pm\left[33S_z^4 - (18s+123)S_z^2 + (s^2+10s+102)\mathbb{I}, S_+^2 \pm S_-^2\right]_+$
	±3	$c_\pm\left[11S_z^3 - (3s+59)S_z, S_+^3 \pm S_-^3\right]_+$
	±4	$c_\pm\left[11S_z^2 - (s+38)\mathbb{I}, S_+^4 \pm S_-^4\right]_+$
	±5	$c_\pm\left[S_z, S_+^5 \pm S_-^5\right]_+$
	±6	$c_\pm(S_+^6 \pm S_-^6)$

$[A,B]_+$ indicates the symmetrized product $(AB+BA)/2$, and $s = S(S+1)$, $c_+ = 1/2$, $c_- = 1/2\mathrm{i}$.

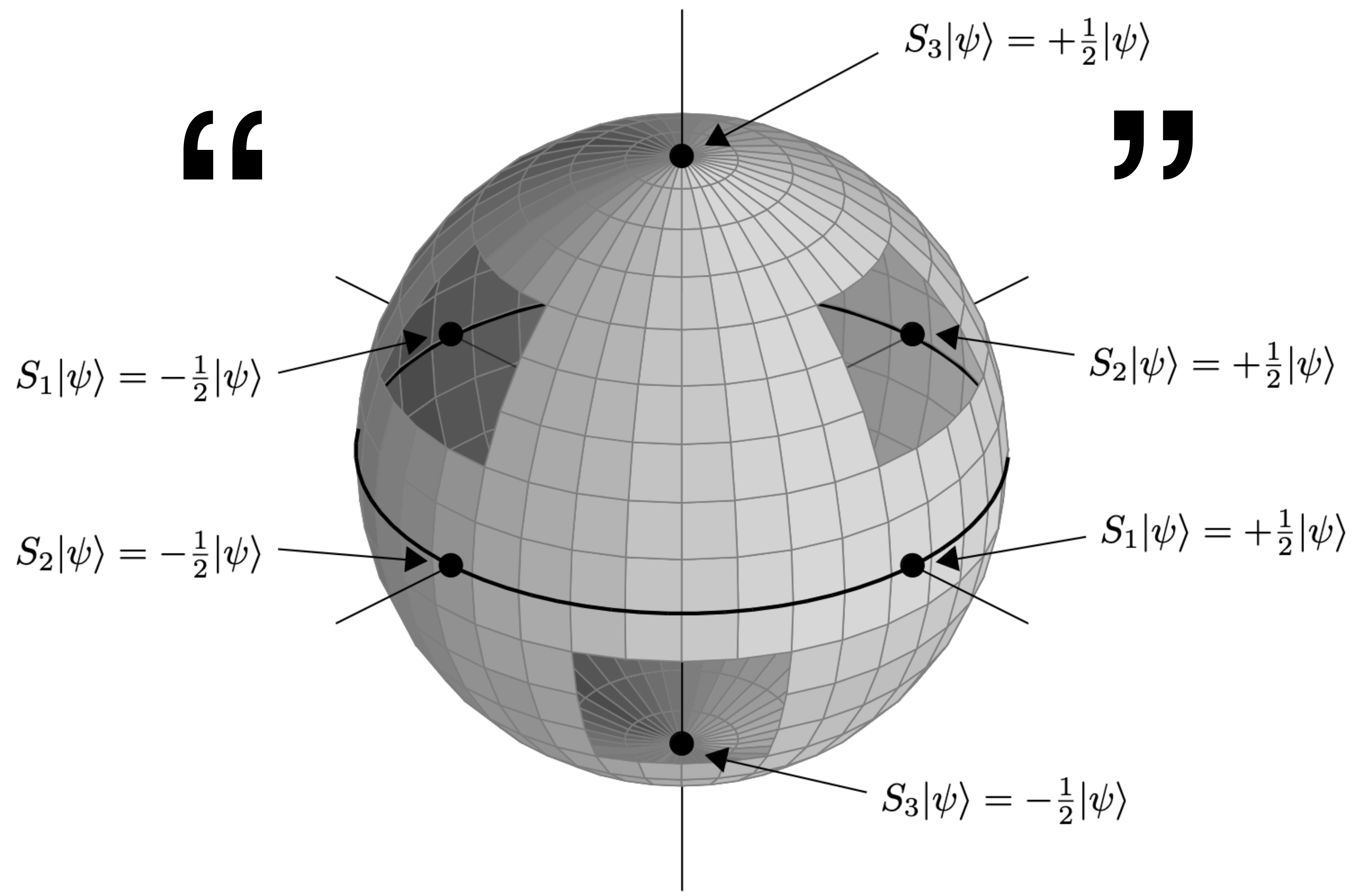
Source: https://easyspin.org/documentation/stevensoperators.html

I. SU(*N*) semiclassics

$CP^1 \rightarrow CP^{N-1}$

- There is a correspondence between all these states (and any N-level state) with points on a sphere on CP^{N-1}

"



"

$$|\Psi\rangle \leftrightarrow \langle\Psi|\hat{T}^\alpha|\Psi\rangle \equiv n^\alpha$$

SU(N) coherent state ⟵ One-to-one correspondence ⟶ Real (N^2-1) vector on CP^{N-1}

I. SU(*N*) semiclassics

- Send $M \to \infty$ and $\hbar \to 0$ (while holding $\hbar M$ constant)
  - Operators become more commutative
  - SU(*N*) coherent states become more orthogonal
  - A factorization rule obtains
  - Regardless of representation, get the same dynamics on the same manifold

I. SU(*N*) semiclassics

- Begin by assuming a product state of SU(*N*) coherent states.

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

- Derive equations of motion in the Heisenberg picture.

$$i\hbar \frac{d\hat{T}^\alpha}{dt} = \left[\hat{T}_j^\alpha, \hat{H}(\mathbf{T})\right]$$

$$= i\hbar f_{\alpha\beta\gamma} \frac{\partial \hat{H}(\mathbf{T})}{\partial \hat{T}_j^\beta} \hat{T}_j^\gamma$$

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I. SU(N) semiclassics

- Next take the expectation value in a product of coherent states and evaluate in $M \to \infty$ limit.

$$\frac{d\langle \Omega_j | \hat{T}_j^\alpha | \Omega_j \rangle}{dt} = f_{\alpha\beta\gamma} \frac{\partial \langle \Omega | \hat{H}(\mathbf{T}) | \Omega \rangle}{\partial \langle \Omega_j | \hat{T}_j^\beta | \Omega_j \rangle} \langle \Omega_j | \hat{T}_j^\gamma | \Omega_j \rangle$$

- After some notational adjustments, this becomes the Generalized Landau-Lifshitz equations.

$$\frac{d\mathbf{n}_j}{dt} = -\,\mathbf{n}_j \star \frac{dH_{\text{cl}}(\mathbf{n})}{d\mathbf{n}_j}$$

I. SU(*N*) semiclassics

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$$\frac{d\langle\Omega_j|\hat{T}_j^\alpha|\Omega_j\rangle}{dt} = f_{\alpha\beta\gamma}\frac{\partial\langle\Omega|\hat{H}(\mathbf{T})|\Omega\rangle}{\partial\langle\Omega_j|\hat{T}_j^\beta|\Omega_j\rangle}\langle\Omega_j|\hat{T}_j^\gamma|\Omega_j\rangle$$

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H. Zhang and C. Batista, “Classical spin dynamics based on SU(N) coherent states,” PRB 104 (2021).

I. SU(N) semiclassics

- Recall we can identify vector of expectation values with an operator.

$$\mathbf{n}_j \longrightarrow \mathfrak{n}_j = \sum_\alpha n_j^\alpha \hat{T}^\alpha \longrightarrow \rho_j = \mathfrak{n}_j/\tau + cI$$

- We can similarly associate the gradient of the classical Hamiltonian with an operator.

$$\frac{dH_{\text{cl}}(\mathbf{n})}{d\mathbf{n}_j} \longrightarrow \mathfrak{H}_j = \sum_\alpha \frac{dH_{\text{cl}}}{dn_j^\alpha}\hat{T}^\alpha$$

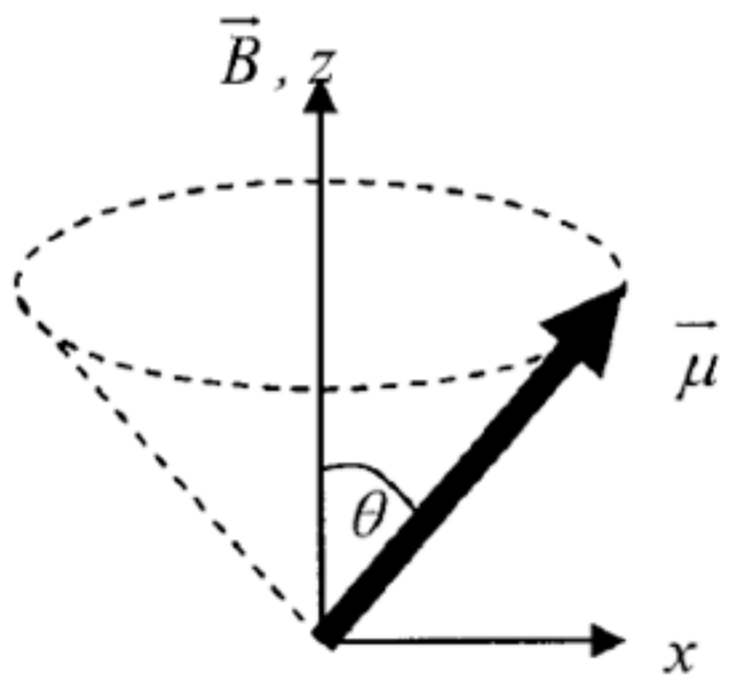
- We can then consider time evolution *in the Schrödinger picture* via the Liouville-von Neumann equation

$$\frac{d\rho_j}{dt} = \mathrm{i}\left[\rho_j, \mathfrak{H}_j\right]$$

I. SU(*N*) semiclassics

- Since evolving a pure state, reduces to an ordinary Schrödinger equation

$$\frac{d|\Omega_j\rangle}{dt} = -\mathrm{i}\mathfrak{H}_j|\Omega_j\rangle \qquad \mathfrak{H}_j = \sum_\alpha \frac{dH_{\mathrm{cl}}}{dn_j^\alpha}\hat{T}^\alpha$$



$$\frac{d\mathbf{n}_j}{dt} = -\mathbf{n}_j \star \frac{dH_{\mathrm{cl}}(\mathbf{n})}{d\mathbf{n}_j}$$

DD, C. Miles, H. Zhang, C.D.Batista, K. Barros, "Langevin dynamics of generalized spins as SU(N) coherent states," PRB 106 (2022).

I. SU(N) semiclassics

“Nonlinear” terms — onsite

- Recall our simple, single-site, $S = 1$ Hamiltonian:

$$\hat{H} = D\left(\hat{S}^z\right)^2$$

$$= D\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

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

$$\langle 0 | \hat{H} | 0 \rangle = 0$$

I. SU(*N*) semiclassics

"Nonlinear" terms — onsite

- Now consider dynamics for $\hat{H} = D\left(\hat{S}^z\right)^2$, recalling $(\hat{S}^z)^2 = \sum_\alpha c_\alpha \hat{T}^\alpha$

Classical Hamiltonian

$$
\begin{aligned}
H_{\text{cl}} &= \lim_{M\to\infty} D\langle\Omega\,|\,(\hat{S}^z)^2\,|\,\Omega\rangle \\
&= D\sum_\alpha c_\alpha \lim_{M\to\infty} \langle\Psi\,|\,\hat{T}^\alpha\,|\,\Psi\rangle \\
&= D\sum_\alpha c_\alpha n^\alpha
\end{aligned}
$$

I. SU(*N*) semiclassics

"Nonlinear" terms — onsite

- Now consider dynamics for $\hat{H} = D\left(\hat{S}^z\right)^2$, recalling $(\hat{S}^z)^2 = \sum_\alpha c_\alpha \hat{T}^\alpha$

Classical Hamiltonian

$$H_{\mathrm{cl}} = \lim_{M\to\infty} D\langle\Omega\,|\,(\hat{S}^z)^2\,|\,\Omega\rangle$$

$$= D\sum_\alpha c_\alpha \lim_{M\to\infty}\langle\Psi\,|\,\hat{T}^\alpha\,|\,\Psi\rangle$$

$$= D\sum_\alpha c_\alpha n^\alpha$$

SU(3) Effective Field

$$\frac{dH_{cl}}{dn^\alpha} = Dc_\alpha$$

$$\mathfrak{H} = \sum_\alpha \frac{dH_{cl}}{dn^\alpha}\hat{T}^\alpha$$

$$= D\sum_\alpha c_\alpha \hat{T}^\alpha$$

I. SU(N) semiclassics

"Nonlinear" terms — onsite

- Now consider dynamics for $\hat{H} = D\left(\hat{S}^z\right)^2$, recalling $(\hat{S}^z)^2 = \sum_\alpha c_\alpha \hat{T}^\alpha$

Classical Hamiltonian

$$H_{\mathrm{cl}} = \lim_{M\to\infty} D\langle\Omega|(\hat{S}^z)^2|\Omega\rangle$$
$$= D\sum_\alpha c_\alpha \lim_{M\to\infty}\langle\Psi|\hat{T}^\alpha|\Psi\rangle$$
$$= D\sum_\alpha c_\alpha n^\alpha$$

SU(3) Effective Field

$$\frac{dH_{cl}}{dn^\alpha} = Dc_\alpha$$
$$\mathfrak{H} = \sum_\alpha \frac{dH_{cl}}{dn^\alpha}\hat{T}^\alpha$$
$$= D\sum_\alpha c_\alpha \hat{T}^\alpha$$

Equations of Motion

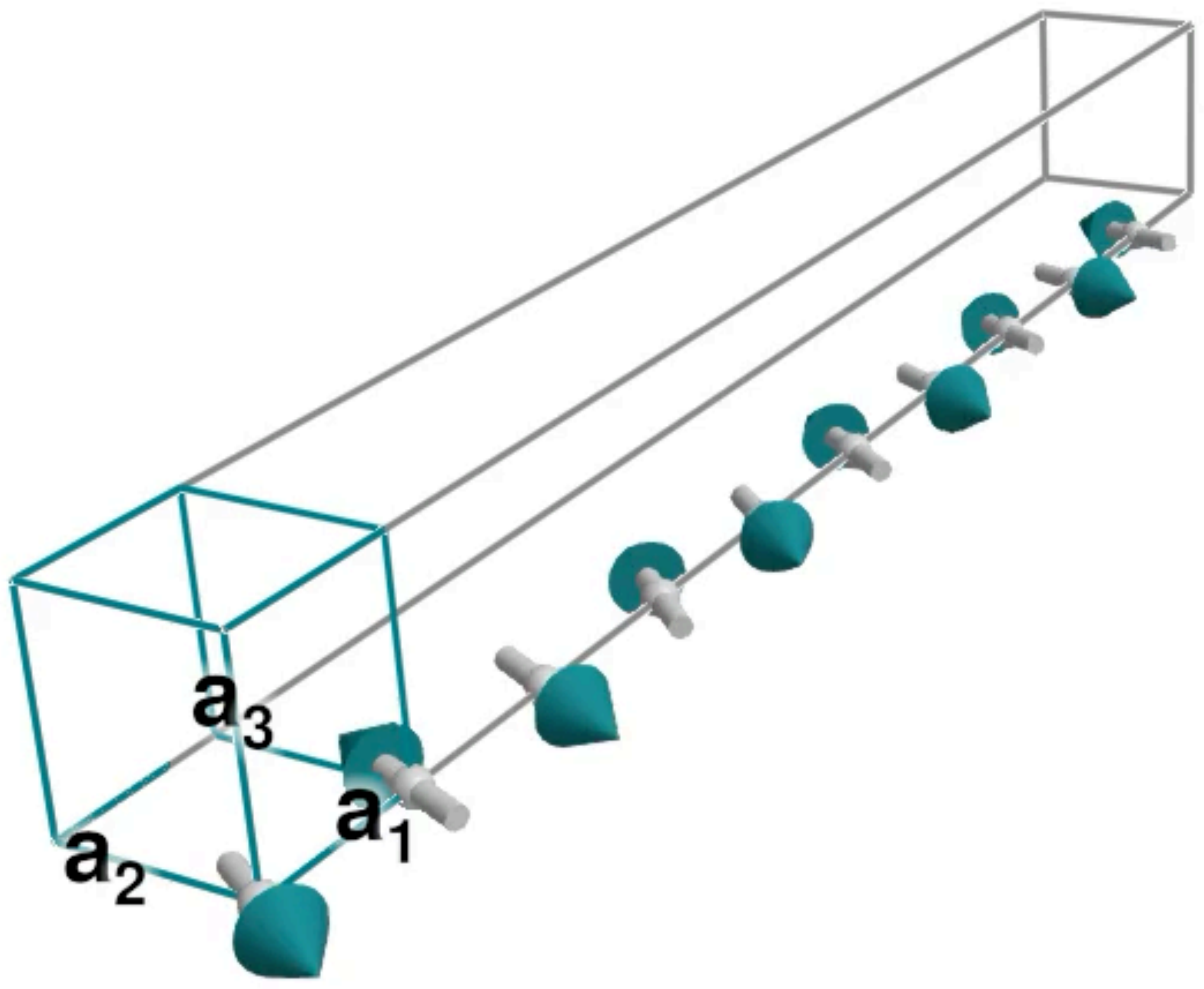
$$\frac{d\mathbf{Z}}{dt} = -\mathrm{i}\mathfrak{H}\mathbf{Z}$$

$$\frac{d}{dt}\begin{pmatrix} z_1 \\ z_2 \\ z_3 \end{pmatrix} = -\mathrm{i}\begin{pmatrix} D & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & D \end{pmatrix}\begin{pmatrix} z_1 \\ z_2 \\ z_3 \end{pmatrix}$$

I. SU(*N*) semiclassics

$SU(2), \quad S \to \infty$ **limit**

$$\hat{\mathscr{H}} = J \sum_{j,\delta} \hat{S}_j^{\alpha} \hat{S}_{j+\delta}^{\alpha} + D \sum_j \left(\hat{S}_j^z\right)^2$$

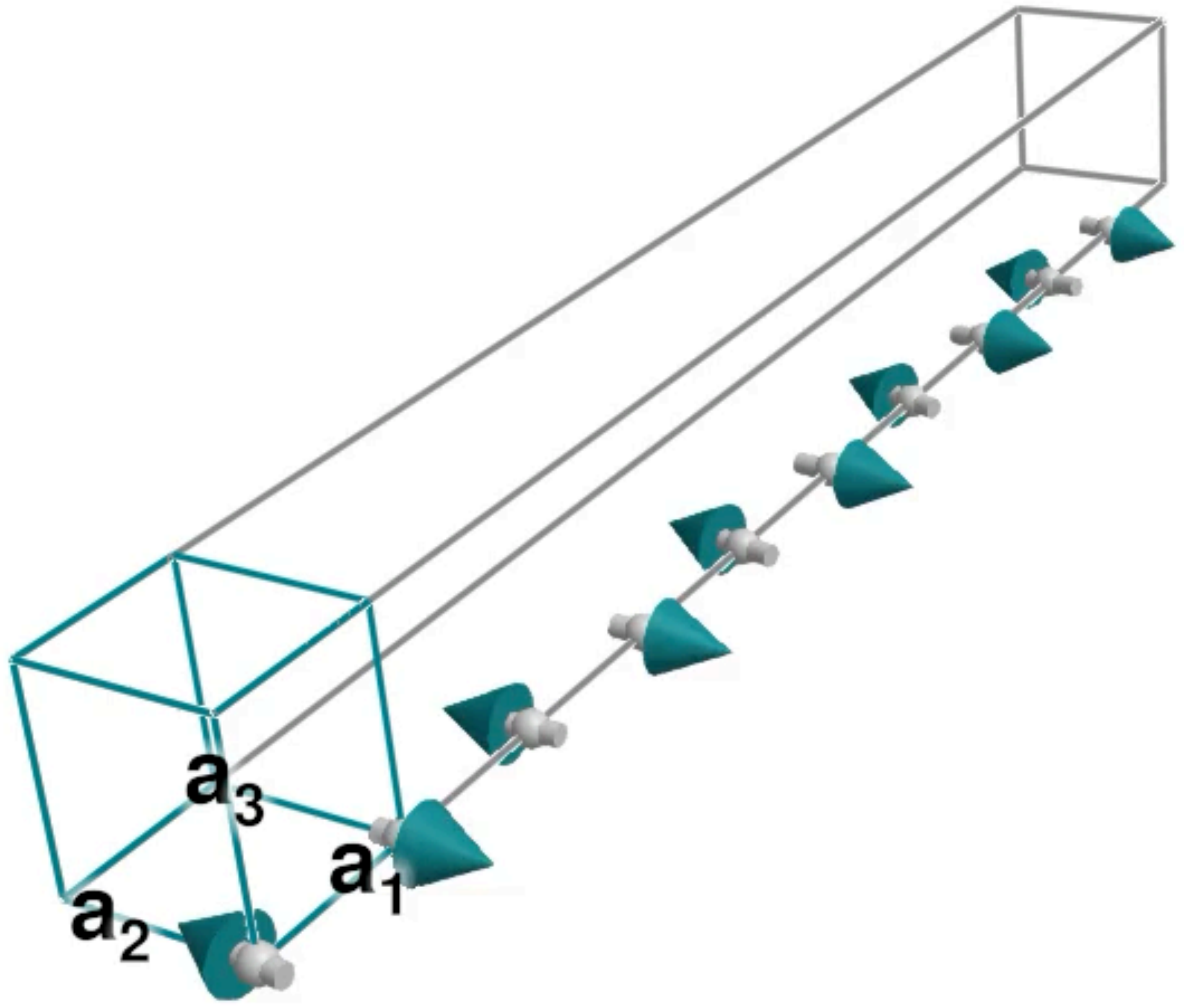


$$\mathfrak{H}_{j,S\to\infty} = J\left(s_{j-1}^x + s_{j+1}^x\right)\hat{S}_j^x + J\left(s_{j-1}^y + s_{j+1}^y\right)\hat{S}^y + \left[J\left(s_{j-1}^z + s_{j+1}^z\right) + 2Ds_j^z\right]\hat{S}^z$$

I. SU(*M*) semiclassics

$SU(3), \quad M \to \infty$ **limit**

$$\hat{\mathscr{H}} = J \sum_{j,\delta} \hat{S}_j^{\alpha} \hat{S}_{j+\delta}^{\alpha} + D \sum_j \left(\hat{S}_j^z \right)^2$$



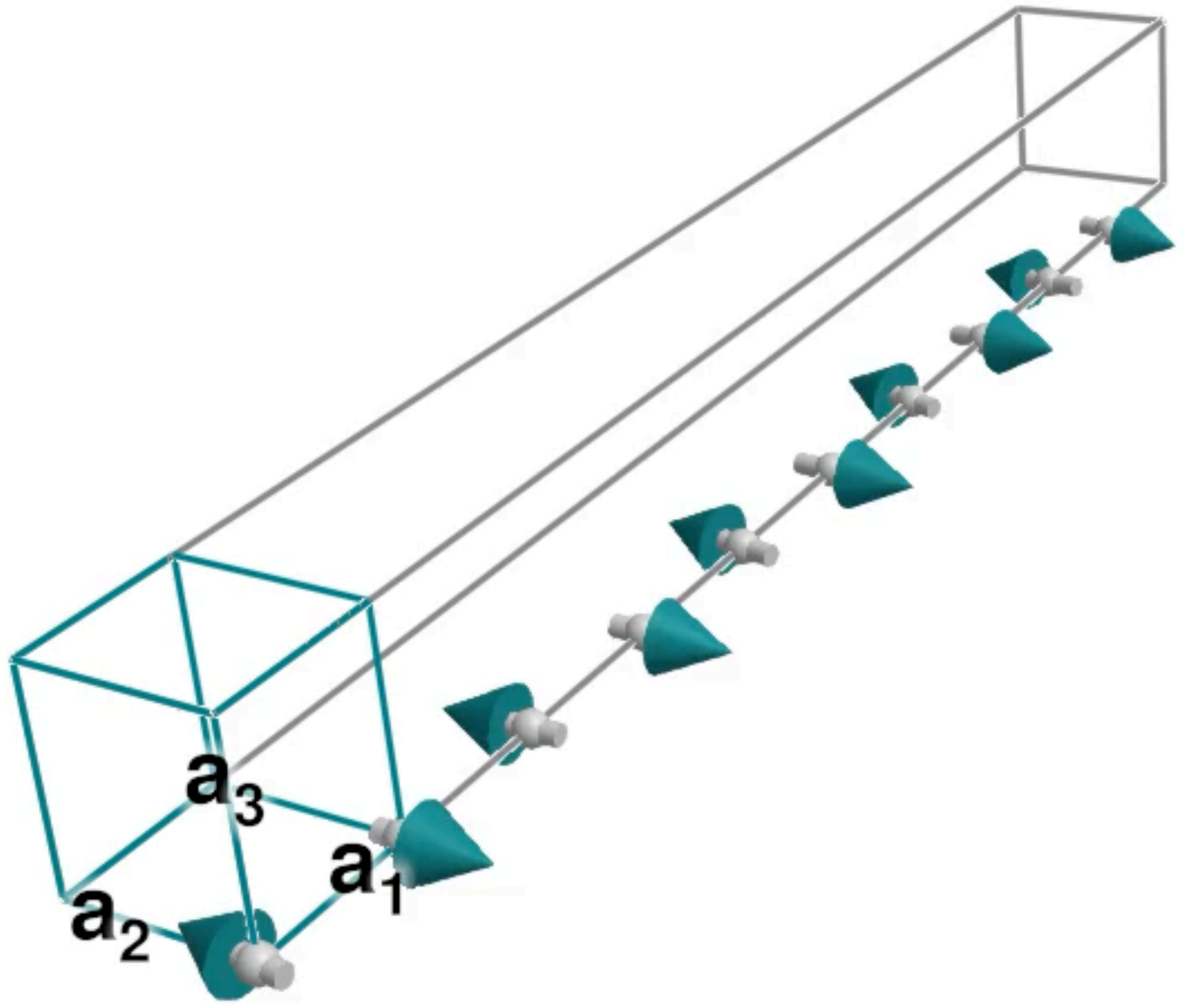
$$\mathfrak{H}_{j,M\to\infty} = J \left(s_{j-1}^x + s_{j+1}^x \right) \hat{S}_j^x + J \left(s_{j-1}^y + s_{j+1}^y \right) \hat{S}^y + \left[J \left(s_{j-1}^z + s_{j+1}^z \right) + 2D \right] \hat{S}^z$$

I. SU(*M*) semiclassics

$SU(3), \quad M \to \infty$ **limit**

$$\hat{\mathcal{H}} = J \sum_{j,\delta} \hat{S}_j^{\alpha} \hat{S}_{j+\delta}^{\alpha} + D \sum_j \left(\hat{S}_j^z \right)^2$$

$$\mathfrak{H}_{j,M\to\infty} = \mathfrak{H}_{j,\mathrm{exch}}(t) + D(\hat{S}^z)^2$$



I. SU(*N*) semiclassics

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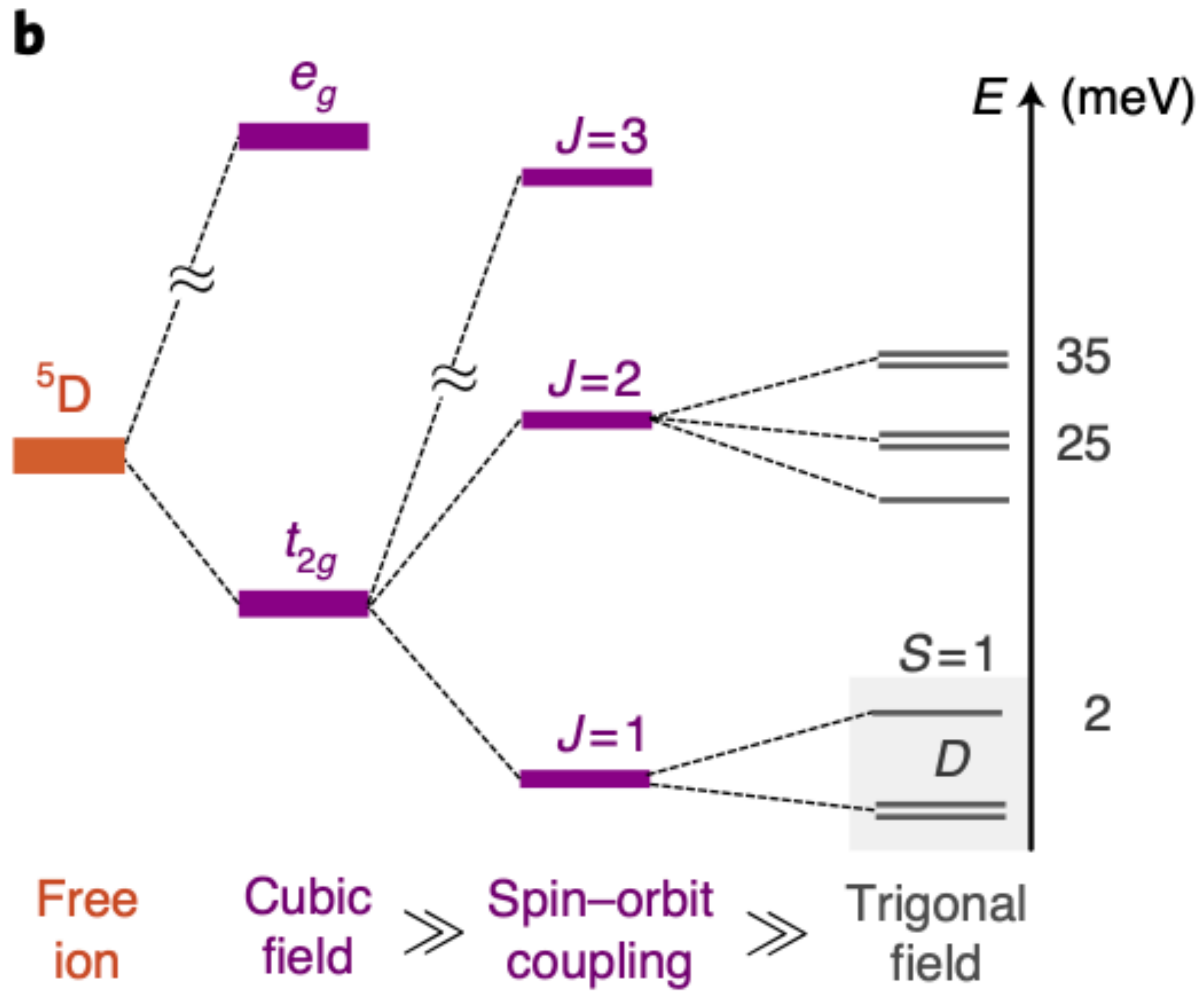
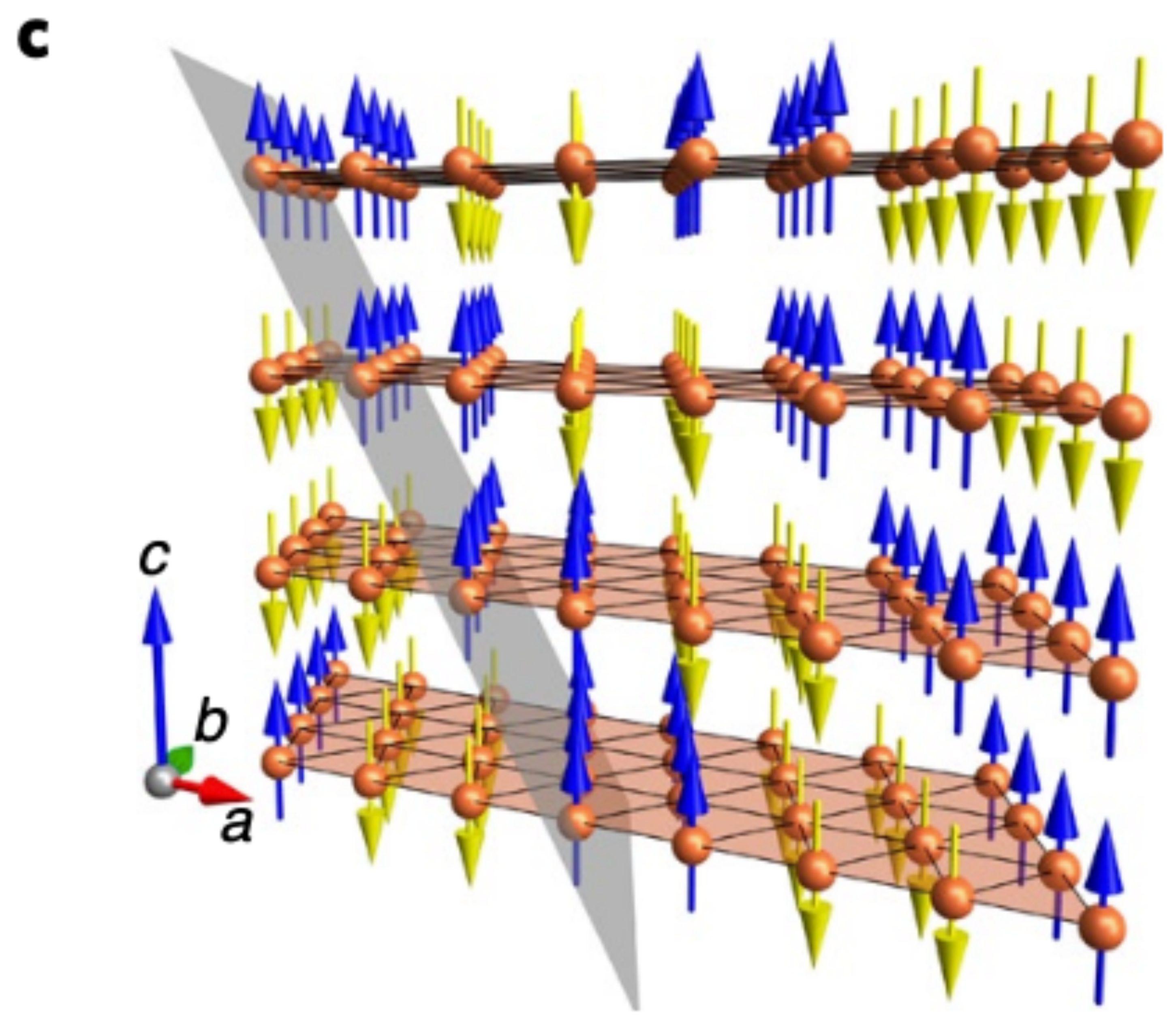
II. Applications of SU(*N*) dynamics

FeI_2 at finite temperature

$$\mathcal{H} = \sum_{\langle ij \rangle} \sum_{\mu\nu} S_i^\mu \mathcal{J}_{ij}^{\mu\nu} S_j^\nu - D \sum_i Q_i^{zz}$$

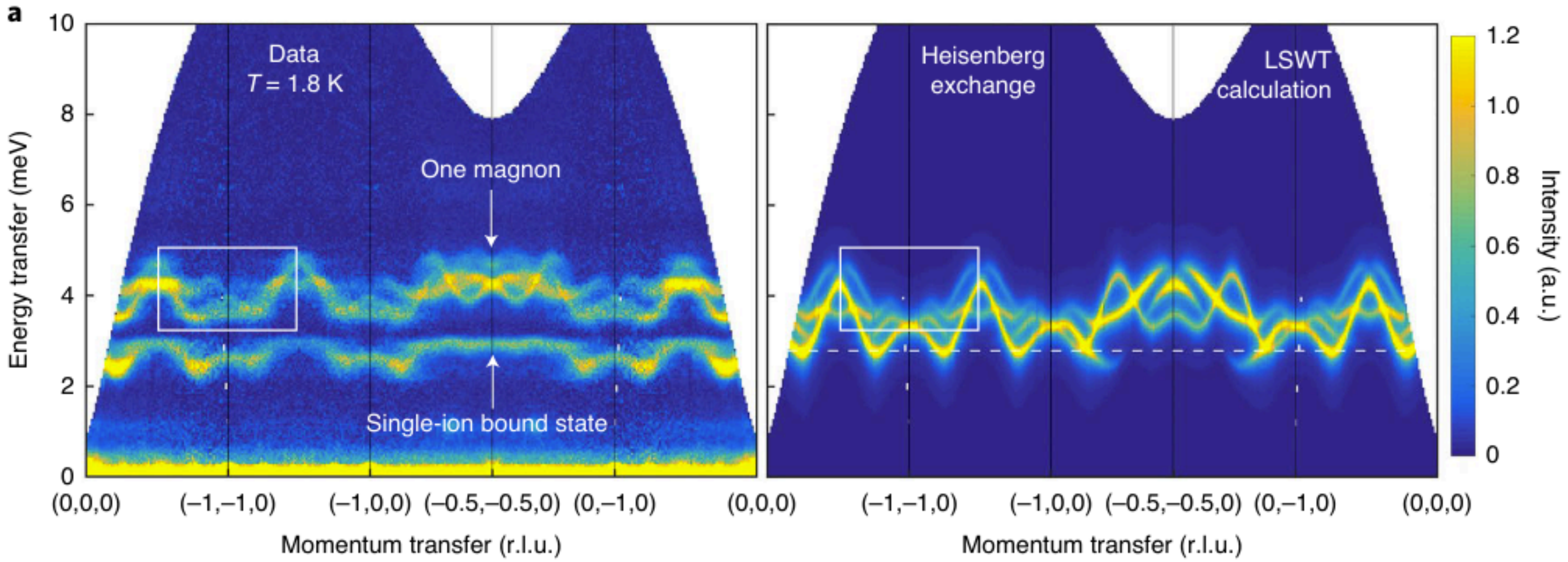




Xiaojian Bai et al. “Hybridized quadrupolar excitations…”, Nature Physics (2021).

II. Applications of SU(*N*) dynamics

FeI_2 at finite temperature



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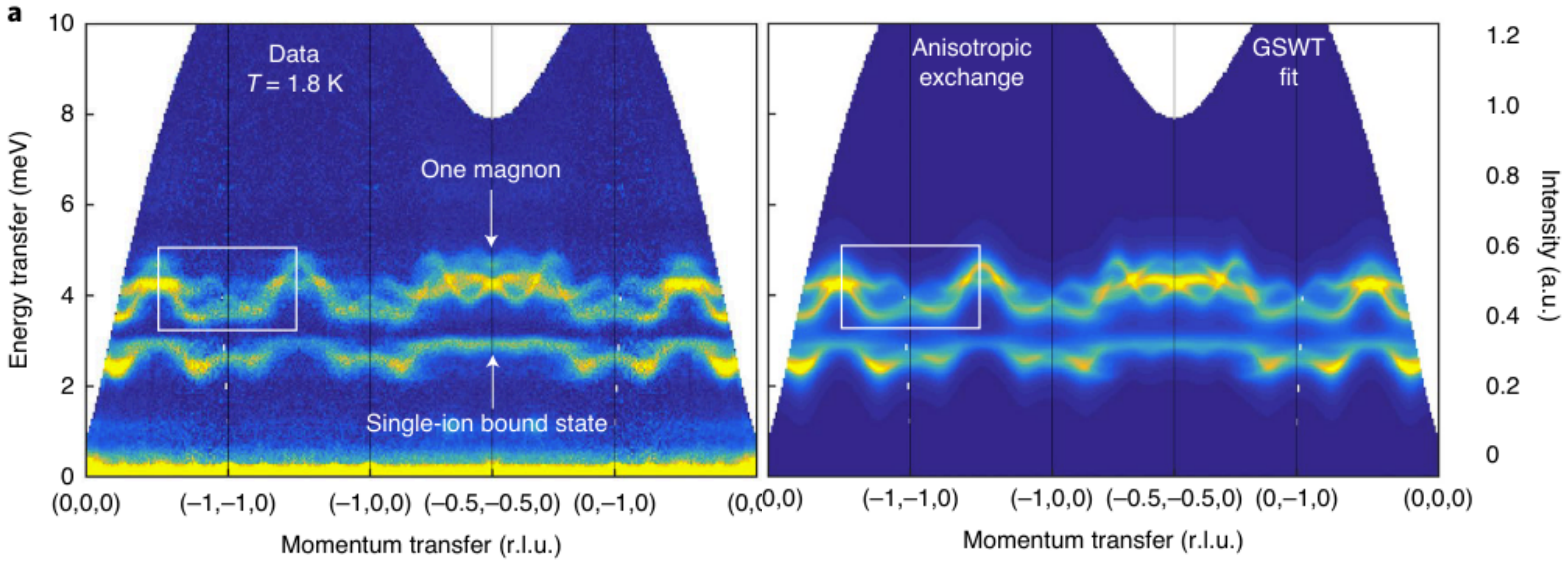
FeI_2 at finite temperature



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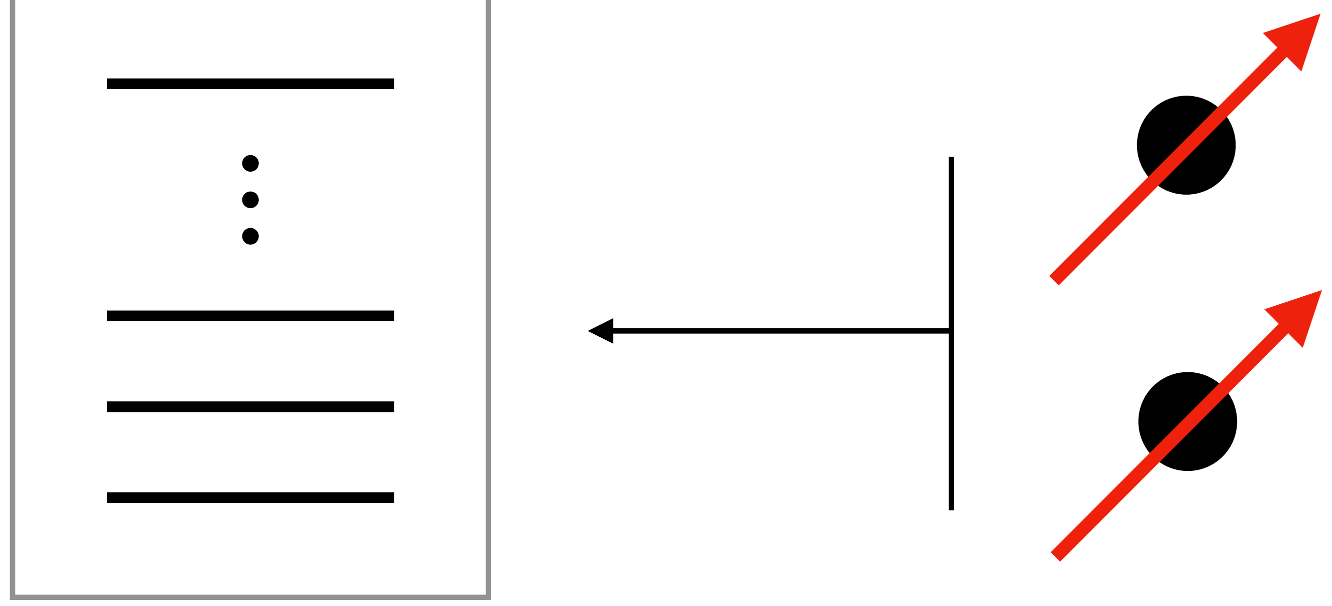
II. Applications of SU(N) dynamics

Capturing local entanglement effects

- When performing a product space decomposition in terms of sites, we systematically neglect entanglement between sites.
- Can instead decompose into dimers, trimers, etc.

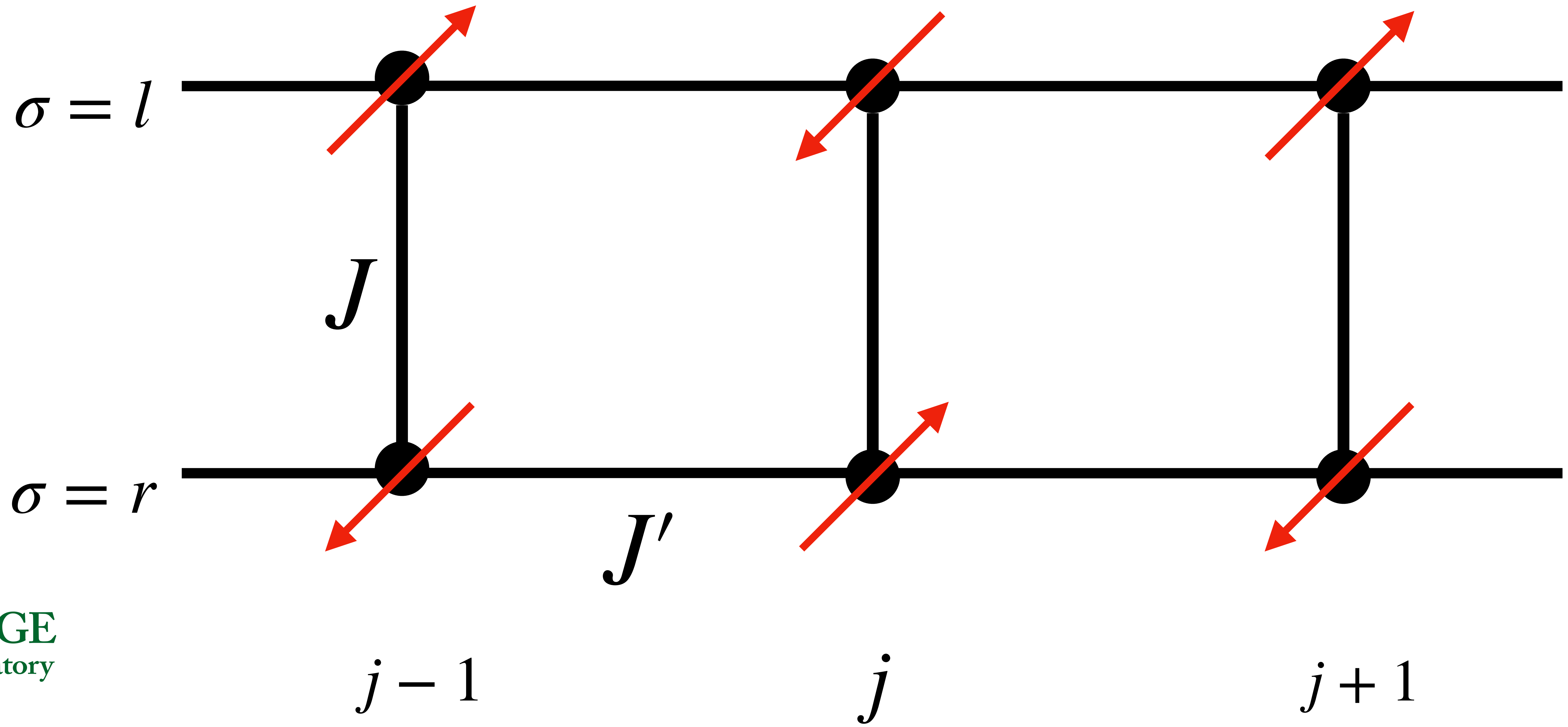


II. Applications of SU(*N*) dynamics

Capturing local entanglement effects

- AFM $S = 1/2$ spin ladder

$$\hat{\mathcal{H}} = J \sum_j \hat{S}^{\beta}_{j,l} \hat{S}^{\beta}_{j,r} + J' \sum_j \left(\hat{S}^{\beta}_{j,l} \hat{S}^{\beta}_{j+1,l} + \hat{S}^{\beta}_{j,r} \hat{S}^{\beta}_{j+1,r} \right)$$



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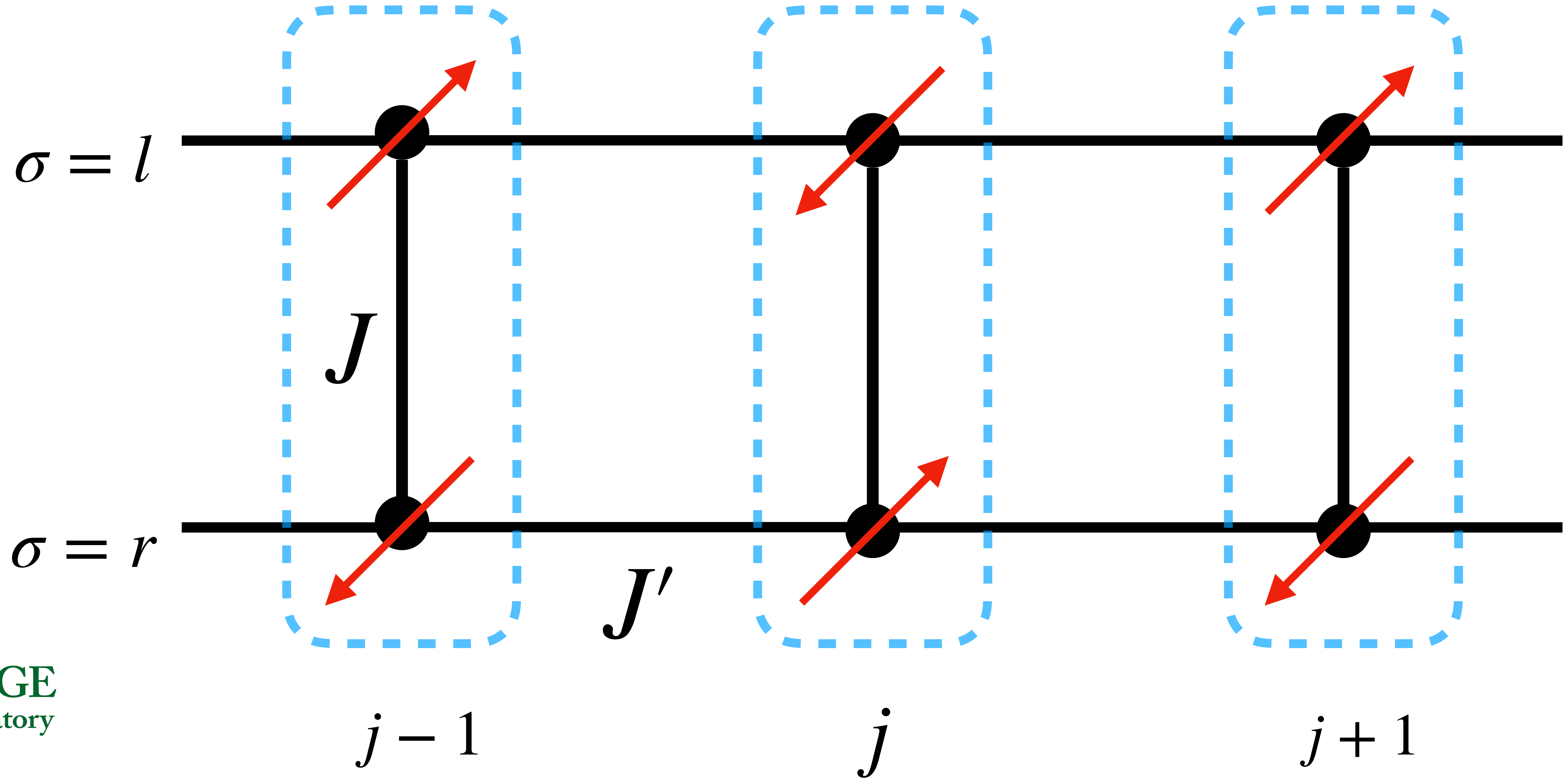


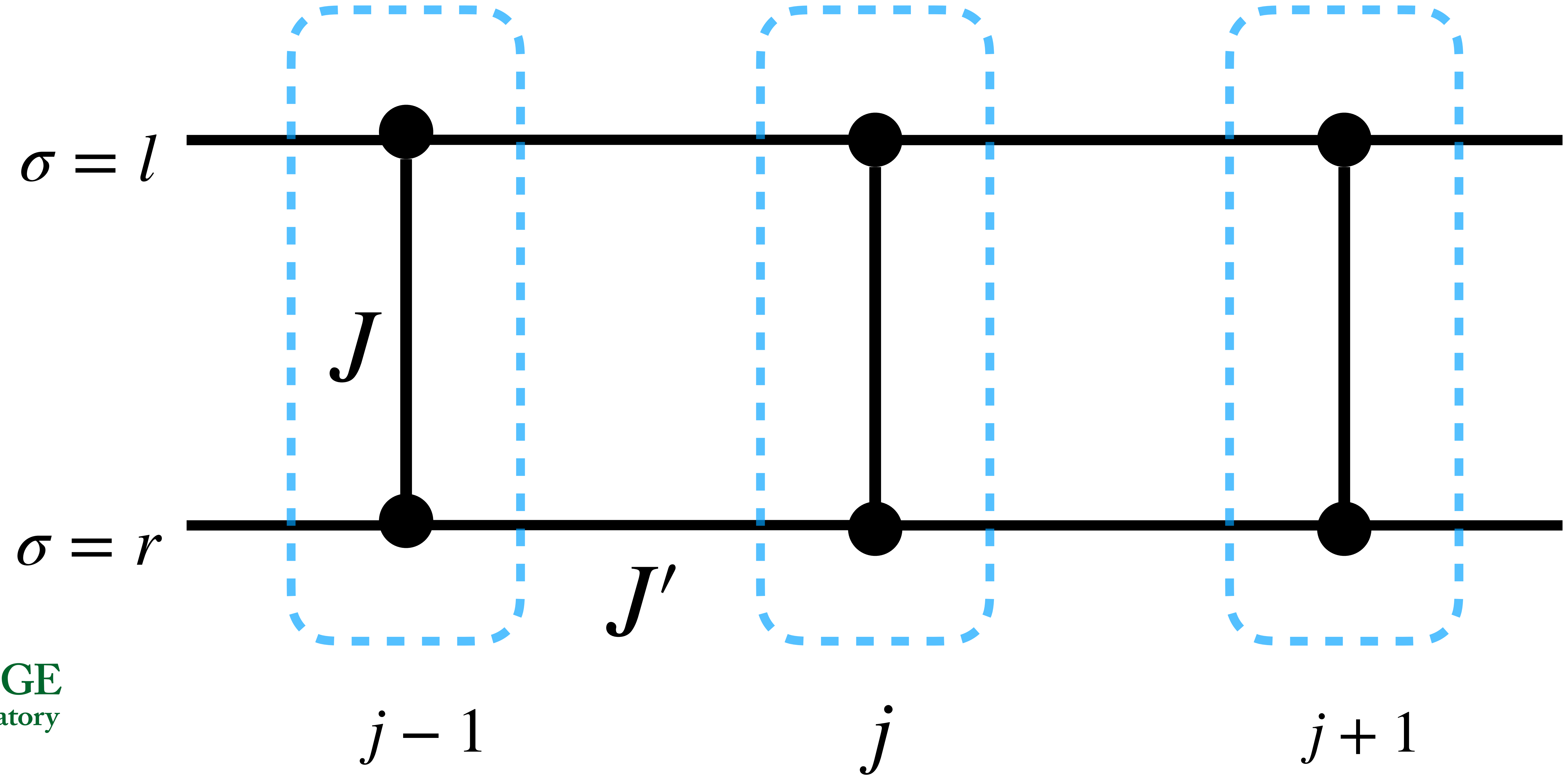
$J' < J$

II. Applications of SU(N) dynamics

Capturing local entanglement effects

- AFM $S = 1/2$ spin ladder

$$\hat{\mathcal{H}} = J\sum_j \hat{S}^{\beta}_{j,l}\hat{S}^{\beta}_{j,r} + J'\sum_j \left(\hat{S}^{\beta}_{j,l}\hat{S}^{\beta}_{j+1,l} + \hat{S}^{\beta}_{j,r}\hat{S}^{\beta}_{j+1,r}\right)$$

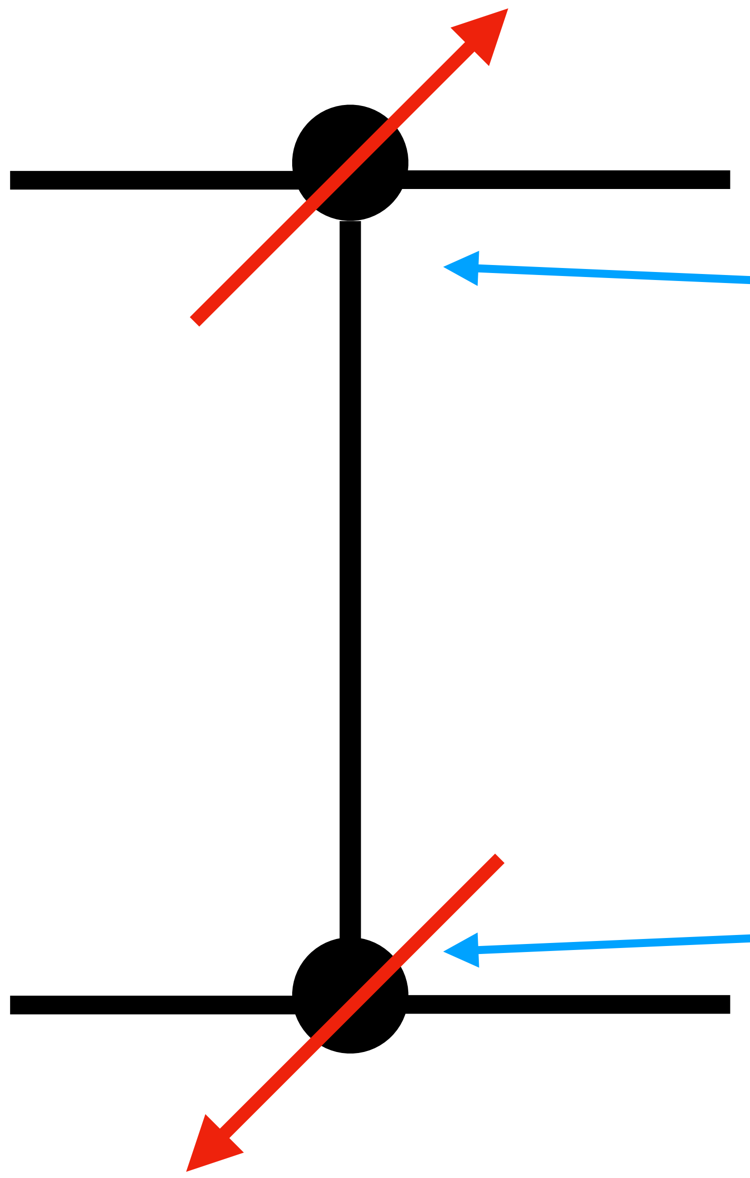


$J' < J$

II. Applications of SU(*N*) dynamics

Capturing local entanglement effects

- In the traditional approach, decomposed into two spin-1/2: $\mathbb{C}^2 \oplus \mathbb{C}^2$



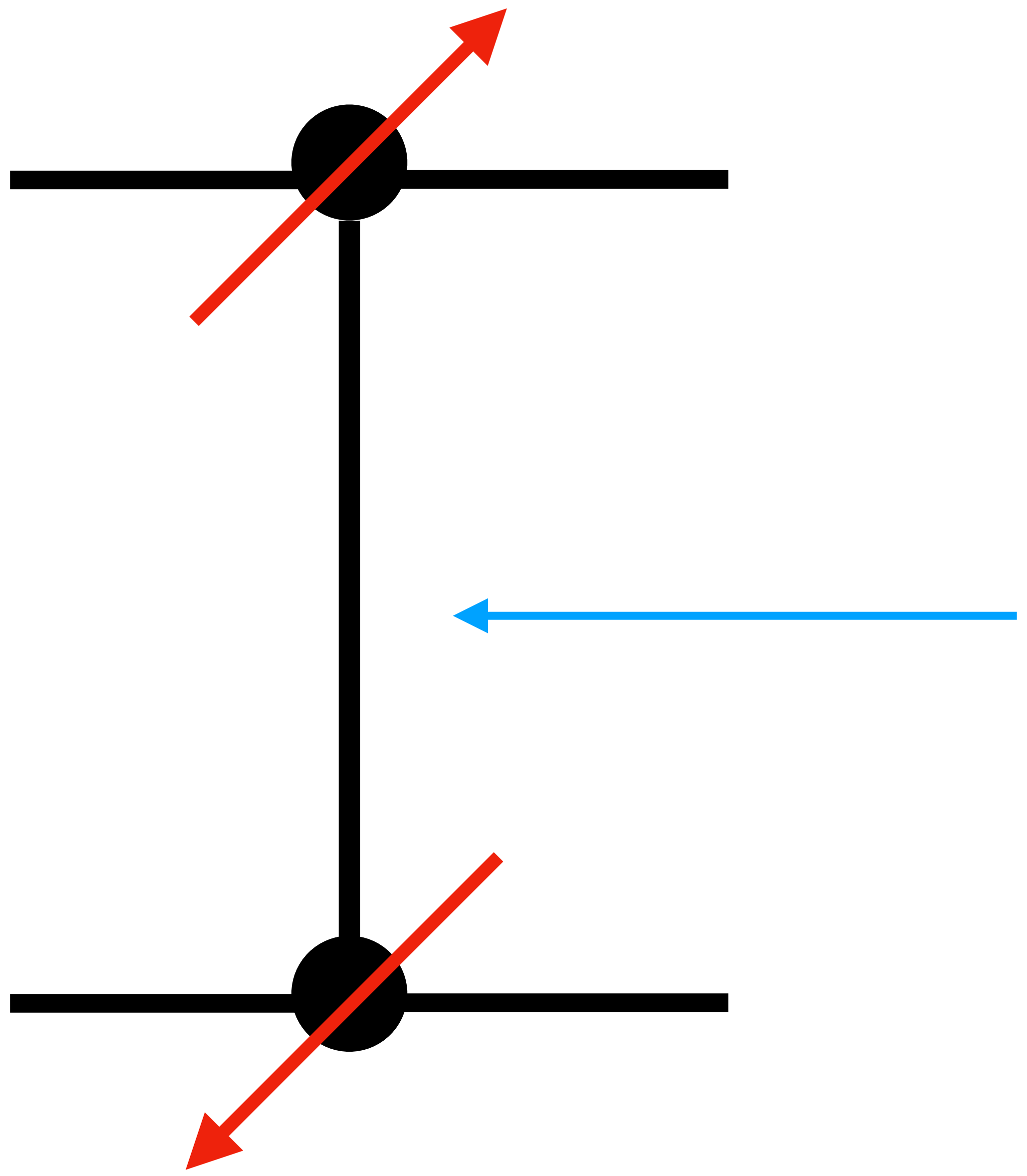
$$\begin{pmatrix} \alpha_{j,l} \\ \beta_{j,l} \end{pmatrix} = \alpha_{j,l} | \uparrow \rangle + \beta_{j,l} | \downarrow \rangle$$

$$\begin{pmatrix} \alpha_{j,r} \\ \beta_{j,r} \end{pmatrix} = \alpha_{j,r} | \uparrow \rangle + \beta_{j,r} | \downarrow \rangle$$

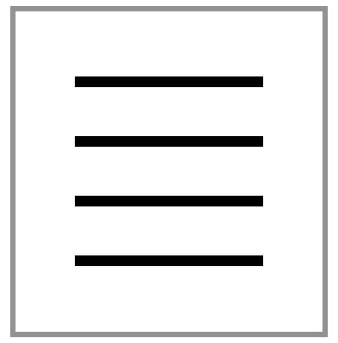
II. Applications of SU(N) dynamics

Capturing local entanglement effects

- Here we instead we decompose based on bonds: $\mathbb{C}^2 \otimes \mathbb{C}^2 = \mathbb{C}^4$

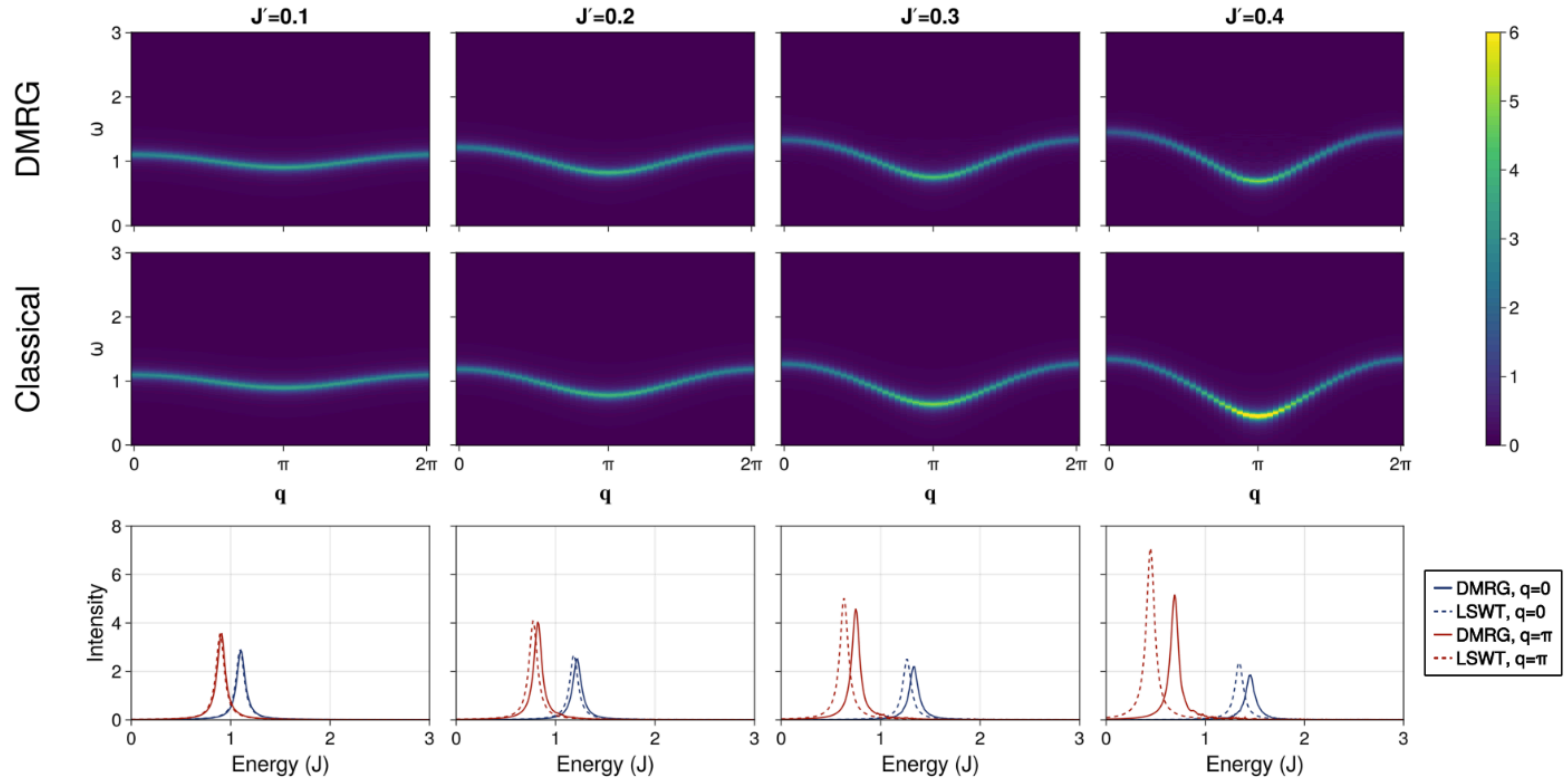


$$\begin{pmatrix}\alpha_j\\ \beta_j\\ \gamma_j\\ \delta_j\end{pmatrix} = \alpha_j|\uparrow\uparrow\rangle + \beta_j|\downarrow\uparrow\rangle + \gamma_j|\uparrow\downarrow\rangle + \delta_j|\downarrow\downarrow\rangle$$



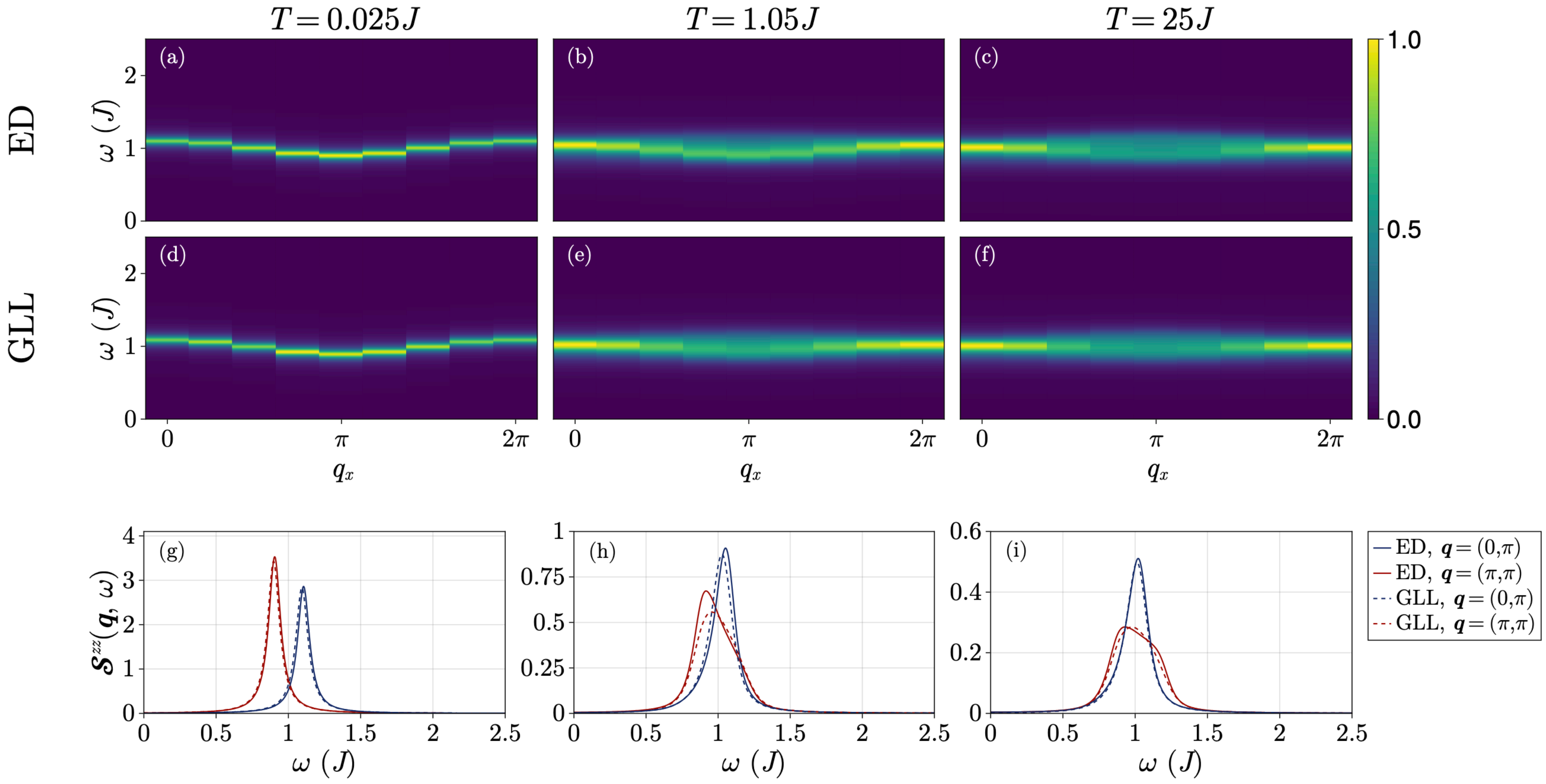
II. Applications of SU(*N*) dynamics

Capturing local entanglement effects



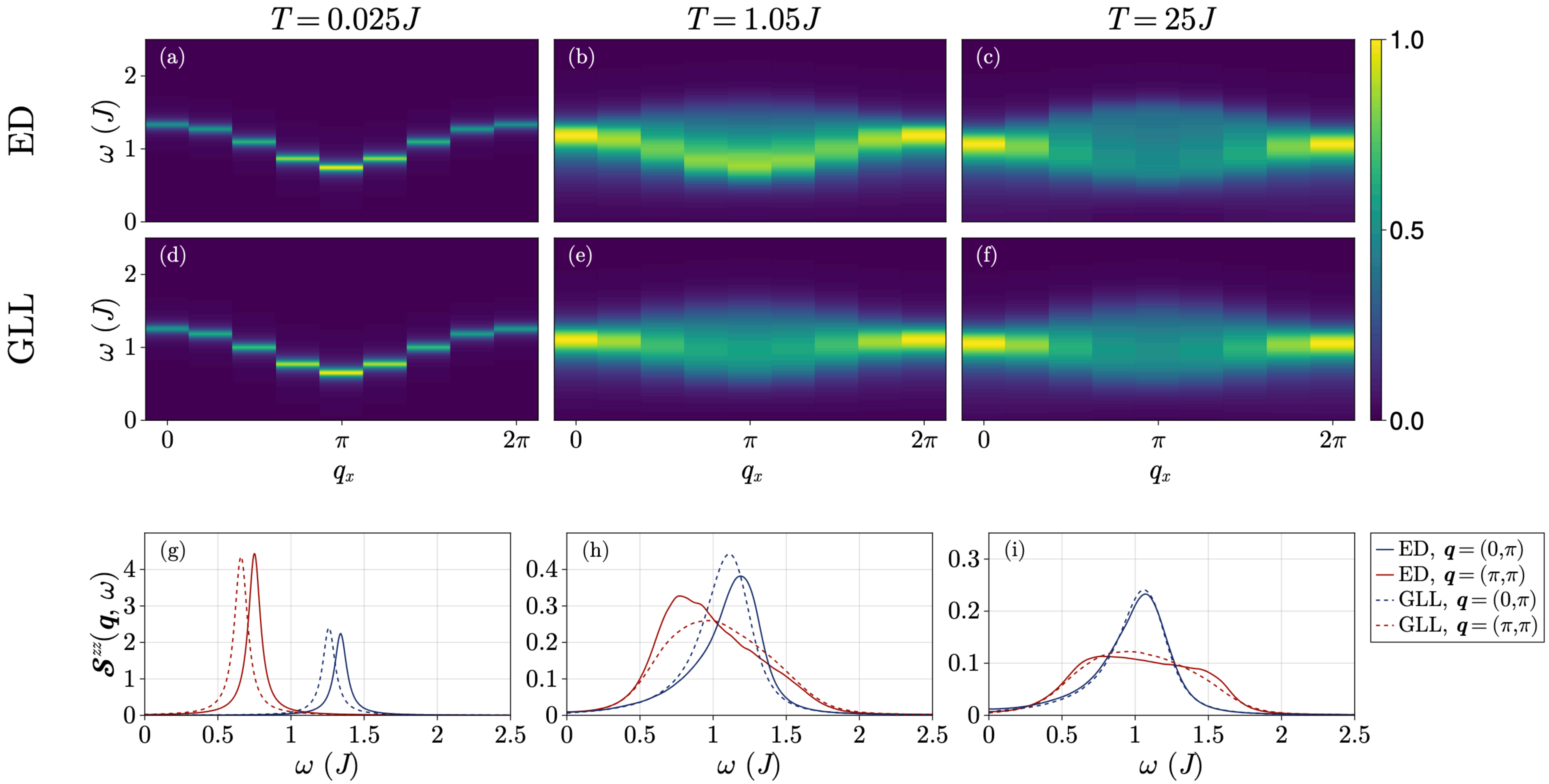
II. Applications of SU(*N*) dynamics

Capturing local entanglement effects



II. Applications of SU(*N*) dynamics

Capturing local entanglement effects



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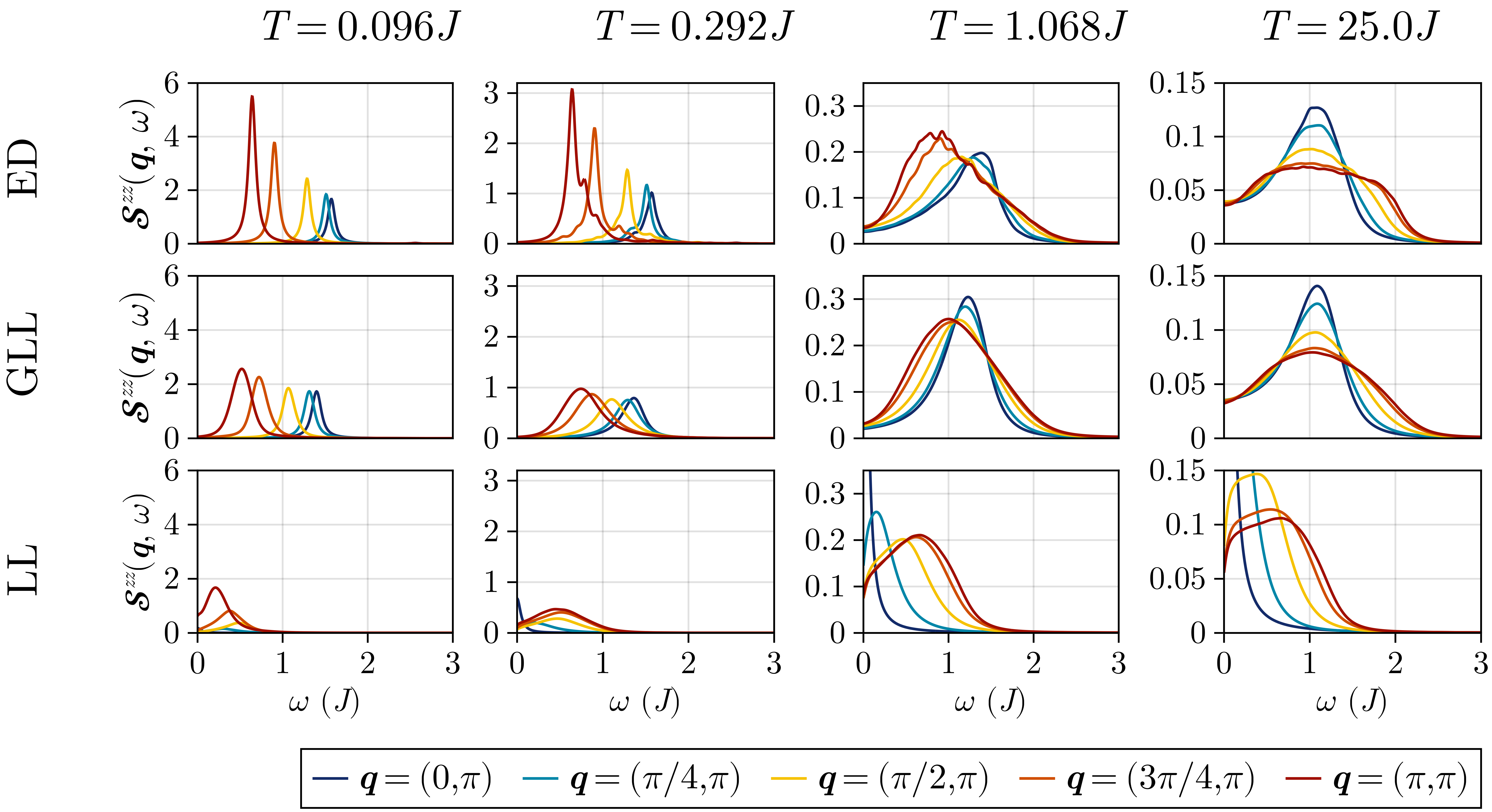
Capturing local entanglement effects



Recap of Part II

- Neutron scattering gives an excellent picture of the structure and dynamics of magnetic systems.

- Intuition about many magnets can already be gleaned from a classical picture.

- The typical classical limit always gives a picture of “dipoles” on each site, but this can be generalized.

- The SU(*N*) formalism enables one to employ a classical limit that captures all the structure of an *N*-level quantum system on each site.