Ideas behind Sunny.jl

Extending classical and semiclassical techniques

David Dahlbom (ORNL) & Cristian Batista (UTK, LANL, ORNL) — April 15th, 2024

Sunny

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

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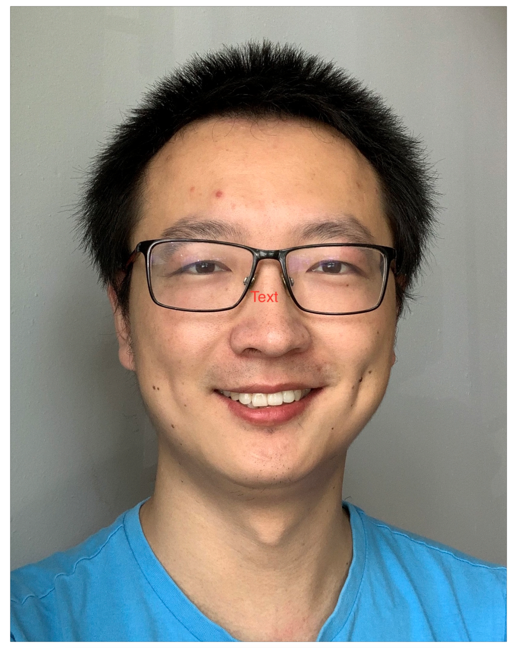

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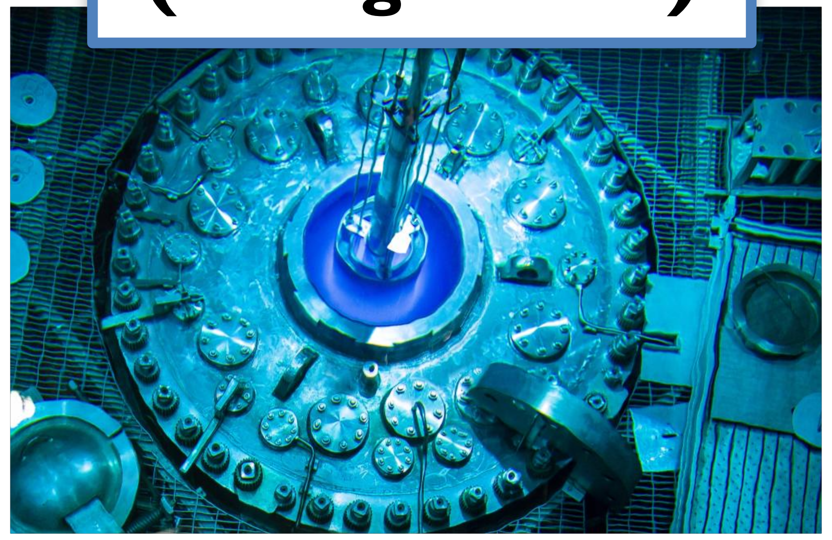

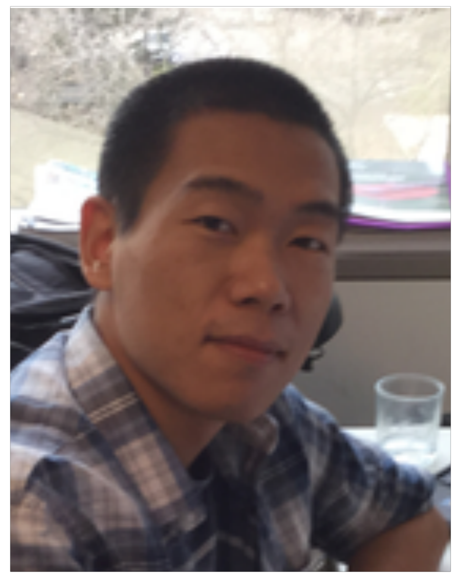

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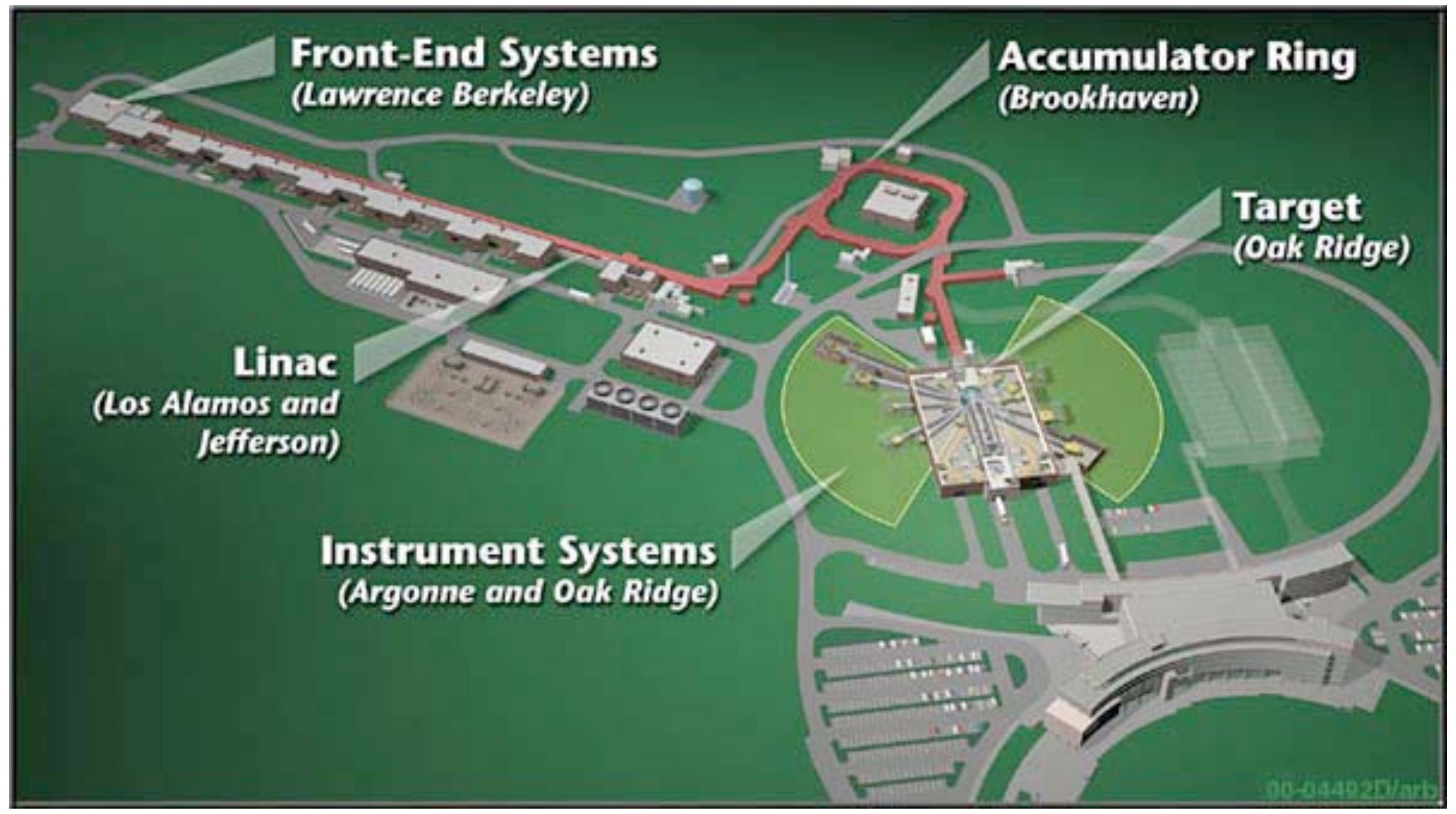
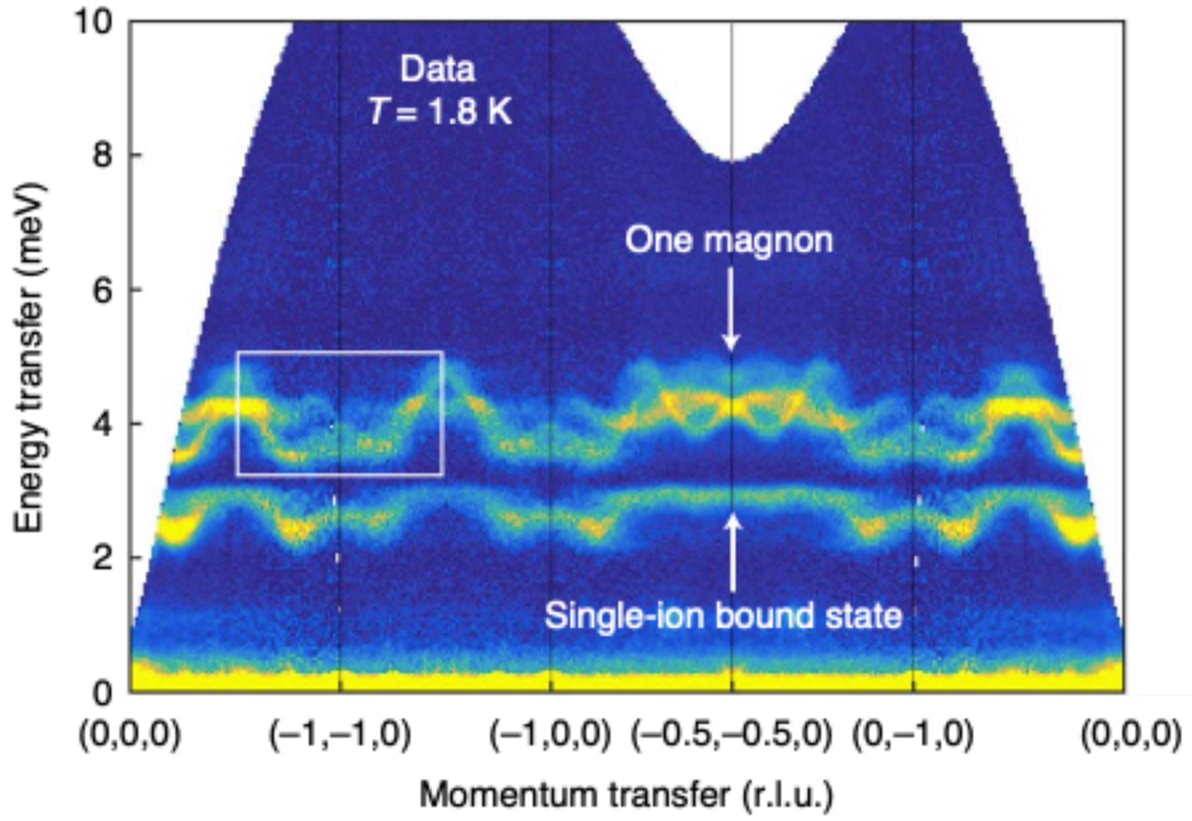
Motivation for developing Sunny

Experiment

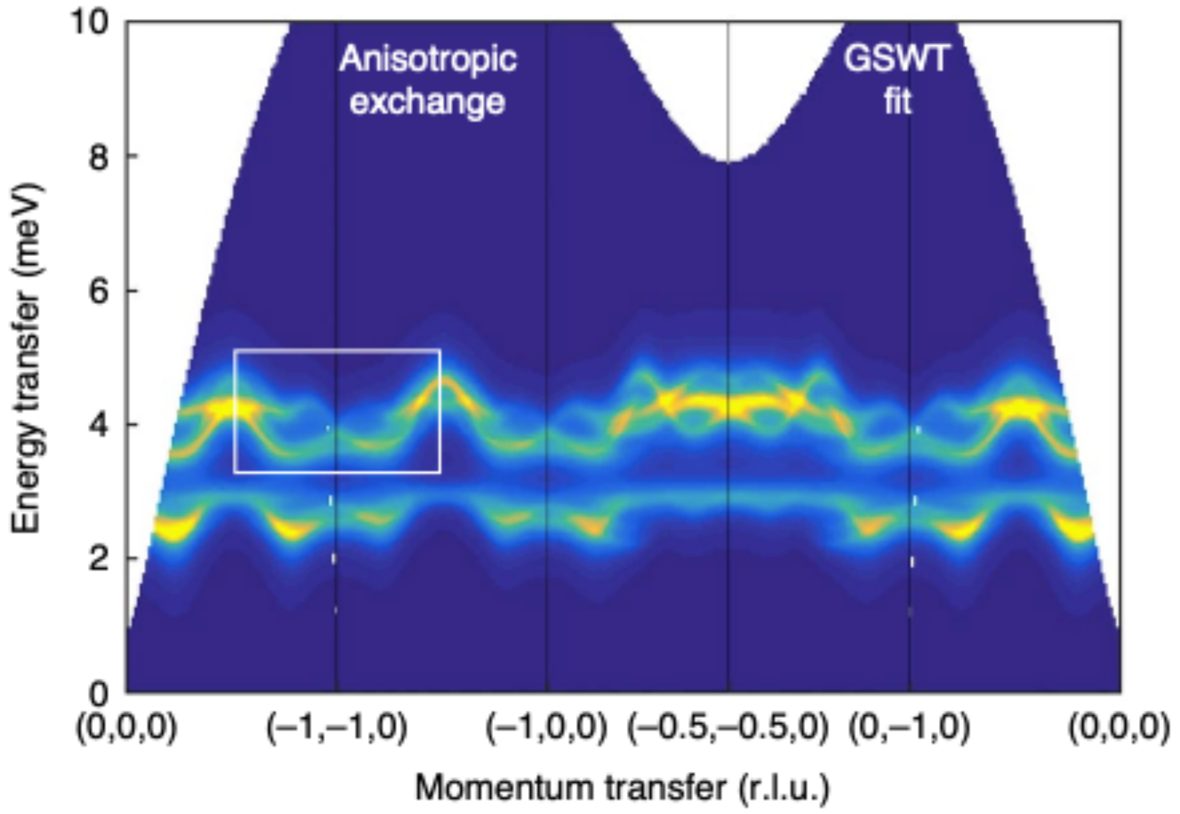




Theory

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

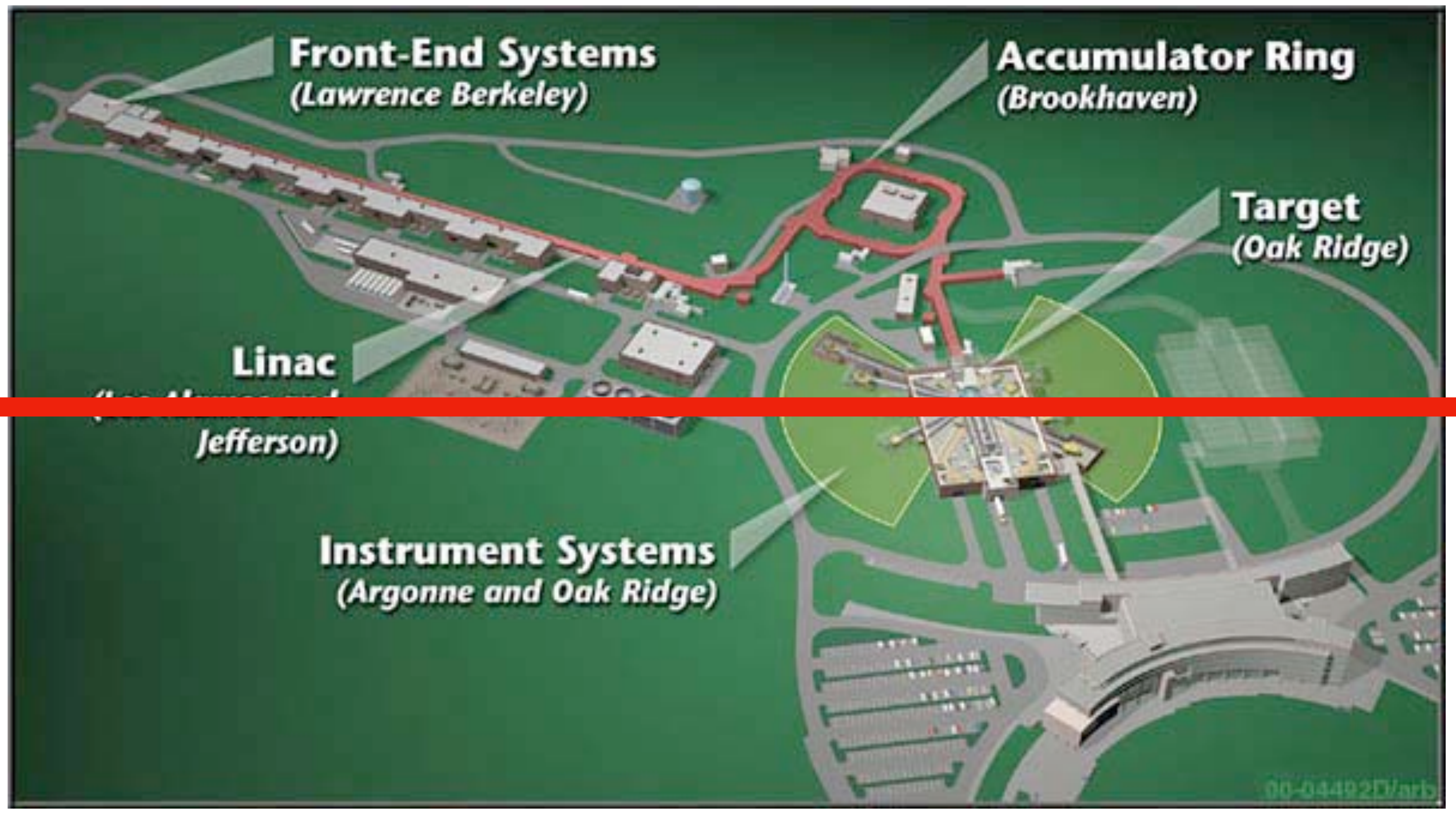
$$i\hbar \frac{d}{dt} \left|\Psi\right\rangle = \hat{\mathcal{H}} \left|\Psi\right\rangle$$

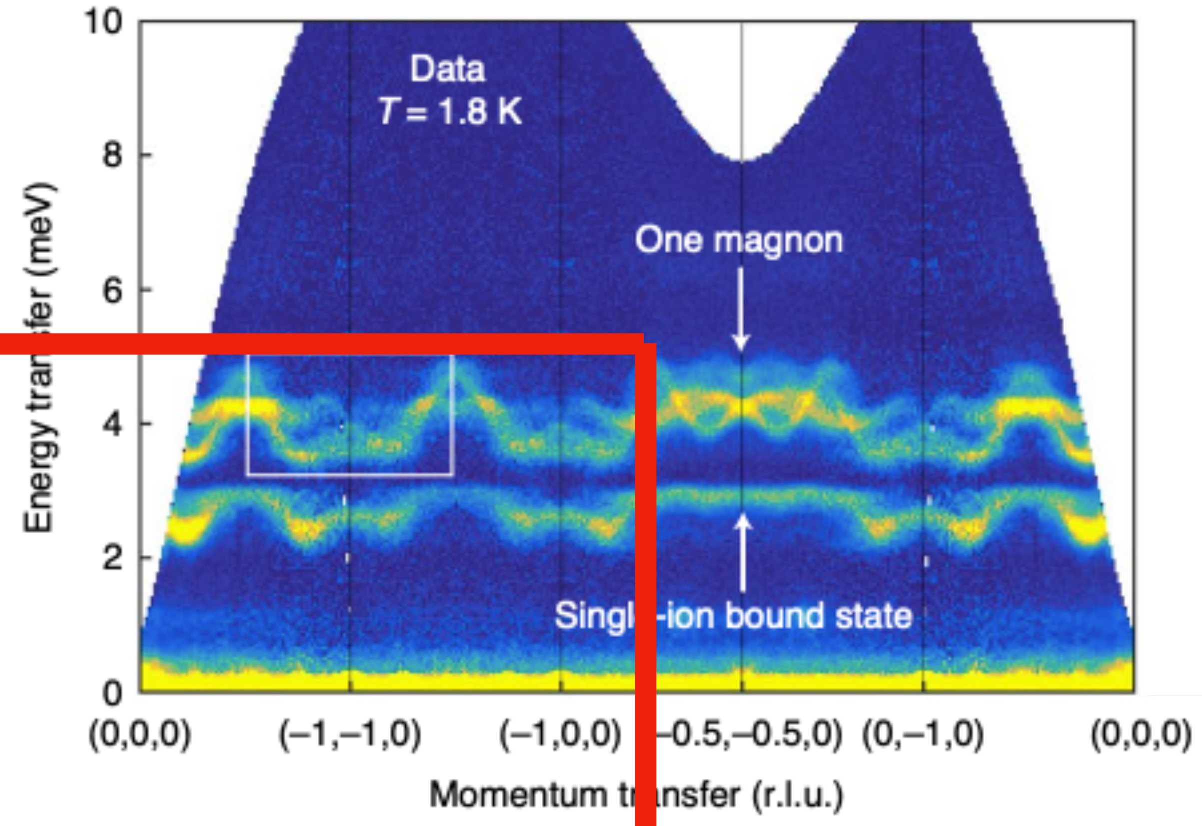


Xiaojian Bai, et al. Nature Physics, 17, 467-472 (2021)

Motivation for developing Sunny

Experiment





Theory

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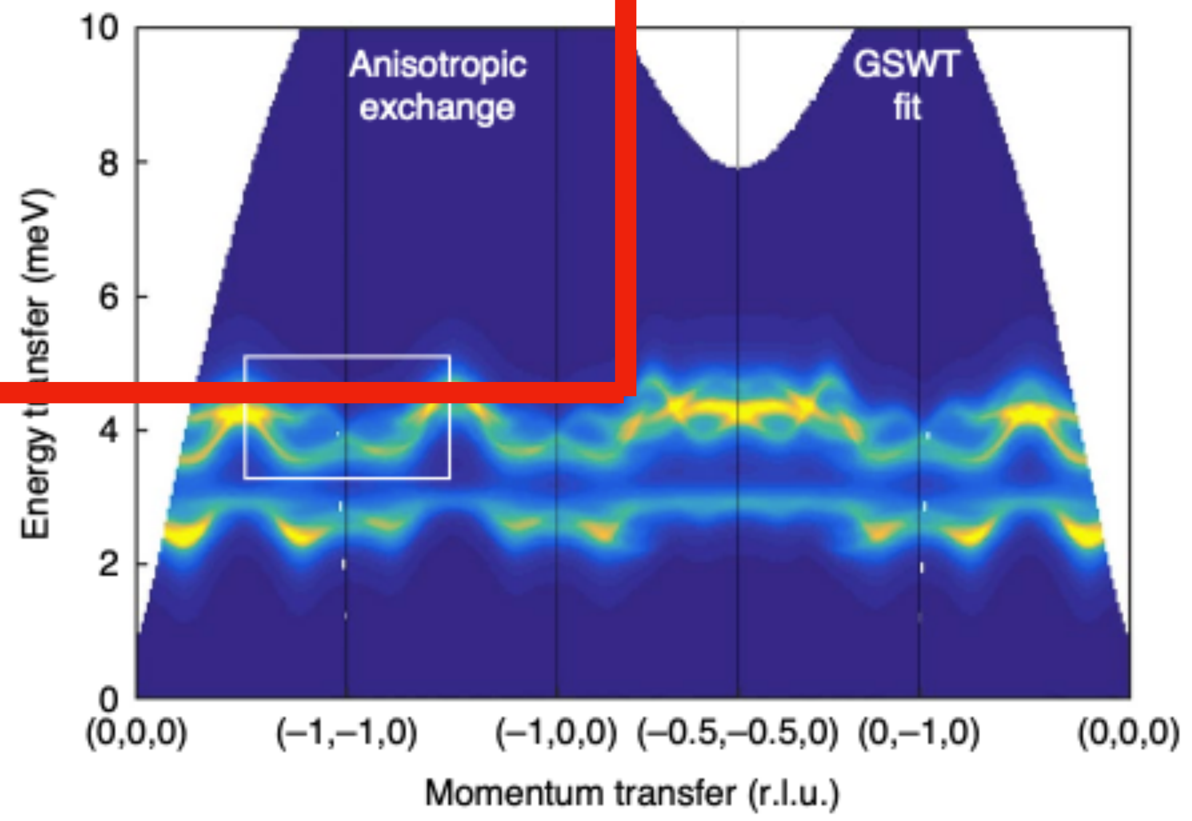
$$i\hbar \frac{d}{dt} |\Psi\rangle = \hat{\mathcal{H}} |\Psi\rangle$$



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Motivation for developing Sunny

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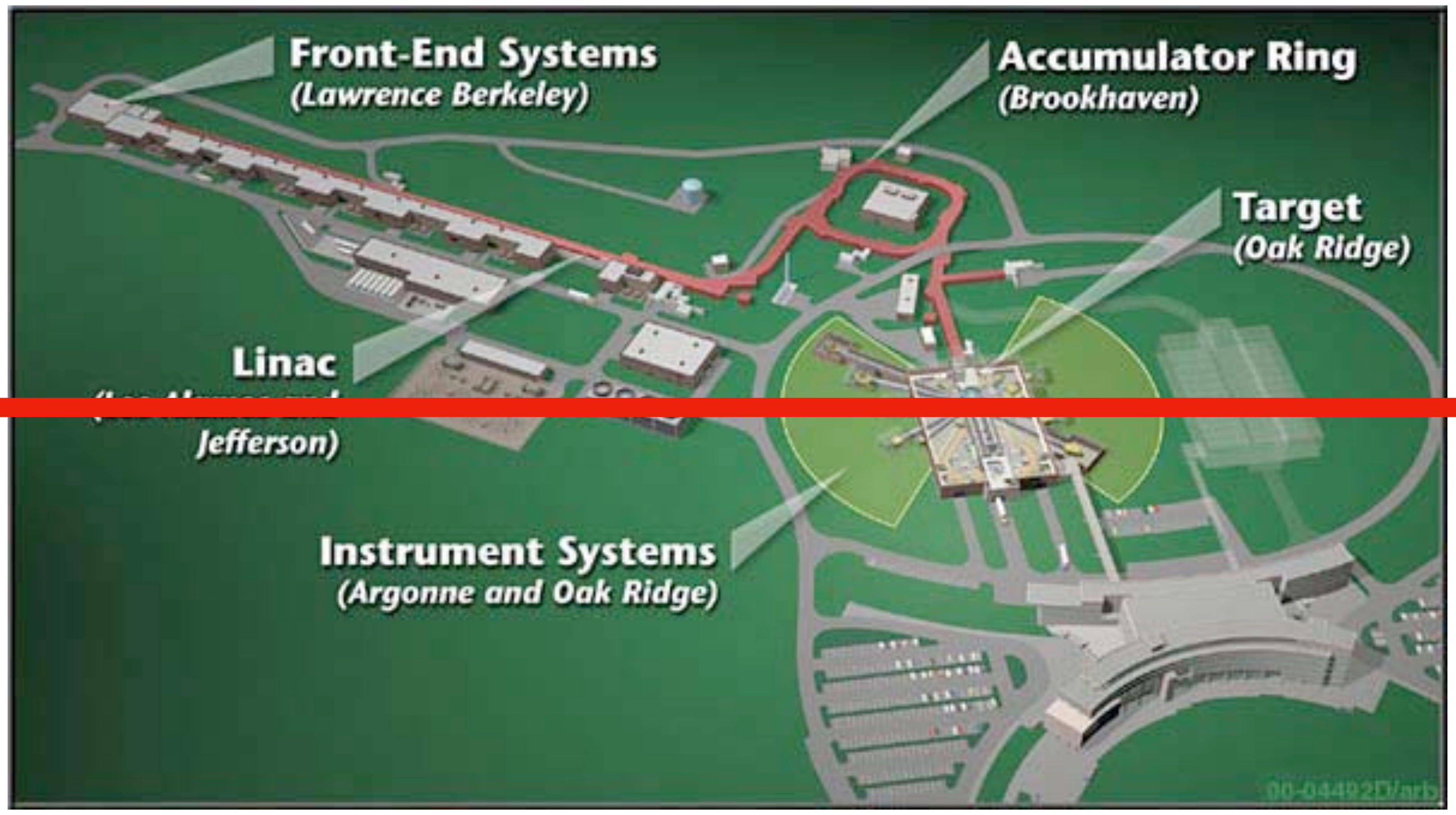

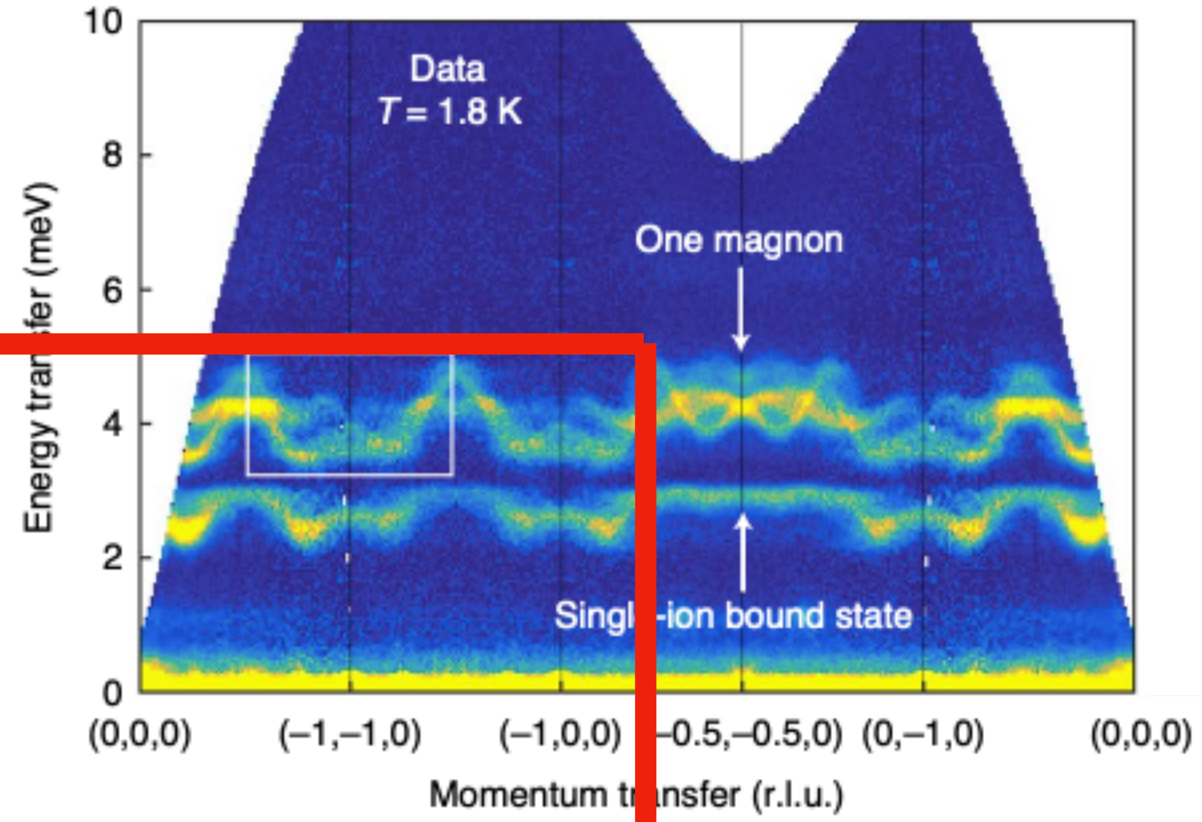

Theory

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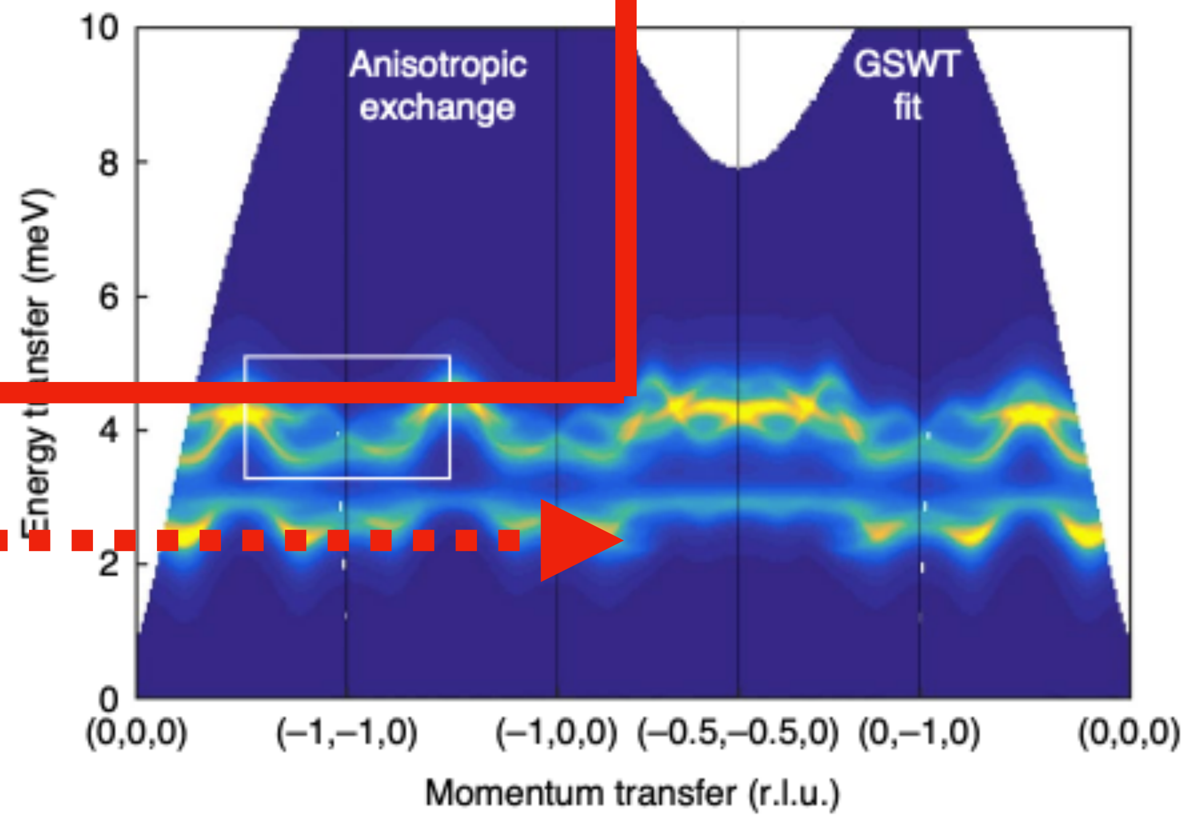
$$i\hbar \frac{d}{dt} |\Psi\rangle = \hat{\mathcal{H}} |\Psi\rangle$$



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

Scattering cross section

- What actually comes out of the scattering process is

$$\boxed{\frac{d^2\sigma}{dEd\Omega} = \frac{k_f}{k_i} r_m^2 \sum_{\alpha,\beta} \left(\delta_{\alpha\beta} - \frac{Q_\alpha Q_\beta}{Q^2}\right) \sum_{j,j'} g_{\alpha,j} \frac{F_j^*(\mathbf{Q})}{2} g_{\beta,j'} \frac{F_{j'}(\mathbf{Q})}{2} \int_{-\infty}^{\infty} e^{-i\omega t} e^{-i\mathbf{Q}\cdot\left(\mathbf{R}_j - \mathbf{R}_{j'}\right)} \left\langle S_j^\alpha S_{j'}^\beta(t) \right\rangle \frac{dt}{2\pi\hbar}}$$

- Contains the dynamical spin structure factor (DSSF)

$$\boxed{\mathcal{S}^{\alpha\beta}(\mathbf{Q},\omega) = \sum_{j,j'} \int_{-\infty}^{\infty} e^{-i\omega t} e^{-i\mathbf{Q}\cdot\left(\mathbf{R}_j - \mathbf{R}_{j'}\right)} \left\langle S_j^\alpha S_{j'}^\beta(t) \right\rangle \frac{dt}{2\pi\hbar}}$$

Calculating the DSSF

- Calculating the DSSF (in the Lehmann representation)

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

- But there's a clear problem, for N_s $S=1/2$ spins we have 2^{N_s} eigenvectors
- In general impossible to calculate for large number of spins

Approximation methods

- General (unbiased) approaches
  - Exact Diagonalization (ED)
  - Density matrix renormalization group (DMRG)
  - Quantum Monte Carlo (QMC)

- Physically “interpretable” approaches with strong assumptions
  - Classical and semiclassical (e.g., Spin Wave Theory)
  - Schwinger-Boson formalism

Role of classical and semiclassical methods

- Reasons for enduring usefulness of classical and semiclassical methods:
  - Many materials do behave rather “classically” (due to large coordination number or large S)
  - Computational cost grows *linearly* in N_S due to product space assumption.

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

Ideas behind Sunny.jl

Lecture 1: Traditional Classical and Semiclassical approaches to spin systems

David Dahlbom (ORNL) & Cristian Batista (UTK, LANL, ORNL) — April 15th, 2024

Points that will be covered

- Both classical and semiclassical methods assume system can be decomposed into product state.
- In the traditional approaches, the constituents of this product space are dipoles.
- Formally, dipoles are coherent states of SU(2). This is where S comes from (labels irreps of SU(2)).
- Given a product state of SU(2) coherent states, one can either develop a classical theory or perform a semiclassical expansion
- All this corresponds to `:dipole_large_S` mode in Sunny.

Brief review of structure of QM

- The basic components of the theory are:
  - the **state and state space** (the wave function and Hilbert space).
  - elements of an **algebra** (observables and Hamiltonians)
  - **group actions** (generated by the Hamiltonian in time)

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

$$\boxed{\left|\Psi\left(t\right)\right\rangle = \exp\left[-\frac{i\hat{\mathcal{H}}t}{\hbar}\right] \left|\Psi\left(0\right)\right\rangle}$$

Brief review of structure of QM

State

- A state is an element of a Hilbert space that fully specifies state of system (expectation value of all observables)
- For an S=1/2 problem the Hilbert space is
  - 2D complex vector space, $\mathbb{C}^2$
  - $|\Psi\rangle = \alpha|1\rangle + \beta|2\rangle$
- For harmonic oscillator, it is
  - Space of square summable functions, l^2
  - $\Psi(x) = \sum_n c_n \psi_n(x)$, where eigenfunction are Hermite polynomials

Brief review of structure of QM

Algebra

- The observables that make up a Hamiltonian, which belong to a collection of observables that are closed under commutation.

Brief review of structure of QM

Algebra

- The observables that make up a Hamiltonian, which belong to a collection of observables that are closed under commutation.

Hamiltonian

$$\hat{\mathcal{H}} = B_x \hat{S}^x + B_y \hat{S}^y + B_z \hat{S}^z = \sum_{\alpha} B_\alpha \hat{S}^\alpha$$

Algebra

$$\left[\hat{S}^\alpha, \hat{S}^\beta\right] = i\hbar \epsilon_{\alpha\beta\gamma} \hat{S}^\gamma \qquad \text{“}\mathfrak{su}\,(2)\text{”}$$

Brief review of structure of QM

Algebra

- The observables that make up a Hamiltonian, which belong to a collection of observables that are closed under commutation.

<u>Hamiltonian</u>	<u>Algebra</u>	
$\hat{\mathcal{H}} = B_x \hat{S}^x + B_y \hat{S}^y + B_z \hat{S}^z = \sum_\alpha B_\alpha \hat{S}^\alpha$	$\left[\hat{S}^\alpha, \hat{S}^\beta\right] = i\hbar \epsilon_{\alpha\beta\gamma} \hat{S}^\gamma$	“$\mathfrak{su}(2)$”
$\hat{\mathcal{H}} = \frac{1}{2m}\hat{p}^2 + \frac{m\omega^2}{2}\hat{q}^2$	$[\hat{q}, \hat{p}] = i\hbar$	“$\mathfrak{h}_3$”

Brief review of structure of QM

Group actions

- The group actions are what the Hamiltonian does

$$\hat{\mathcal{H}} = B_x \hat{S}^x + B_y \hat{S}^y + B_z \hat{S}^z = \sum_\alpha B_\alpha \hat{S}^\alpha$$

$$U(t) = \exp\left[-\frac{i\hat{\mathcal{H}}t}{\hbar}\right] = \exp\left[-\frac{it\sum_\alpha B_\alpha \hat{S}^\alpha}{\hbar}\right] = \begin{pmatrix} \cos\frac{t}{2} - iB_z \sin\frac{t}{2} & (-iB_x - B_y)\sin\frac{t}{2} \\ (iB_x + B_y)\sin\frac{t}{2} & \cos\frac{t}{2} + iB_z \sin\frac{t}{2} \end{pmatrix}$$

Brief review of structure of QM

Group actions

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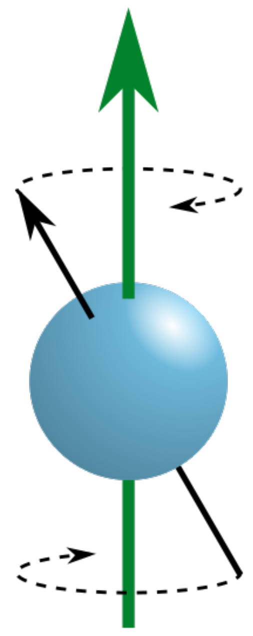
$$\hat{\mathcal{H}} = B_x \hat{S}^x + B_y \hat{S}^y + B_z \hat{S}^z = \sum_\alpha B_\alpha \hat{S}^\alpha$$

$$U(t) = \exp\left[-\frac{i\hat{\mathcal{H}}t}{\hbar}\right] = \exp\left[-\frac{it\sum_\alpha B_\alpha \hat{S}^\alpha}{\hbar}\right] = \underbrace{\begin{pmatrix} \cos\frac{t}{2} - iB_z \sin\frac{t}{2} & (-iB_x - B_y)\sin\frac{t}{2} \\ (iB_x + B_y)\sin\frac{t}{2} & \cos\frac{t}{2} + iB_z \sin\frac{t}{2} \end{pmatrix}}_{\text{Belongs to SU(2)}}$$



Coherent states

- Coherent states are collections of “special” states
  - They “saturate the uncertainty” principle
  - They are (over)-complete
  - They are intimately tied with a classical limit
  - They may be generated with a simple “recipe”

Perelomov A 1972 Commun. Math. Phys. 26 222

Coherent state recipe

(1) Consider the relevant algebra (what's in your Hamiltonian)

$$\mathfrak{h}_3 = \left\{1, \hat{q}, \hat{p}\right\}$$

$$\mathfrak{su}(2) = \left\{\hat{S}^x, \hat{S}^y, \hat{S}^z\right\}$$

$$[\hat{q}, \hat{p}] = i\hbar$$

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

Coherent state recipe

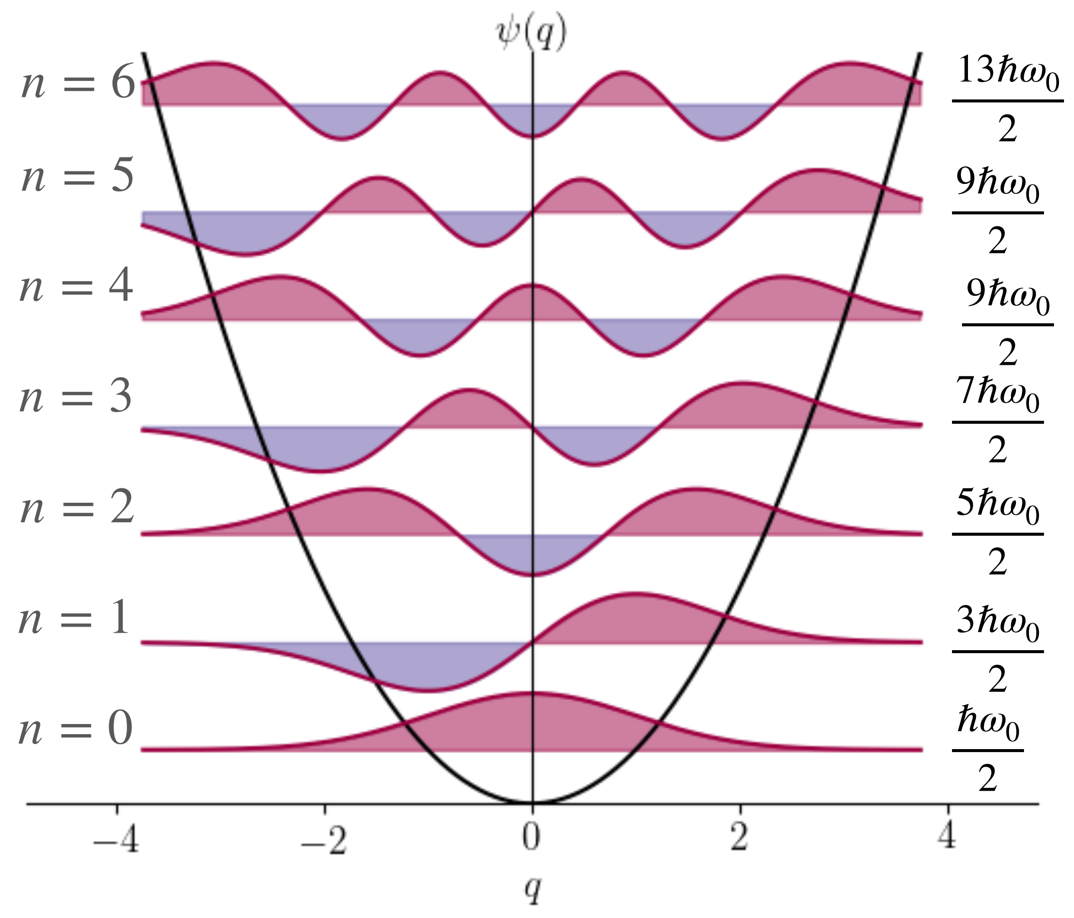
(2) Consider the group associated with that algebra (exponentiate algebra)

H_3	$SU(2)$
$G(X,P) = e^{\frac{2i}{\hbar}\left(P\hat{q} - X\hat{p}\right)}$	$G\left(B_x, B_y, B_z\right) = e^{\frac{i}{\hbar}\sum_\alpha B_\alpha \hat{S}^\alpha}$
	$G(\phi,\theta,\chi) = e^{i\phi\hat{S}^z} e^{i\theta\hat{S}^y} e^{i\chi\hat{S}^z}$

Coherent state recipe

(3) Consider a “special” state as a starting point

H_3



Ground State $|0\rangle$

$SU(2)$

$$|S,-S\rangle, |S,-S+1\rangle, \ldots, |S,S-1\rangle, |S,S\rangle$$

Fully polarized state,
a.k.a. $|\uparrow\rangle$

Coherent state recipe

(4) Apply all the group elements to that reference state to generate another coherent state.

$$H_3 \qquad\qquad SU(2)$$

$$|X, P\rangle = e^{\frac{2i}{\hbar}\left(P\hat{q} - X\hat{p}\right)}|0\rangle$$

$$|\Omega\rangle = e^{i\phi\hat{S}^z}e^{i\theta\hat{S}^z}e^{i\chi\hat{S}^z}|\uparrow\rangle$$

Aside: what group theory has to do with it

- We are talking about groups in a very general way — essentially as the set of "things" that an *arbitrary* Hamiltonian can do
- This is in contrast with what condensed matter physicists usually do: exploit symmetries of particular Hamiltonians to make the problem simpler
- In fact, the formalism we will be developing is most useful for low-symmetry Hamiltonians.

Coherent states of the harmonic oscillator

Original Hamiltonian: $$\hat{H} = \frac{1}{2m}\hat{\pi}^2 + \frac{m\omega^2}{2}\hat{q}^2 \qquad [\hat{q}, \hat{\pi}] = i\hbar$$

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$$\hat{P} = \frac{\hat{\pi}}{\sqrt{2m\omega_0}}, \qquad \hat{X} = \sqrt{\frac{m\omega_0}{2}}\hat{q} \longrightarrow [\hat{X}, \hat{P}] = \frac{i}{2}\hbar$$

$$\hat{a} = \frac{\hat{X}}{\sqrt{\hbar}} + i\frac{\hat{P}}{\sqrt{\hbar}}, \quad \hat{a}^\dagger = \frac{\hat{X}}{\sqrt{\hbar}} - i\frac{\hat{P}}{\sqrt{\hbar}}, \longrightarrow [\hat{a}, \hat{a}^\dagger] = 1$$

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Unitless Hamiltonian: $$\hat{H} = \omega_0(\hat{P}^2 + \hat{X}^2) = \hbar\omega_0\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right)$$

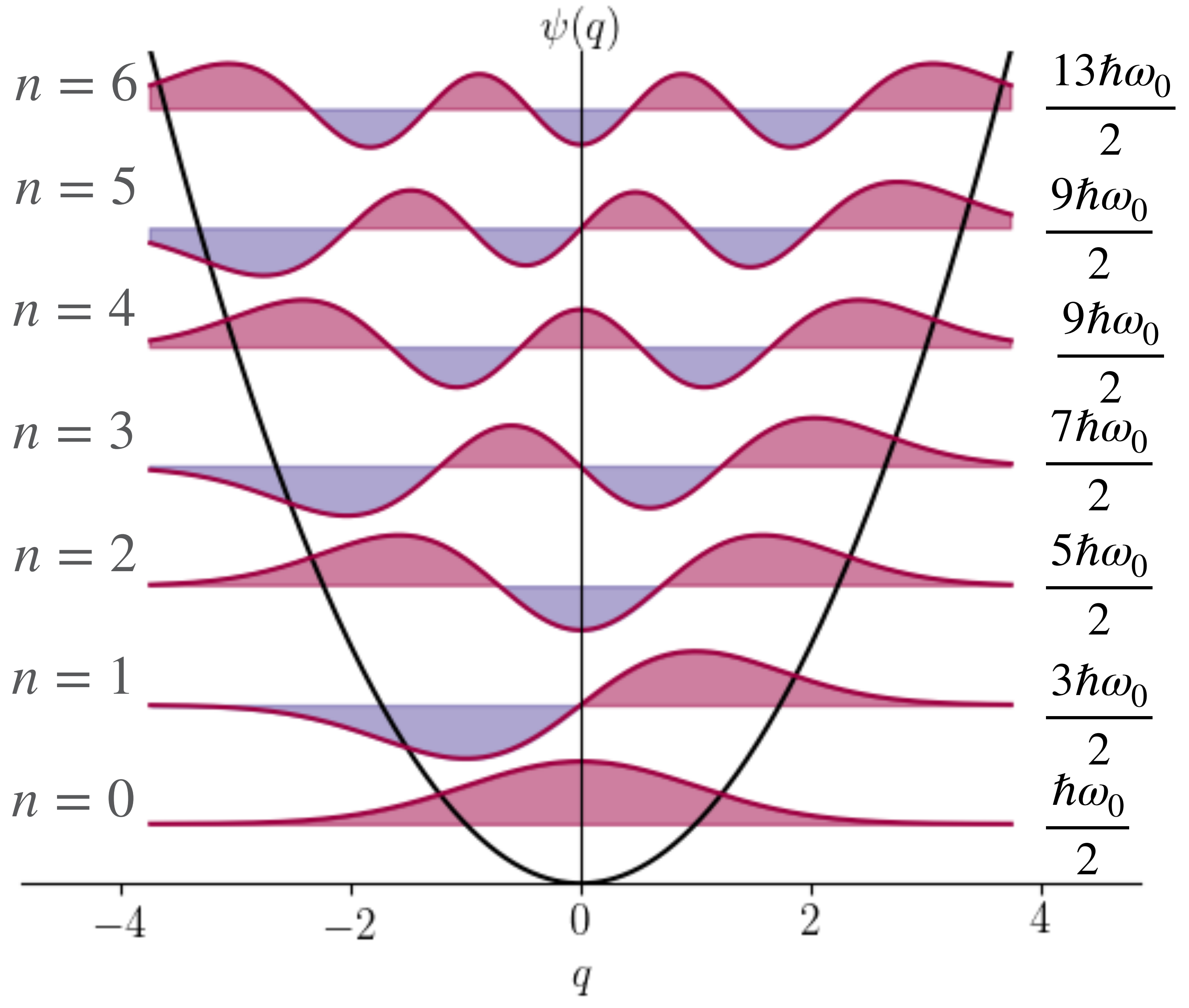
Coherent states of the harmonic oscillator

$$\hat{H} = \omega_0(\hat{P}^2 + \hat{X}^2) = \hbar\omega_0 \left(\hat{a}^\dagger \hat{a} + \frac{1}{2} \right)$$

$$\hat{H}|n\rangle = \left(n + \frac{1}{2} \right) \hbar\omega_0 |n\rangle$$

$$\epsilon_n = \left(n + \frac{1}{2} \right) \hbar\omega_0$$

$$\psi_0(x) = \langle x|0\rangle = \frac{1}{(\pi\hbar)^{1/4}} e^{-\frac{(x-X)^2}{\hbar}}$$



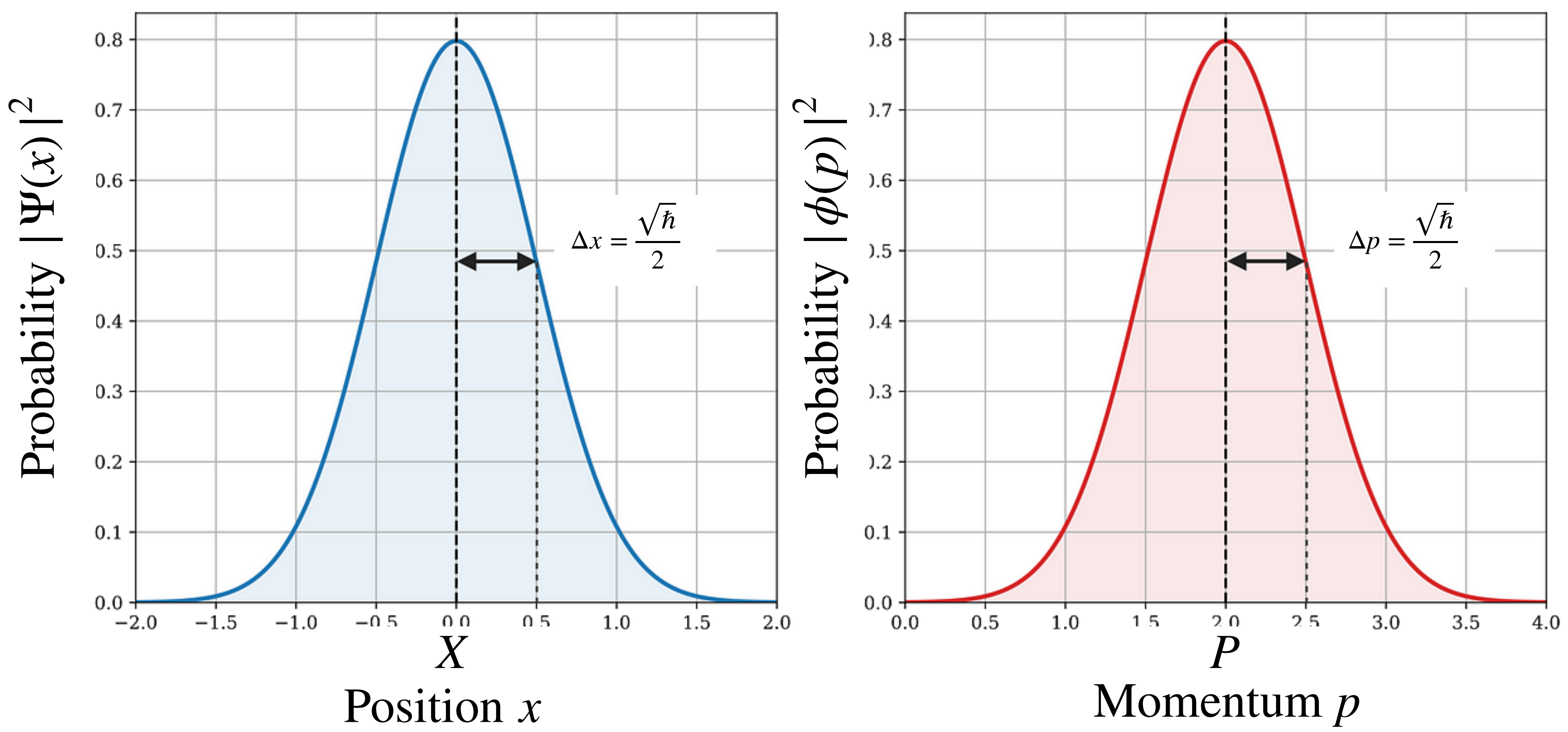
Coherent states of the harmonic oscillator

Generators of Heisenberg-Weyl Lie Algebra h_3: $\{\hat{a}^\dagger, \hat{a}, \hat{1}\}$

Heisenberg-Weyl Group H_3: $\boxed{\hat{G}(\alpha, \bar{\alpha}) = e^{\alpha\hat{a}^\dagger - \bar{\alpha}\hat{a}}}$ $\boxed{\alpha = \hbar^{-1/2}(X + iP)}$

$$|P, X\rangle = |\alpha\rangle = \hat{G}(\alpha)|0\rangle = e^{\alpha\hat{a}^\dagger - \bar{\alpha}\hat{a}}|0\rangle \qquad \langle x|P, X\rangle = \frac{1}{(\pi\hbar)^{1/4}} e^{-\frac{(x-X)^2}{\hbar}} e^{i\frac{Px}{\hbar}}$$

Minimum Uncertainty
Gaussian
Wave Packet centered
around P and X



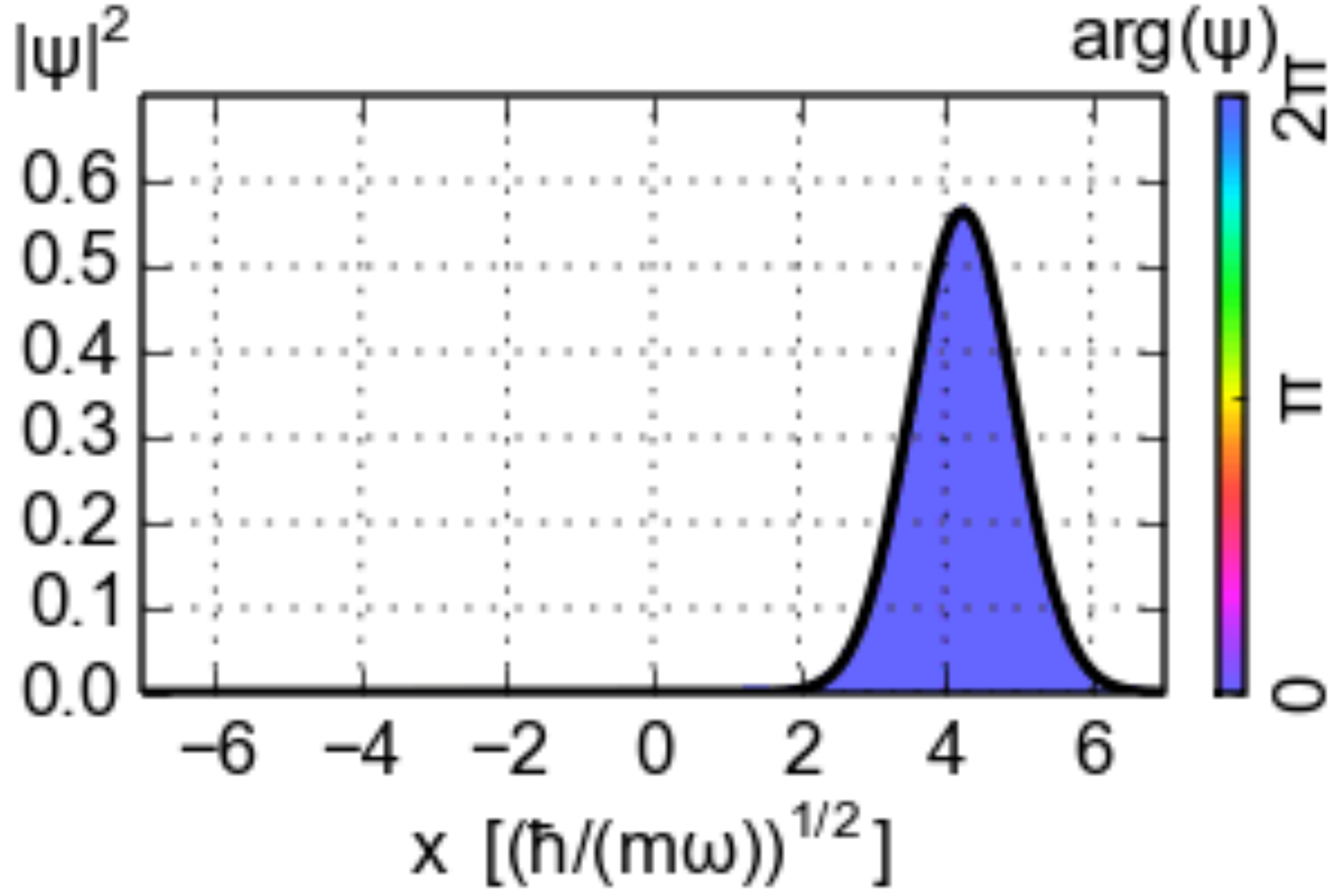
$$\Delta q \Delta \pi = \frac{\hbar}{2}$$

Dynamics of HO coherent states

- Can solve equations of motion for such a state:

$$\langle X, P | x | X, P \rangle = \left| \alpha(0) \right| \sqrt{\frac{2\hbar}{m\omega}} \cos\left(\angle\alpha(0) - \omega t\right)$$

$$\langle X, P | p | X, P \rangle = \left| \alpha(0) \right| \sqrt{2m\hbar\omega} \sin\left(\angle\alpha(0) - \omega t\right)$$

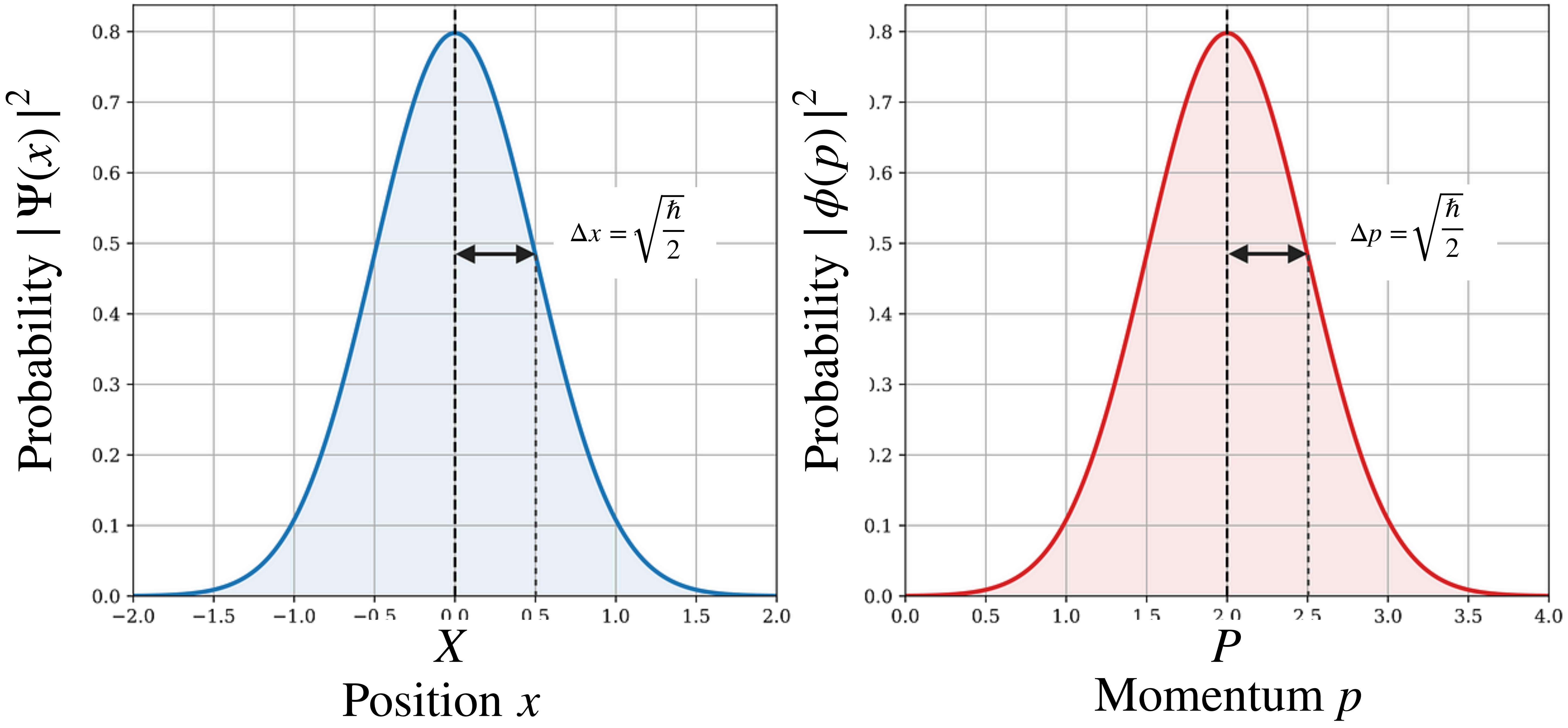


https://upload.wikimedia.org/wikipedia/commons/c/c0/QHO-coherentstate3-animation-color.gif

Classical limit of HO

- Classical limit corresponds to $\hbar \to 0$

$$\langle x | P, X \rangle = \frac{1}{(\pi\hbar)^{1/4}} e^{-\frac{(x-X)^2}{\hbar}} e^{i\frac{Px}{\hbar}}$$



Classical limit of HO

Coherent states become a proper orthonormal basis in process

- One can show that the states $|X, P\rangle$ are complete

$$\hat{1} = \int \frac{dP'dX'}{2\pi\hbar} |P', X'\rangle\langle P', X'|$$

- And in fact over-complete — they overlap with one another

$$\langle X, P | X', P'\rangle = \exp\left\{-\frac{1}{4\hbar}\left[(P - P')^2 + (X - X')^2\right]\right\}$$

Classical limit of HO

Summary of what happens when $\hbar \to 0$

- One may use the resolution of identity to expand the expectation value of operators in terms of $\hbar$ to show:
  - A factorization rule for the expectation of operators

$$\lim_{\hbar \to 0} \langle X, P | \hat{C}\hat{D} | X, P \rangle = \langle X, P | \hat{C} | X, P \rangle \langle X, P | \hat{D} | X, P \rangle$$

  - A correspondence between the commutator and Poisson brackets

$$\{\ ,\ \}_{PB} \leftarrow \frac{[\ ,\ ]}{i\hbar}$$

Coherent states of SU(2)

- We play the same game with the "spin" algebra:

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

- Our reference state is the fully polarized state: $|\uparrow\rangle$

Coherent states of SU(2)

- An SU(2) coherent state may be generated by applying a generic SU(2) group action to a reference state

$$\left|\Omega\right\rangle = G(\phi, \theta, \chi)\left|\uparrow\right\rangle = e^{i\phi\hat{S}^z}e^{i\theta\hat{S}^y}e^{i\chi\hat{S}^z}\left|\uparrow\right\rangle$$

Coherent states of SU(2)

- Before giving an analytical expression for this, recall that the spin algebra has many different representations labeled by S

$S = 1/2$ $$S^x = \frac{1}{2}\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix},\ S^y = \frac{1}{2}\begin{bmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{bmatrix},\ S^z = \frac{1}{2}\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

$S = 1$ $$S^x = \frac{1}{\sqrt{2}}\begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix},\ S^y = \frac{1}{\sqrt{2}}\begin{bmatrix} 0 & -\mathrm{i} & 0 \\ \mathrm{i} & 0 & -\mathrm{i} \\ 0 & \mathrm{i} & 0 \end{bmatrix},\ S^z = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{bmatrix}$$

$$\vdots$$

$S = \dfrac{N-1}{2}$ $$S^x = \begin{bmatrix} 0 & a_1 & & \\ a_1 & 0 & \ddots & \\ & \ddots & \ddots & a_{N-1} \\ & & a_{N-1} & 0 \end{bmatrix},\ S^y = \begin{bmatrix} 0 & -\mathrm{i}\,a_1 & & \\ \mathrm{i}\,a_1 & 0 & \ddots & \\ & \ddots & \ddots & -\mathrm{i}\,a_{N-1} \\ & & \mathrm{i}\,a_{N-1} & 0 \end{bmatrix},\ S^z = \begin{bmatrix} S & & & \\ & S-1 & & \\ & & \ddots & \\ & & & -S \end{bmatrix}$$ $$a_j = \tfrac{1}{2}\sqrt{2(S+1)j - j(j+1)}$$

Coherent states of SU(2)

- After some labor, it can be shown that for any representation we have

$$\left|\Omega(\theta,\phi)\right\rangle = e^{i\phi\hat{S}^z}e^{i\theta\hat{S}^y}e^{i\chi\hat{S}^z}\left|\uparrow\right\rangle = e^{iS\chi}\sqrt{(2S)!}\sum_m \frac{u^{S+m}v^{S-m}}{\sqrt{(S+m)!(S-m)!}}|S,m\rangle$$

$$u(\theta,\phi) = \cos(\theta/2)e^{i\phi/2}$$

$$v(\theta,\phi) = \sin(\theta/2)e^{-i\phi/2}$$

Coherent states of SU(2)

$$\left|\Omega(\theta,\phi)\right\rangle = e^{iS\chi}\sqrt{(2S)!}\sum_m \frac{u^{S+m}v^{S-m}}{\sqrt{(S+m)!(S-m)!}}\,|S,m\rangle$$

$$\Big\downarrow\; S = 1/2$$

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

- This in fact parameterizes all possible 2-level states uniquely. (No need to normalize and remove global phase.)

Coherent states of SU(2)

S=1/2

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

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

SU(2) cohere

← One-to-one →

Real 3-vector

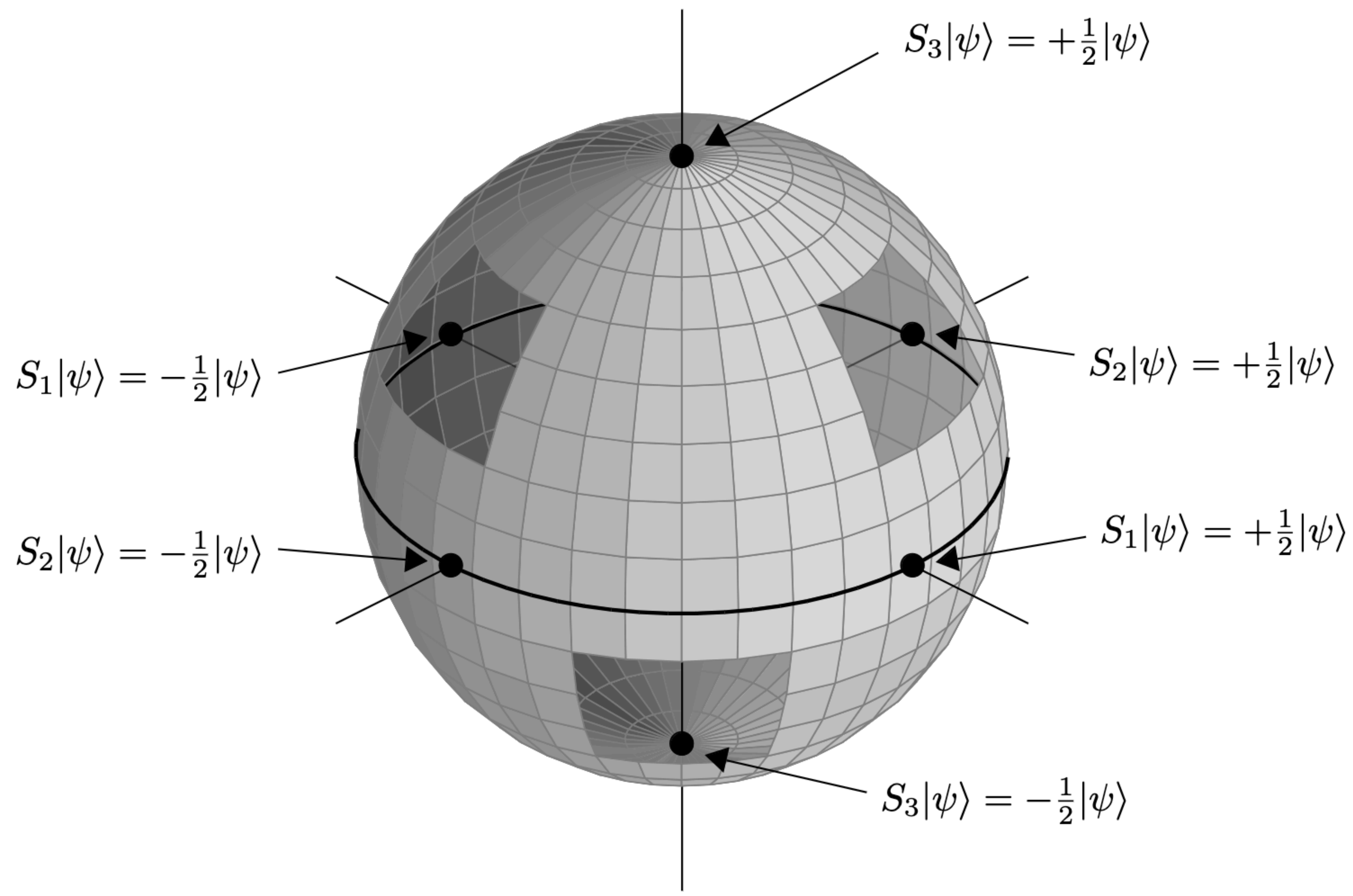


Image from: P. Woit, *Quantum Theory, Groups and Representations (2014)*

Coherent states of SU(2)

$$\left|\Omega(\theta,\phi)\right\rangle = e^{iS\chi}\sqrt{(2S)!}\sum_m \frac{u^{S+m}v^{S-m}}{\sqrt{(S+m)!(S-m)!}}\,|S,m\rangle$$

$$\Big\downarrow \; \text{S=1}$$

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

- These states can be put into one-to-one correspondence with points on a sphere — but they do cover all possible states for a 3-level system. Consider the pure state $|0\rangle$.

Coherent states of SU(2)

Essentially dipolar states

- We may always associate our group action with a unit vector.

$$\mathbf{n}(\theta, \phi) = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$$

- If we evaluate the expectation value of the three spin operators with respect to a coherent state, $|\Omega(\theta, \phi)\rangle$, we get a result proportional to this unit vector:

$$(\langle\Omega|\hat{S}^x|\Omega\rangle, \langle\Omega|\hat{S}^y|\Omega\rangle, \langle\Omega|\hat{S}^z|\Omega\rangle) = (S\sin\theta\cos\phi, S\sin\theta\sin\phi, S\cos\theta)$$

- This is true for all S. $SU(2)$ coherent states are always *dipolar* states, regardless of representation.

Why all the bother about SU(2) coherent states?

- They are, as we've just seen, exclusively dipolar states.
- They are always "present" when we see the label S.
- Any classical or semi-classical method that uses S as a control or expansion parameter likely has SU(2) coherent states at work somewhere.
- This means that any such theory always at least starts with a dipolar state (and potentially expands around this).
- This can be a problem since a generic spin-S state need not be dipolar.

Classical limit for SU(2) coherent states

- The classical limit corresponds to sending $S \to \infty$ while sending $\hbar \to 0$ (while holding $S\hbar$ constant)
- Things become "more classical" as $S \to \infty$

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

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"

Classical limit for SU(2) coherent states

- Similar HO coherent states, one can show that spin coherent states become orthogonal in the $S \to \infty$ limit

$$\Big|\Omega(\theta,\phi)\rangle = e^{iS\chi}\sqrt{(2S)!}\sum_m \frac{u^{S+m}v^{S-m}}{\sqrt{(S+m)!(S-m)!}}\,|S,m\rangle$$

$$\lim_{S\to\infty}\langle\Omega(\theta,\phi)\,|\,\Omega(\theta',\phi')\rangle = \delta_{\theta,\theta'}\delta_{\phi,\phi'}$$

Classical limit "recipe"

- Replace all operators with their expectation values in SU(2) coherent states.

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

- When the operator is linear in the spin algebra, this is just the regular expectation value (since $S\hbar$ is held constant).

- For products of operators, use a factorization rule:

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

Classical Dynamics for SU(2) coherent states

- 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.

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

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

Classical Dynamics for SU(2) coherent states

- 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.

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

Classical Dynamics for SU(2) coherent states

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

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

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

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

Classical Dynamics for SU(2) coherent states

- Let's take a break and consider the Landau-Lifshitz equations in Sunny…

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

FM Spin Chain

Classical limit

- Consider a simple ferromagnetic spin chain with field and anisotropy

$$\hat{H} = -J\sum_j \hat{\mathbf{S}}_j \cdot \hat{\mathbf{S}}_j - D\sum_j \left(\hat{S}_z\right)^2 - B\sum_j \hat{S}_j^z$$

- Use our classical limit “recipe”

$$H_{\mathrm{cl}} = -J\sum_j \mathbf{s}_j \cdot \mathbf{s}_j - D\sum_j \left(s_z\right)^2 - B\sum_j s_j^z$$

FM Spin Chain

Dynamics

- This classical Hamiltonian,

$$H_{\mathrm{cl}} = -J \sum_j \mathbf{s}_j \cdot \mathbf{s}_j - D \sum_j \left(s_z\right)^2 - B \sum_j s_j^z$$

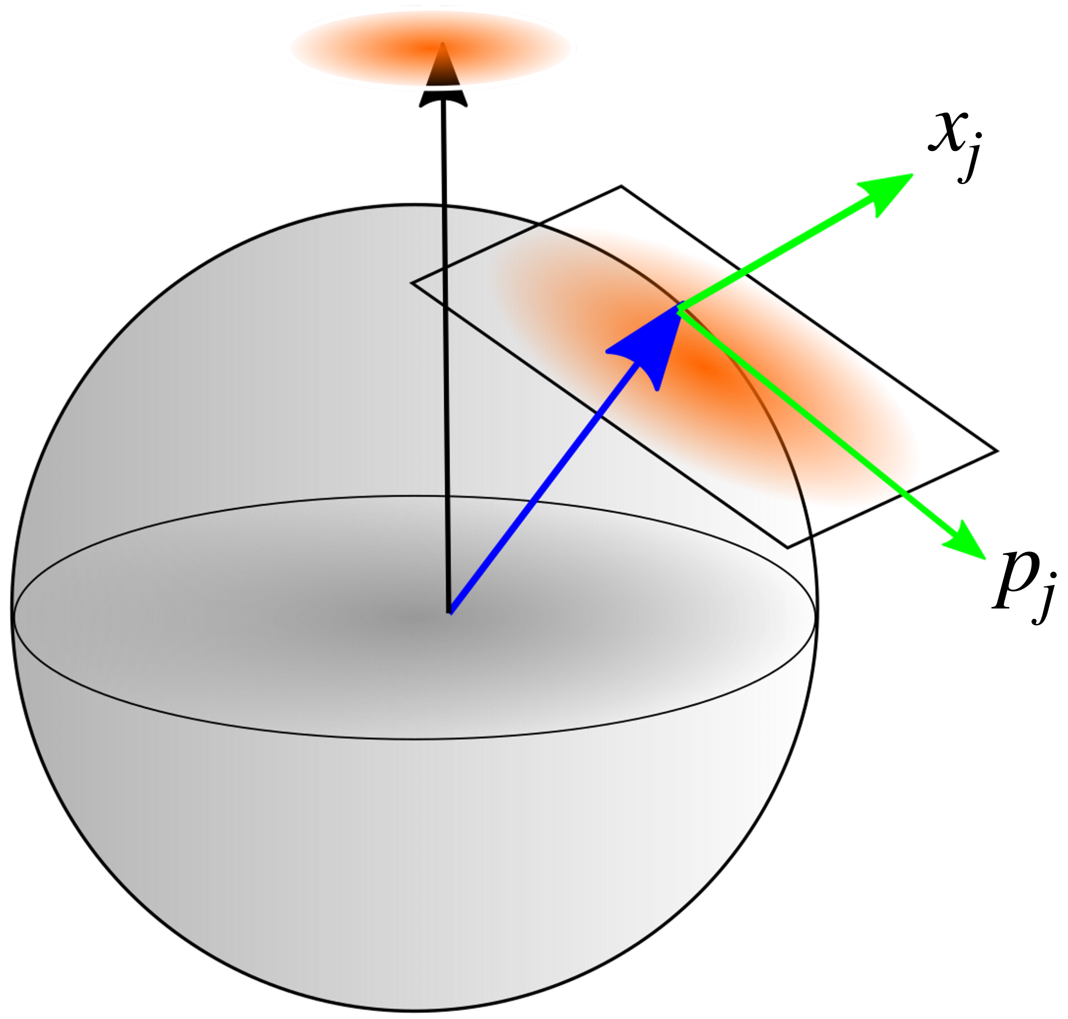
- will drive the Landau-Lifshitz equations:

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

FM Spin Chain

Linearize

- The resulting equations of motion may be linearized about the ground state, $s_{0,j}$, resulting in an effective field $\mathbf{B}_j$ on each site.
- Then we may consider small perturbations about this ground state.



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

FM Spin Chain

Linearize

- The translation invariance of the chain can be exploited by introducing a Fourier transform

$$\delta \mathbf{s}_j = \frac{1}{\sqrt{N}} \sum_j e^{ijk} \delta \mathbf{s}_k$$

- Which will decouple the normal modes, yielding equations

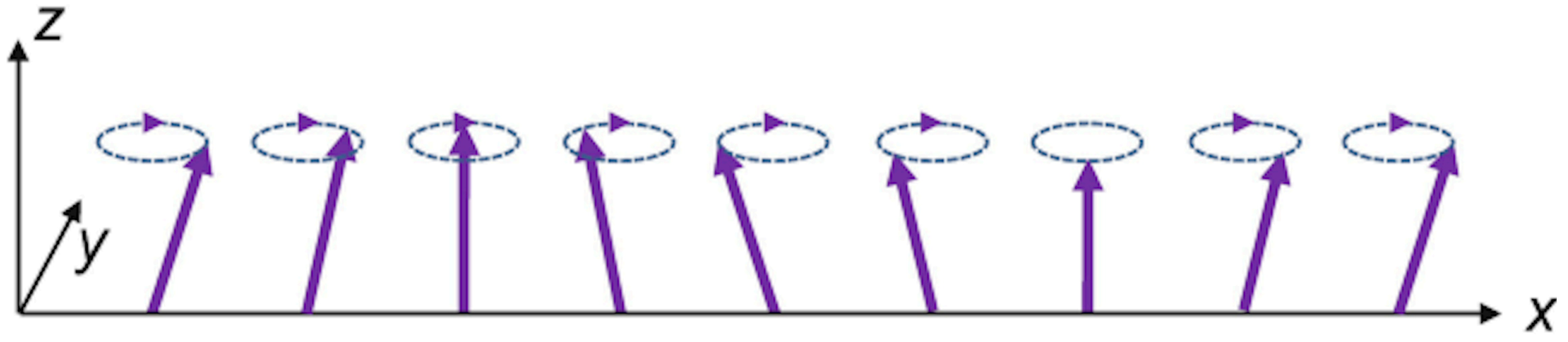
$$\delta \dot{\mathbf{s}}_k = \delta \mathbf{s}_k \times \mathbf{B}_k$$

FM Spin Chain

Linearize

- Which can be solved to yield a dispersion relation

$$\omega_k = |\tilde{\boldsymbol{B}}_k| = \left[\frac{2JS}{\hbar}[1 - \cos(ka)] + \frac{(B + 2D)}{\hbar}\right]$$



FM Spin Chain

- Claim: This is exactly the same dispersion relation that one gets from Linear Spin Wave Theory (LSWT).
- Suggests that one can "quantize" the normal mode of the linearized classical theory to recover the LSWT results.
- This correspondence depends on both theories being "S" theories (i.e. based on states that can be reached by SU(2) group actions).
- Let's make this plausible in Sunny

Takeaways I

Theoretical ideas

- There's a general recipe for generating coherent states.
- These are a large set of special states generated by a group.
- Which group is relevant depends on what operators are in your Hamiltonian.
- The coherent states serve as a basis for a corresponding classical theory.

Takeaways II

Relation between classical dynamics and spin wave theory

- The classical theory corresponding to dipolar spins ($SU(2)$ theory) is the Landau-Lifshitz equations.
- If these classical equations are linearized about the ground state, we get one harmonic oscillator per site.
- The associated dispersion relation is identical to what one gets from traditional LSWT.

Takeaways III

Uses of classical dynamics

- If LSWT is a good approximation, so is LL.
- LL, however, includes all nonlinearities.
- Classical dynamics therefore particularly useful for:
  - Capturing nonlinear effects at high-temperature
  - Studying out-of-equilibrium dynamics

Foreshadowing

- But we have seen hints that $SU(2)$ coherent states may not be sufficient
  - Cannot represent arbitrary spin-S states
  - Impose a “factorization rule” when taking classical limits.
- Next time we will extend our coherent state framework to the groups $SU(N)$, where $N > 2$.

Ideas behind Sunny.jl

Lecture 2: Generalizing the classical methods to “higher” spins and entangled units

David Dahlbom (ORNL) & Cristian Batista (UTK, LANL, ORNL) — April 16th, 2024

Brief recap

- Yesterday we discussed:
  - How the presence of S indicates the role SU(2) coherent states
  - This “bakes in” the assumption of a fully dipolar state
  - Sending $S \to \infty$ yields a classical theory, namely Landau-Lifshitz equations
  - S may also be used as an expansion parameter for SWT
  - In the $T \to \infty$ limit, the linearized classical theory and linear SWT essentially “agree”.

SU(2) algebra revisited

- Recall that the algebra of SU(2) consists of

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

- We can "complexify" this algebra in a manner similar to what we did with the harmonic oscillator

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

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

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

SU(2) algebra revisited

Schwinger Bosons

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

$$n_0 = b_0^\dagger b_0$$

$$n_1 = b_1^\dagger b_1$$

$$n_0 + n_1 = 2S$$

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

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

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

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

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

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

SU(2) algebra revisited

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$$n_0 = b_0^\dagger b_0$$

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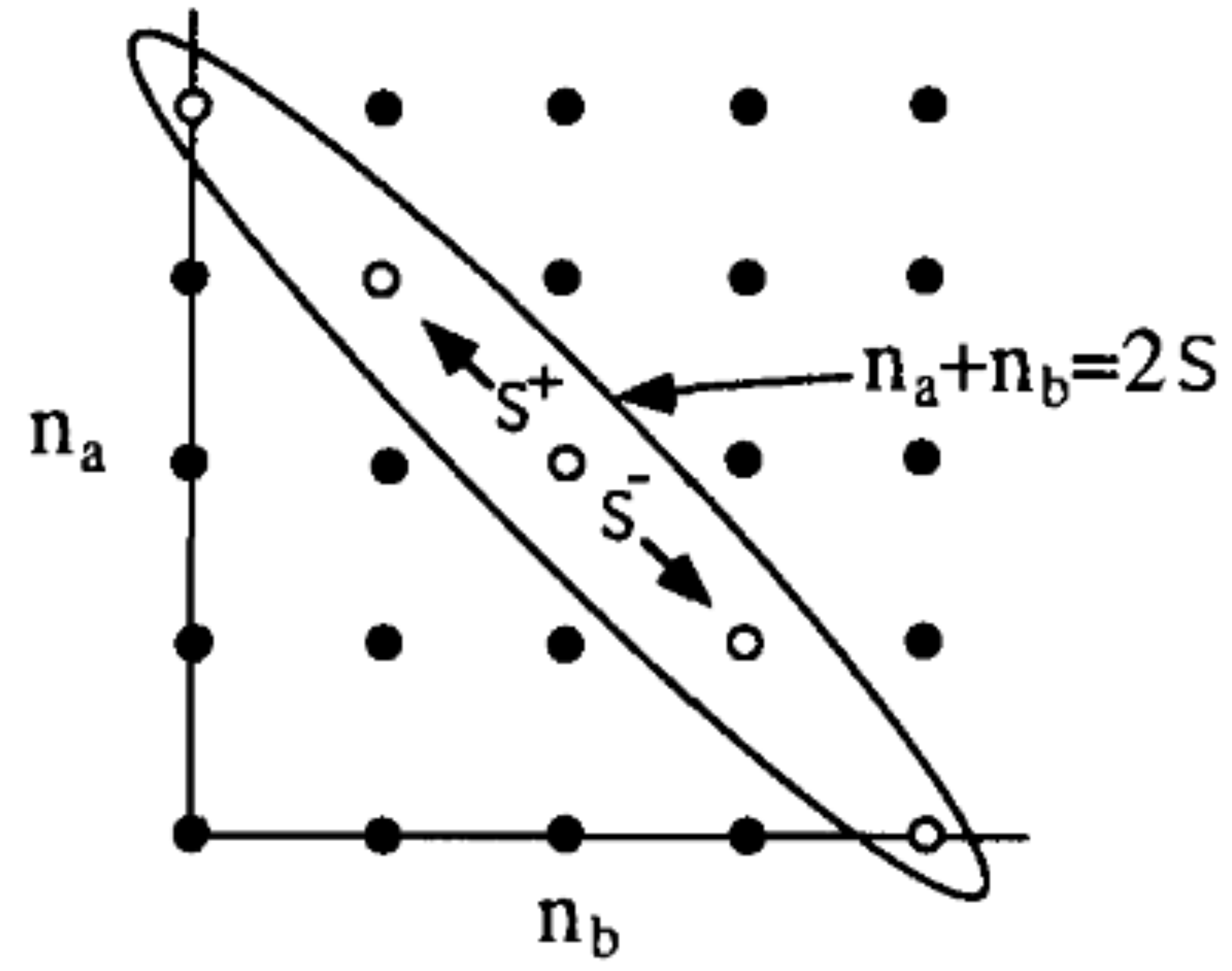
$$n_0 + n_1 = 2S$$



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

SU(2) algebra revisited

- The Schwinger 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.

SU(2) LSWT recipe

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)

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4. Fourier transform on the lattice
5. Para-diagonalize if necessary (Bogoliubov transformation)

SU(2) LSWT recipe

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).

$$\hat{S}_j^{\alpha} \to U_j^{\dagger}\left(\theta, \phi\right) \hat{S}_j^{\alpha} U_j\left(\theta, \phi\right)$$

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

SU(2) LSWT recipe
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.

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

SU(2) LSWT recipe

Bosonize

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

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

- Then "condense" the ground state boson.

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

Use as criterion to evaluated validity of any expansion.

SU(2) LSWT recipe

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

SU(2) LSWT recipe
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, $b_{j,1}^{\dagger} = \hat{X}_j + i\hat{P}_j$, per site

The SU(N) generalization

- Yesterday, we focused on the concept of classical limits and coherent states with respect to the harmonic oscillator and $SU(2)$
- Today we will follow the same program for $SU(N)$

The SU(N) generalization

- An $SU(N)$ coherent state faithfully represents the structure of an N-level system
- The choice of N depends on the local physics (the local “degrees” of freedom)
- Example: for a general spin-J site, N should be $2J + 1$
- Example: For a “site” containing two spin-$1/2$, N should 4

One motivation: Nonlinear terms

- The formalism of $SU(2)$coherent states — a classical theory based on fixed magnitude dipole — is not well matched to Hamiltonians that have terms that are nonlinear in the spin operators

- Consider a simple, single-site, $S = 1$ Hamiltonian:

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

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

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

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

One motivation: nonlinear terms

- 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:

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

The SU(N) coherent states

Recall the recipe

- Yesterday, we spoke about the algebra for $SU(2)$: $\hat{S}^x, \hat{S}^y, \hat{S}^z$
- For $SU(N)$, we will in general have an algebra of $N^2 - 1$ generators (observables): $\hat{T}^1, \hat{T}^2, \ldots, \hat{T}^{N^2-1}$
- SU(N) coherent states may be generated by exponentiating linear combinations of these generators

$$\left|\Omega_{\mathrm{SU}(N)}\right\rangle = e^{i\left(\sum_\alpha c_\alpha \hat{T}^\alpha\right)} \left|\uparrow\right\rangle$$

The SU(N) coherent states

Sources of SU(N) generators (observables)

- 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

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

The 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	$c_\pm\left[S_z, S_+ \pm S_-\right]_+$
	± 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

Parameterizing SU(N) Coherent States

- The manifold of SU(2) coherent states is ultimately a 2-dimensional object

$$\left|\Omega_{\mathrm{SU}(2)}\left(\theta,\phi\right)\right\rangle$$

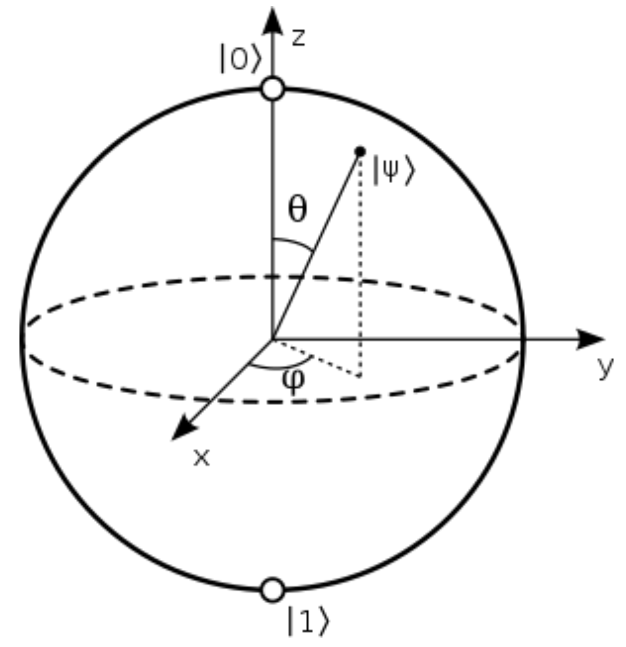
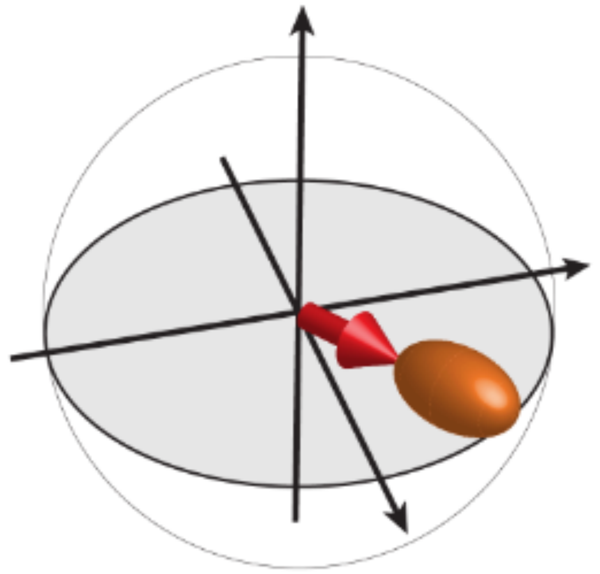
- Similarly, the manifold of SU(N) coherent states is 2(N-1)-dimensional

$$\left|\Omega_{\mathrm{SU(N)}}\left(\theta_1,\phi_1,\ldots,\theta_{N-1},\phi_{N-1}\right)\right\rangle$$

K. Nemoto, "Generalised coherent states for SU(N) systems," J. Phys. A, 33.17 (2000).

SU(N) coherent states

Summary of “how to think about” coherent states of $SU(N)$

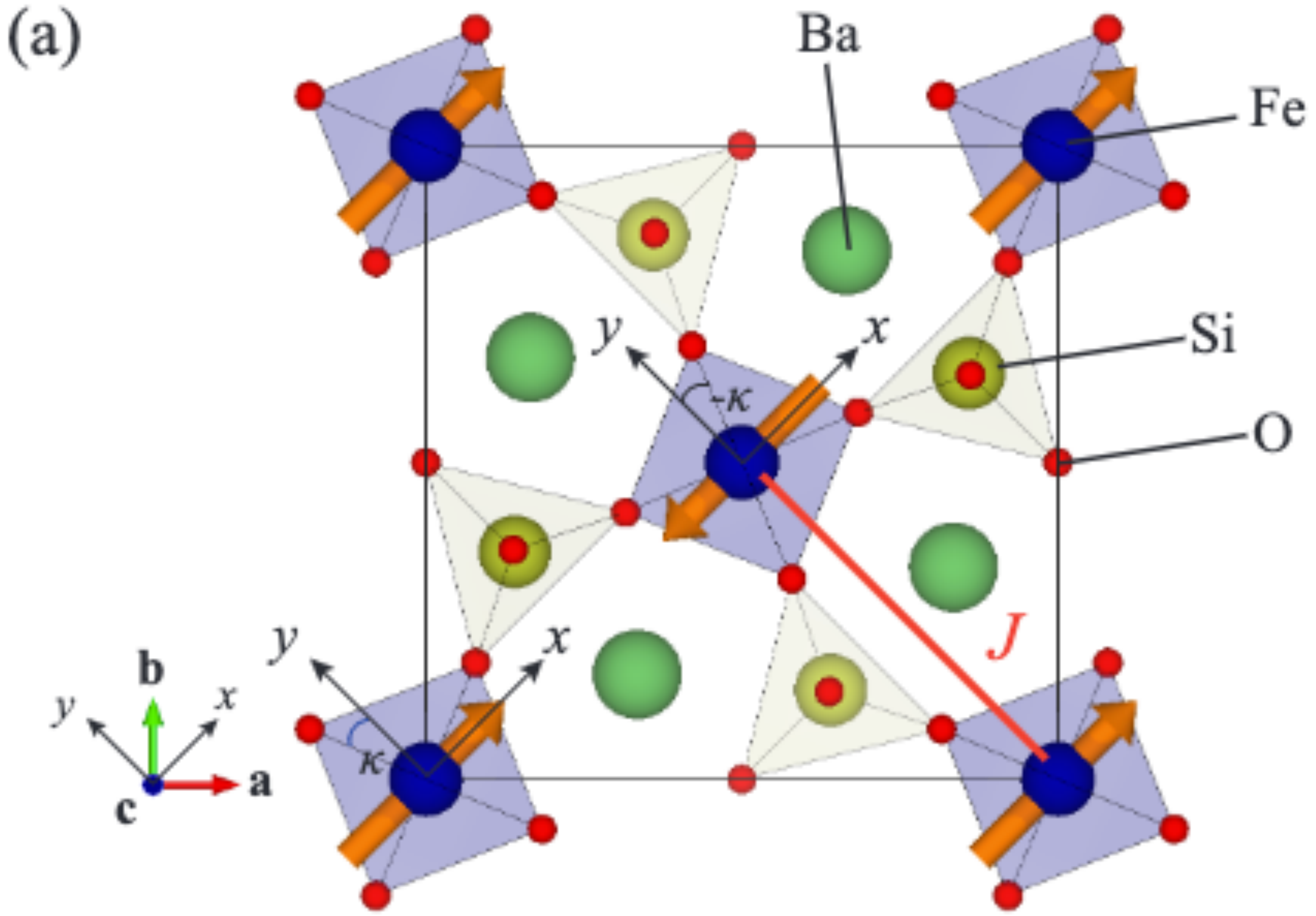
S	N	Dimension	# of observables	Illustration	Corresponds to	Angle Parametrization
1/2	2	2	3		Complex 2-vector	$\vert\Omega(\theta_1, \phi_1)\rangle$
1	3	4	8		Complex 3-vector	$\vert\Omega(\theta_1, \phi_1, \theta_2, \phi_2)\rangle$
3/2	4	6	15	?	Complex 4-vector	$\vert\Omega(\theta_1, \phi_1, \theta_2, \phi_2, \theta_3, \phi_3)\rangle$

Magnetization $Ba_2FeSi_2O_7$

Behavior of more generalized $S = 2$ spin (Sunny example)

- AFM, highly-anisotropic, easy-plane, square lattice

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

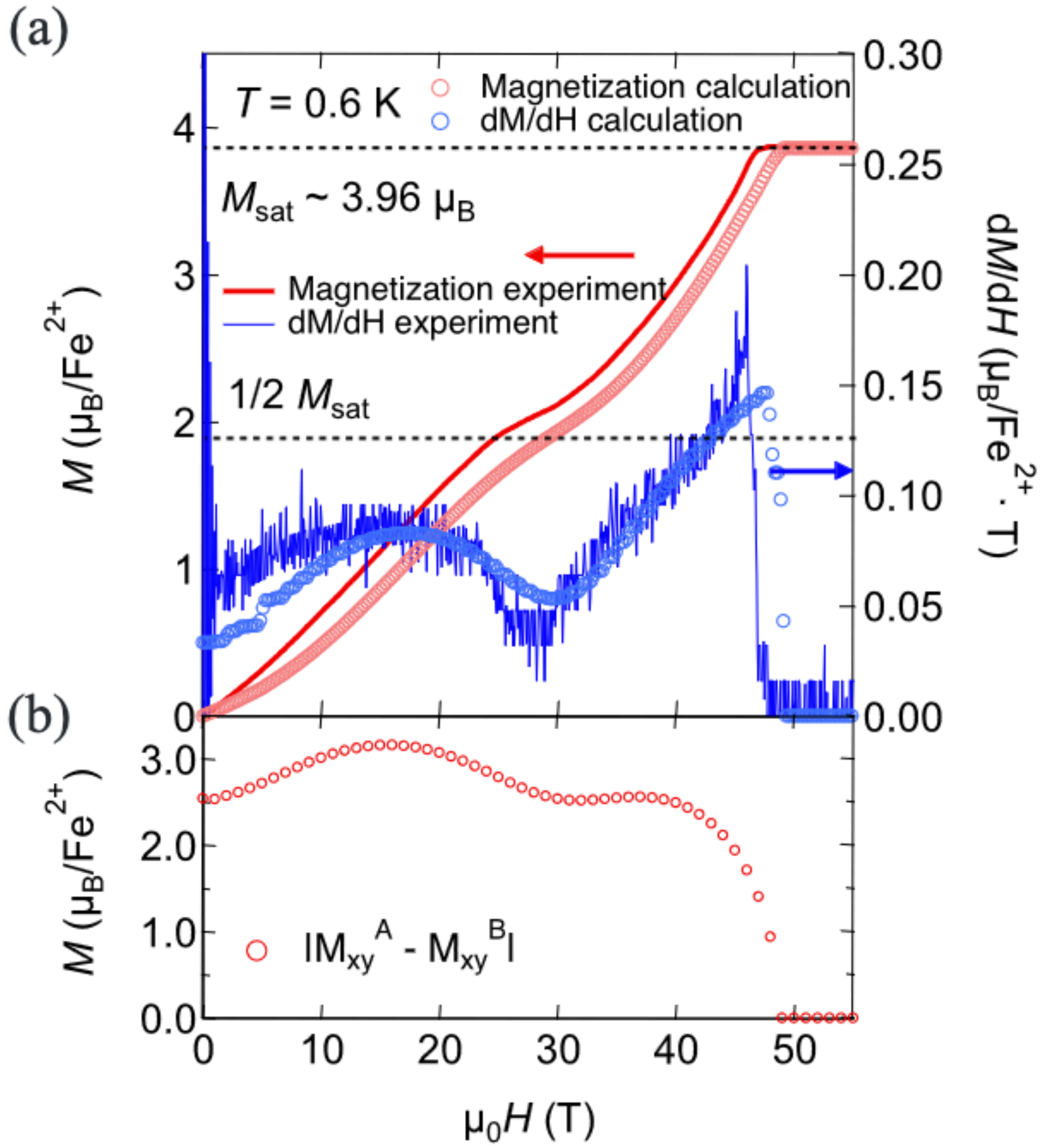


- S=2, so use SU(5): $|2\rangle\,, |1\rangle\,, |0\rangle\,, |-1\rangle\,, |-2\rangle$

M. Lee,…, **DD**, et al. Phys. Rev. B 107 (2023)

Magnetization $Ba_2FeSi_2O_7$

- Zero field: $|1\rangle\,,|0\rangle$
- Applied field: $|2\rangle\,,|0\rangle$
- Fully saturated: $|2\rangle$



Where the LL Equations Come From

Quick derivation

- Consider many-body spin Hamiltonian. Neglect entanglement between sites by restricting to tensor product basis of coherent states of SU(2)

$$|Z\rangle = \bigotimes_k |Z_k\rangle$$

Where the LL Equations Come From

Quick derivation

- Consider many-body spin Hamiltonian. Neglect entanglement between sites by restricting to tensor product basis of coherent states of SU(2)

$$|Z\rangle = \bigotimes_k |Z_k\rangle$$

- Derive equations of motion in Heisenberg picture

$$\begin{aligned} i\hbar \frac{dS_i^\alpha}{dt} &= \left[S_i^\alpha, \mathcal{H}\left(\mathbf{S}\right)\right] \\ &= i\hbar \epsilon_{\alpha\beta\gamma} \frac{\partial \mathcal{H}\left(\mathbf{S}\right)}{\partial S_i^\beta} S_i^\gamma \end{aligned}$$

Where the LL Equations Come From

Quick derivation

- Go to infinite representation limit, replace operators with expectation values

$$\frac{d \langle Z| S_i^\alpha |Z\rangle}{dt} = \epsilon_{\alpha\beta\gamma} \frac{\partial \langle Z| \mathcal{H}(\mathbf{S}) |Z\rangle}{\partial \langle Z| S_i^\beta |Z\rangle} \langle Z| S_i^\gamma |Z\rangle$$

Where the LL Equations Come From

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- Go to infinite representation limit, replace operators with expectation values

$$\frac{d\left\langle Z\right| S_i^{\alpha} \left|Z\right\rangle}{dt} = \boxed{\epsilon_{\alpha\beta\gamma}} \frac{\partial \left\langle Z\right| \mathcal{H}\left(\mathbf{S}\right) \left|Z\right\rangle}{\partial \left\langle Z\right| S_i^{\beta} \left|Z\right\rangle} \left\langle Z\right| S_i^{\gamma} \left|Z\right\rangle$$

- After some notational adjustments, this simply becomes the LL equations

$$\frac{d\mathbf{s}_j}{dt} = -\mathbf{s}_j \boxed{\times} \nabla_{\mathbf{s}_j} \mathcal{H}_{cl}\left(\mathbf{s}\right)$$

Generalizing the LL Equations

How to do it

- Coherent states of other groups, in particular SU(N), generated in analogous manner to SU(2).
- Consider complete set of generators of SU(N)

$$S^x, S^y, S^z \longrightarrow T^1, T^2, \ldots, T^{N^2-1}$$

- These generate group actions in turn generate the manifold of coherent states

$$|Z\rangle = e^{i(a_x S^x + a_y S^y + a_z S^z)} |\uparrow\rangle \longrightarrow |Z\rangle = e^{i \sum_\alpha c_\alpha T^\alpha} |\uparrow\rangle$$

Generalizing the LL Equations

How to do it

- We again have a one-to-one correspondence between coherent states and a vector of real values

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

$$\downarrow$$

$$|Z\rangle \leftrightarrow \left(\langle Z| T^1 |Z\rangle , \langle Z| T^2 |Z\rangle , \dots , \langle Z| T^{N^2-1} |Z\rangle\right) \equiv \vec{\mathbf{n}}$$

- The coherent states form a larger manifold, here CP^{N-1} instead of the (Bloch) sphere

Generalizing the LL Equations

How to do it

- We again consider a product basis (in coherent states of SU(N)!) and derive the equations of motion.

$$
\begin{aligned}
i\hbar\frac{dS_i^\alpha}{dt} &= \left[S_i^\alpha, \mathcal{H}\left(\mathbf{S}\right)\right] \\
&= i\hbar\epsilon_{\alpha\beta\gamma}\frac{\partial\mathcal{H}\left(\mathbf{S}\right)}{\partial S_i^\beta}S_i^\gamma
\end{aligned}
\longrightarrow
\begin{aligned}
i\hbar\frac{dT_i^\alpha}{dt} &= \left[T_i^\alpha, \mathcal{H}\left(\mathbf{T}\right)\right] \\
&= i\hbar f_{\alpha\beta\gamma}\frac{\partial\mathcal{H}\left(\mathbf{T}\right)}{\partial T_i^\beta}T_i^\gamma
\end{aligned}
$$

Generalizing the LL Equations

How to do it

- We again consider a product basis (in coherent states of SU(N)!) and derive the equations of motion.

$$
\begin{aligned}
i\hbar \frac{dS_i^\alpha}{dt} &= \left[S_i^\alpha, \mathcal{H}\left(\mathbf{S}\right)\right] \\
&= i\hbar \epsilon_{\alpha\beta\gamma} \frac{\partial \mathcal{H}\left(\mathbf{S}\right)}{\partial S_i^\beta} S_i^\gamma
\end{aligned}
\quad \longrightarrow \quad
\begin{aligned}
i\hbar \frac{dT_i^\alpha}{dt} &= \left[T_i^\alpha, \mathcal{H}\left(\mathbf{T}\right)\right] \\
&= i\hbar f_{\alpha\beta\gamma} \frac{\partial \mathcal{H}\left(\mathbf{T}\right)}{\partial T_i^\beta} T_i^\gamma
\end{aligned}
$$

$$\left[T^\alpha, T^\beta\right] = f_{\alpha\beta\gamma} T^\gamma$$

Generalizing the LL Equations

How to do it

- Taking the classical limit (sending irreps of SU(N) to infinity)
- $$\frac{d \langle Z| T_j^\alpha |Z\rangle}{dt} = f_{\alpha\beta\gamma} \frac{\partial \langle Z| \mathcal{H}(\mathbf{T}) |Z\rangle}{\partial \langle Z| T_j^\beta |Z\rangle} \langle Z| T_j^\gamma |Z\rangle$$
- With some notational changes, this becomes

$$\boxed{\frac{d\mathbf{n}_j}{dt} = -\mathbf{n}_j \star \nabla_{\mathbf{n}_j} \mathcal{H}_{SU(N)}} \qquad \mathcal{H}_{SU(N)} = \langle Z| \mathcal{H}(\mathbf{T}) |Z\rangle$$

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

Generalizing the LL Equations

What did we get?

- The resulting equations can represent spin states that cannot be represented by the LL formalism
- There is no longer any need to invoke the factorization rule when taking the classical limit

$$\mathcal{H} = (S^z)^2 = \sum_\alpha c_\alpha T^\alpha$$

$$\langle Z| \mathcal{H} |Z\rangle = \langle Z| (S^z)^2 |Z\rangle = \sum_\alpha c_\alpha \langle Z| T^\alpha |Z\rangle$$

Numerical obstacles

- The number of generators, T^{α}, for SU(N) is $N^2 - 1$. So the number of variables grows rapidly.

$$\mathfrak{su}(2)$$

$$\begin{bmatrix} 0 & -h^z & h^y \\ h^z & 0 & -h^x \\ -h^y & h^x & 0 \end{bmatrix} \longrightarrow$$

$$\mathfrak{su}(3)$$

$$\begin{bmatrix}
0 & -B^3 & B^2 & -B^7 & \left(B^6+\sqrt{3}B^8\right) & -B^5 & B^4 & -\sqrt{3}B^5 \\
B^3 & 0 & -B^1 & \left(B^6-\sqrt{3}B^8\right) & B^7 & -B^4 & -B^5 & \sqrt{3}B^4 \\
-B^2 & B^1 & 0 & -B^5 & B^4 & -2B^7 & 2B^6 & 0 \\
B^7 & -\left(B^6-\sqrt{3}B^8\right) & B^5 & 0 & -B^3 & B^2 & -B^1 & -\sqrt{3}B^2 \\
-\left(B^6+\sqrt{3}B^8\right) & -B^7 & -B^4 & B^3 & 0 & B^1 & B^2 & \sqrt{3}B^1 \\
B^5 & B^4 & 2B^7 & -B^2 & -B^1 & 0 & -2B^3 & 0 \\
-B^4 & B^5 & -2B^6 & B^1 & -B^2 & 2B^3 & 0 & 0 \\
\sqrt{3}B^5 & -\sqrt{3}B^4 & 0 & \sqrt{3}B^2 & -\sqrt{3}B^1 & 0 & 0 & 0
\end{bmatrix}$$

Schrödinger Formulation of LL

Hint of alternate formulation

- Recall that we had a one-to-one correspondence between two representations of a coherent state

$$|Z\rangle \leftrightarrow \Big(\langle Z|\, T^1\, |Z\rangle\,, \langle Z|\, T^2\, |Z\rangle\,, \ldots, \langle Z|\, T^{N^2-1}\, |Z\rangle\Big) \equiv \vec{\mathbf{n}}$$

- The expectation value representation is larger than the ket representation

- The latter came from the Heisenberg picture…can we use the former in a Schrödinger formulation (using the fundamental representation)?

Schrödinger Formulation of LL

- In deriving the generalized LL equations, we found

$$\frac{d\left\langle Z\right| T_j^\alpha \left|Z\right\rangle}{dt} = f_{\alpha\beta\gamma}\boxed{\frac{\partial\left\langle Z\right| \mathcal{H}\left(\mathbf{T}\right)\left|Z\right\rangle}{\partial\left\langle Z\right| T_j^\beta \left|Z\right\rangle}}\left\langle Z\right| T_j^\gamma \left|Z\right\rangle$$

- Use this to define a local Hamiltonian operator

$$\mathfrak{H}_j = \sum_\alpha \frac{\partial\left\langle Z\right| \mathcal{H}\left(\mathbf{T}\right)\left|Z\right\rangle}{\partial\left\langle Z\right| T_j^\alpha \left|Z\right\rangle} T^\alpha$$

Schrödinger Formulation of LL

- Then it can be shown that the following dynamics is entirely equivalent to the dynamics derived above

$$\boxed{\frac{d\left|Z_j\right\rangle}{dt} = -i\mathfrak{H}_j\left|Z_j\right\rangle} \qquad \mathfrak{H}_j = \sum_\alpha \frac{\partial\left\langle Z\right|\mathcal{H}\left(\mathbf{T}\right)\left|Z\right\rangle}{\partial\left\langle Z\right|T_j^\alpha\left|Z\right\rangle} T^\alpha$$

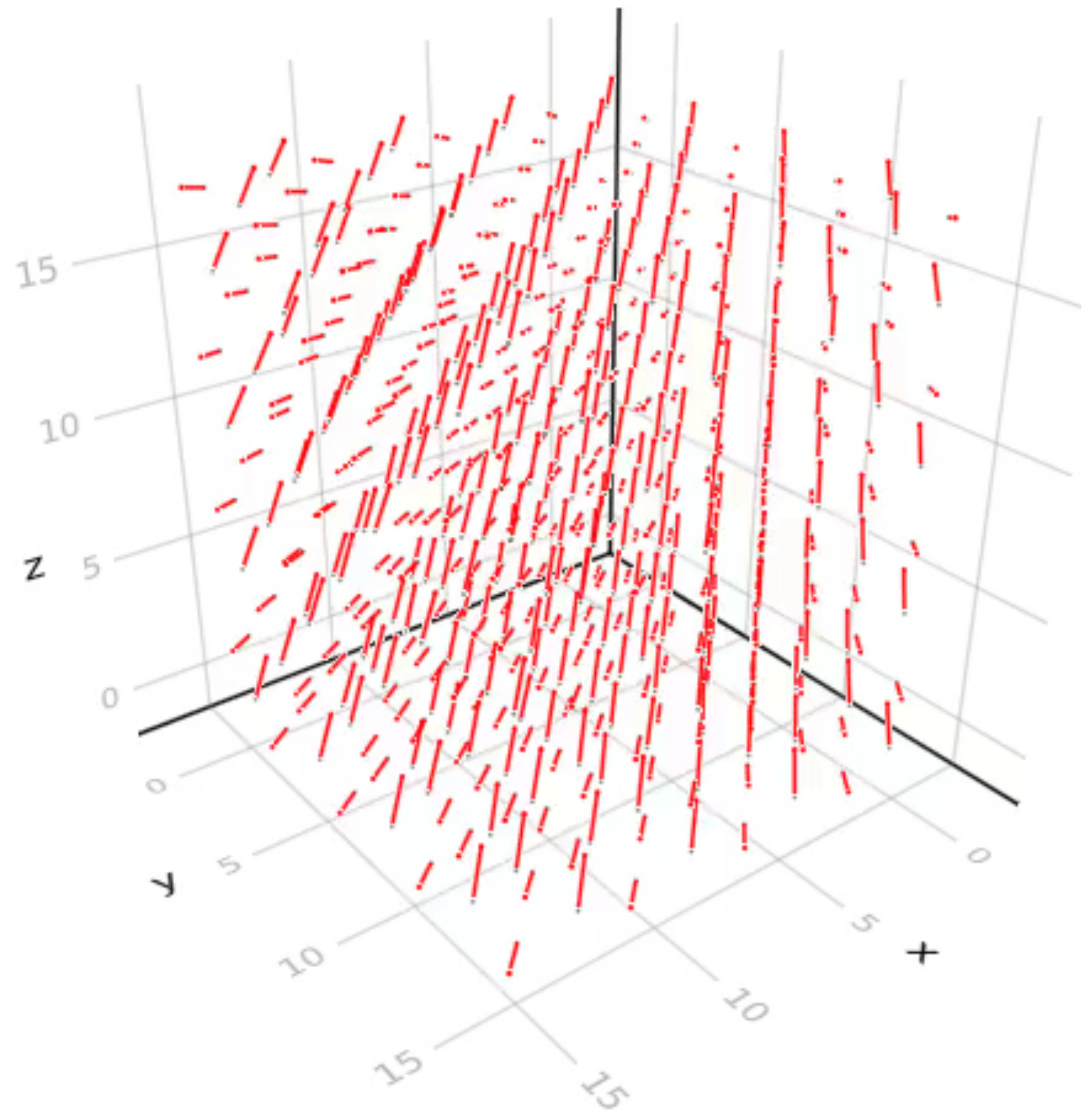
DD, H. Zhang, C. Miles, X. Bai, C.D. Batista, K. Barros. PRB (2022). https://doi.org/10.1103/PhysRevB.106.054423

Schrödinger Formulation of LL

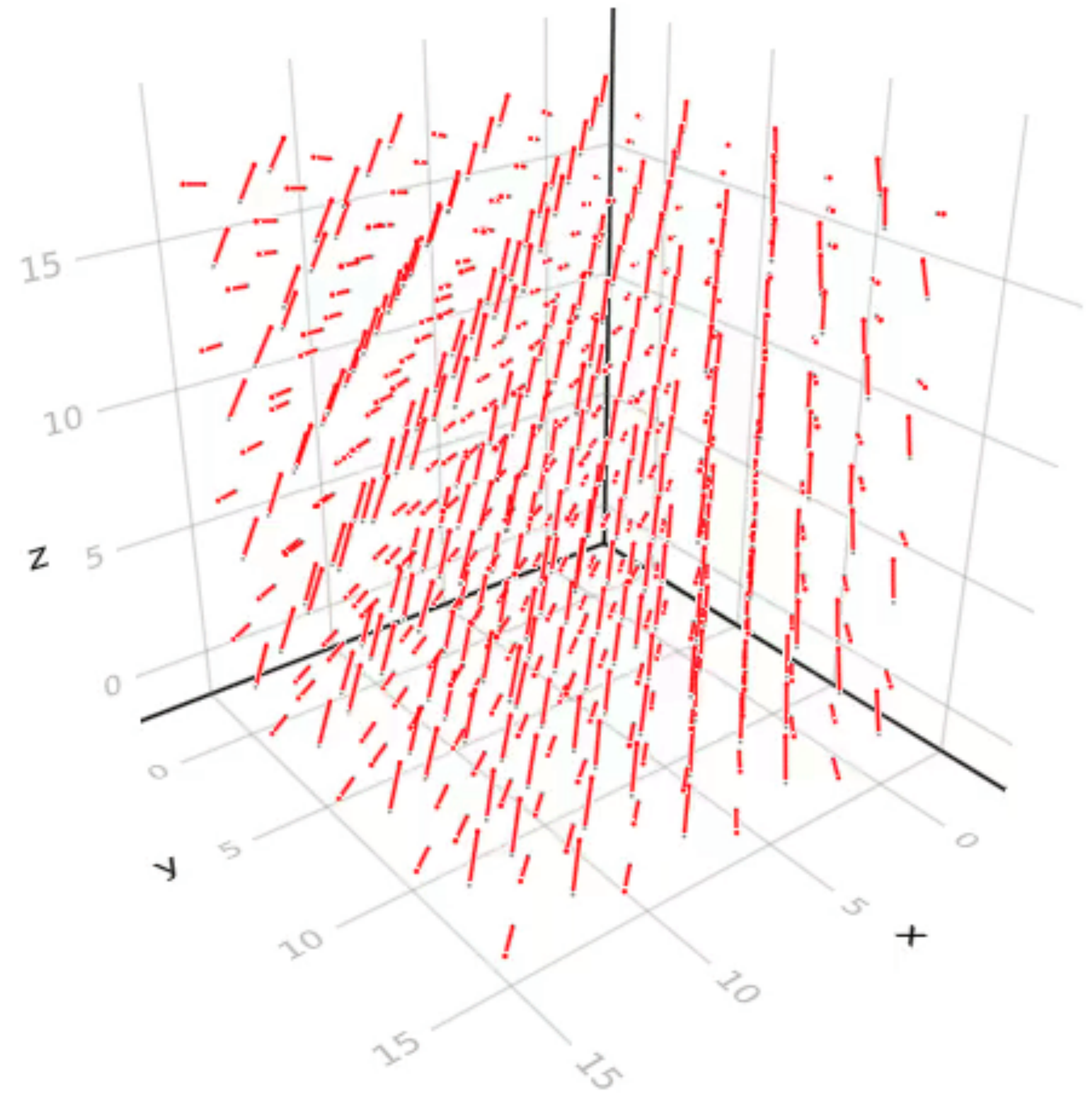
Numerical advantages

- $2N < N^2 - 1$

- Global Hamiltonian structure



Heun (RK-type): Δt = 0.0125



Midpoint (symplectic): Δt = 0.05

Langevin Dynamics

Finite temperature

- The Stochastic LLG equations can be generalized in natural way
- This can be extended to Schrödinger picture formulation

$$\frac{d\mathbf{s}_j}{dt} = -\mathbf{s}_j \times \frac{\partial H}{\partial \mathbf{s}_j} \longrightarrow \frac{d\mathbf{s}_j}{dt} = -\mathbf{s}_j \times \left(\xi_j + \frac{\partial H}{\partial \mathbf{s}_j} - \lambda \mathbf{s}_j \times \frac{\partial H}{\partial \mathbf{s}_j} \right)$$

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$$\frac{d\mathbf{Z}_j}{dt} = -i\mathfrak{H}_j \mathbf{Z}_j \longrightarrow \frac{d\mathbf{Z}_j}{dt} = -iP_j \left[\zeta_j + \left(1 - i\tilde{\lambda}\right) \mathfrak{H}_j \mathbf{Z}_j\right]$$

DD, C. Miles, H. Zhang, C.D. Batista, K. Barros. PRB (2022). https://doi.org/10.1103/PhysRevB.106.235154

SU(N) generalization of LSWT

Organizational principle for multiflavor bosons

- Traditional Schwinger bosons give a language for rewriting the spin operators $\hat{S}^x, \hat{S}^y, \hat{S}^z$ — the generators of $SU(2)$.
- We can introduce additional "flavors" of boson that enable us to rewrite an arbitrary generator of $SU(N)$.
- In general we will need N flavors.
- After condensation, we will have $(N-1)$ modes.
- This is the number of DoF in the corresponding classical theory, where there are $2(N-1)$ angles parameterizing each CS

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

SU(N) generalization of LSWT

Organizational principle for multiflavor bosons

- For SU(2) we had two flavors of boson.
- For SU(N) we have N flavors of boson.

$$\left\{ b_{j,0}, b_{j,1} \right\} \longrightarrow \left\{ b_{j,0}, \ldots, b_{j,N-1} \right\}$$

- For SU(2) we had the constraint.
- For SU(N) we have the constraint.

$$b^\dagger_{0,j} b_{0,j} + b^\dagger_{1,j} b_{1,j} = 2S \longrightarrow \sum_{m=0}^{N-1} b^\dagger_{j,m} b_{j,m} = M$$

SU(N) generalization of LSWT

Transformations associated with ground state

- The ground state is an $SU(2)$ coherent state, i.e., a dipole. This was specified by an $SU(2)$ rotation

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

- Now the ground state is an $SU(N)$ coherent state specified by an $SU(N)$ rotation

$$\hat{T}_j^\alpha \to U_j^\dagger\left(\theta_1,\ldots,\theta_{2(N-1)}\right)\hat{T}_j^\alpha U_j\left(\theta_1,\ldots,\theta_{2(N-1)}\right)$$

SU(N) generalization of LSWT

Bosonize

- For SU(2) LSWT, we used the following substitutions

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

- For SU(N) LSWT, we always have the simple recipe (because work in fundamental representation).

$$\hat{T}_j^\alpha \to \mathbf{b}_j^\dagger \hat{T}_j^\alpha \mathbf{b}_j \qquad \mathbf{b}_j = \begin{pmatrix} b_{j,0} \\ b_{j,1} \\ \vdots \\ b_{j,N-1} \end{pmatrix}$$

SU(N) generalization of LSWT

Bosonize

- For SU(2) LSWT, we used the standard Holstein-Primakoff transformation

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

- For SU(N) LSWT, we use the generalized Holstein-Primakoff transformation

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

SU(N) generalization of LSWT

Collect terms in orders of M

- For $SU(2)$ expanded the Holstein-Primakoff boson in powers of S and collected terms of like order

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

For$SU(N)$, we do the exact same, but in powers of M

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

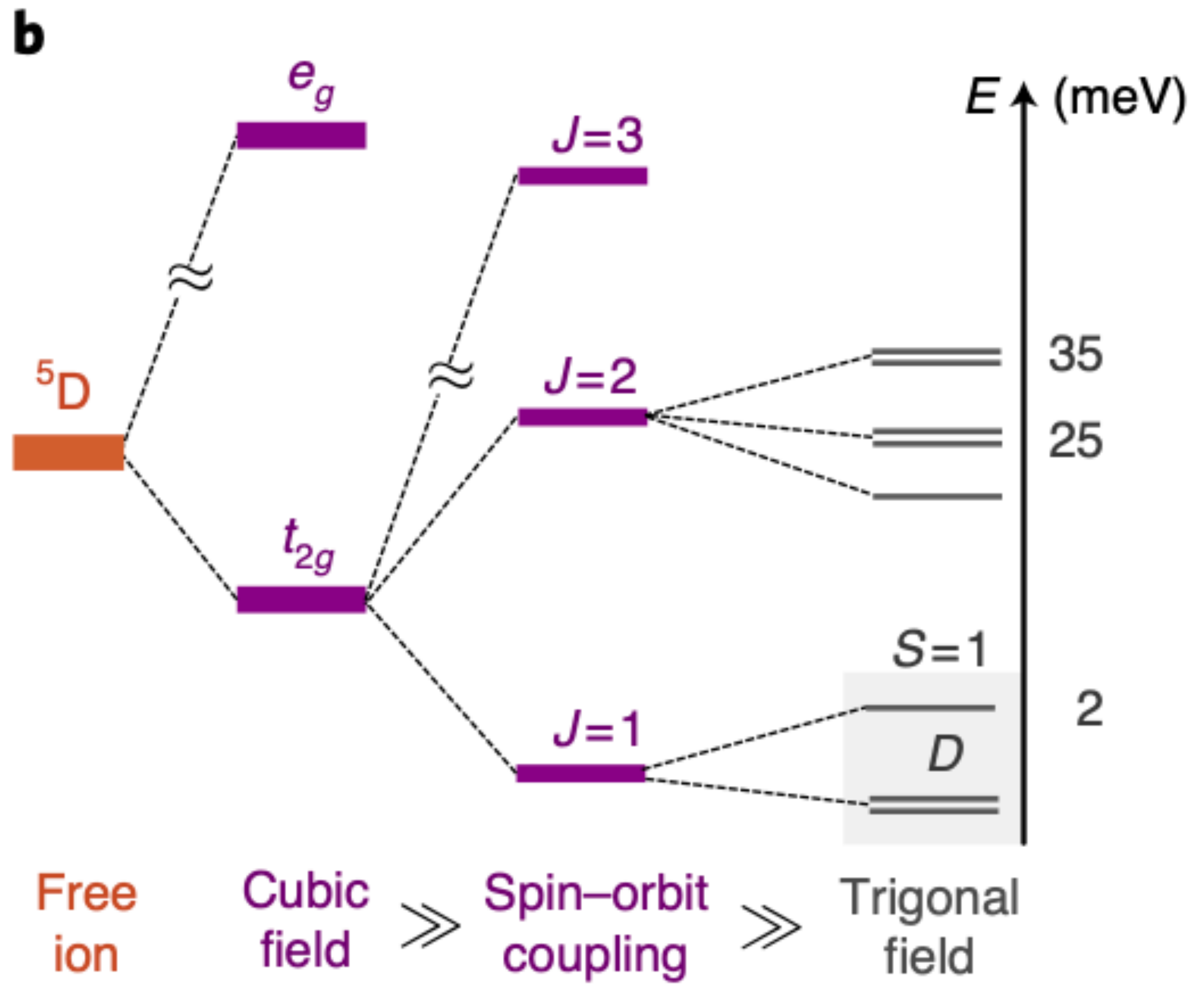
SU(N) generalization of LSWT

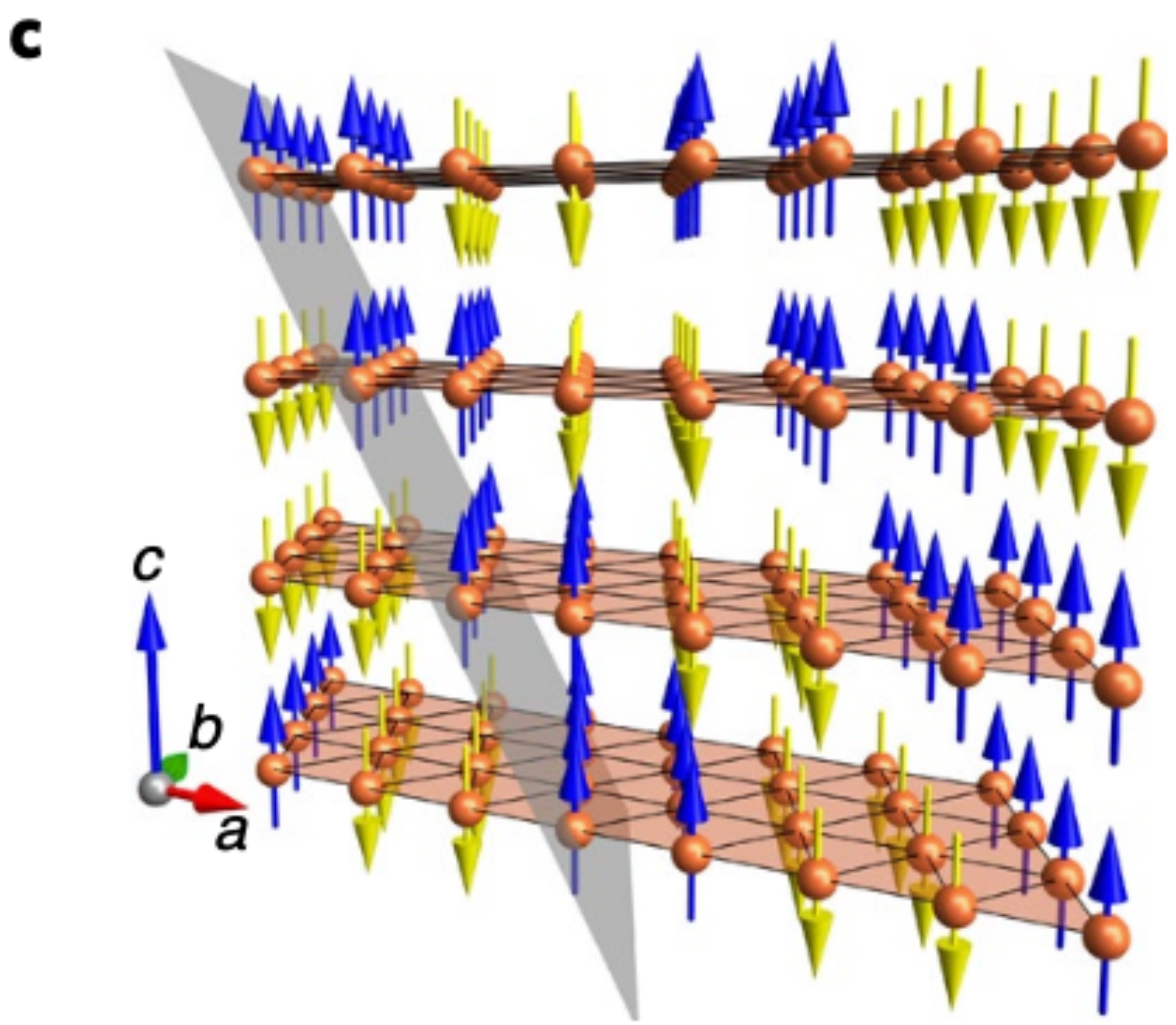
Diagonalize

- The quadratic Hamiltonian $\hat{H}^{(2)}$ can then be diagonalized
  - Exploit translation invariance (Fourier transform on the lattice)
  - Apply a paraunitary (Bogoliubov) transformation
- The $SU(N)$ generalization introduces no essential changes to these steps.

S=1 example: FeI_2

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

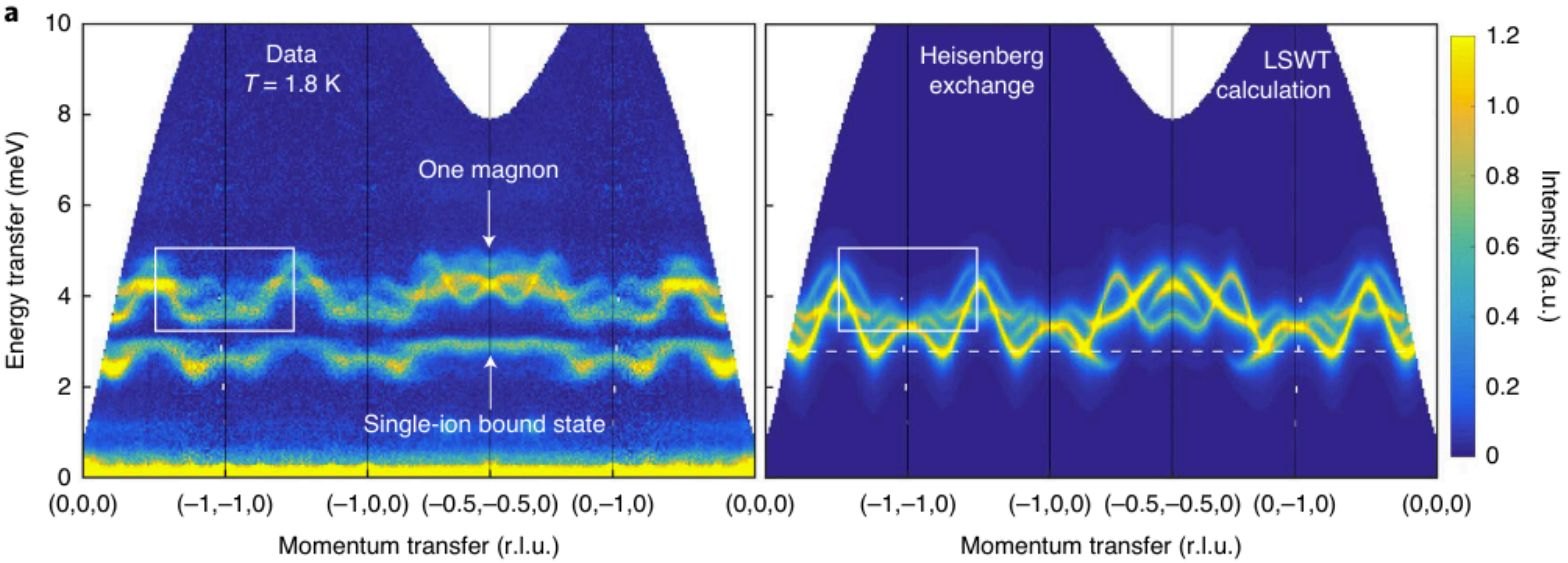




Xiaojian Bai et al. “Hybridized quadrupolar excitations…”, Nature Physics (2021).

S=1 example: FeI_2

Prediction from SU(3) theory



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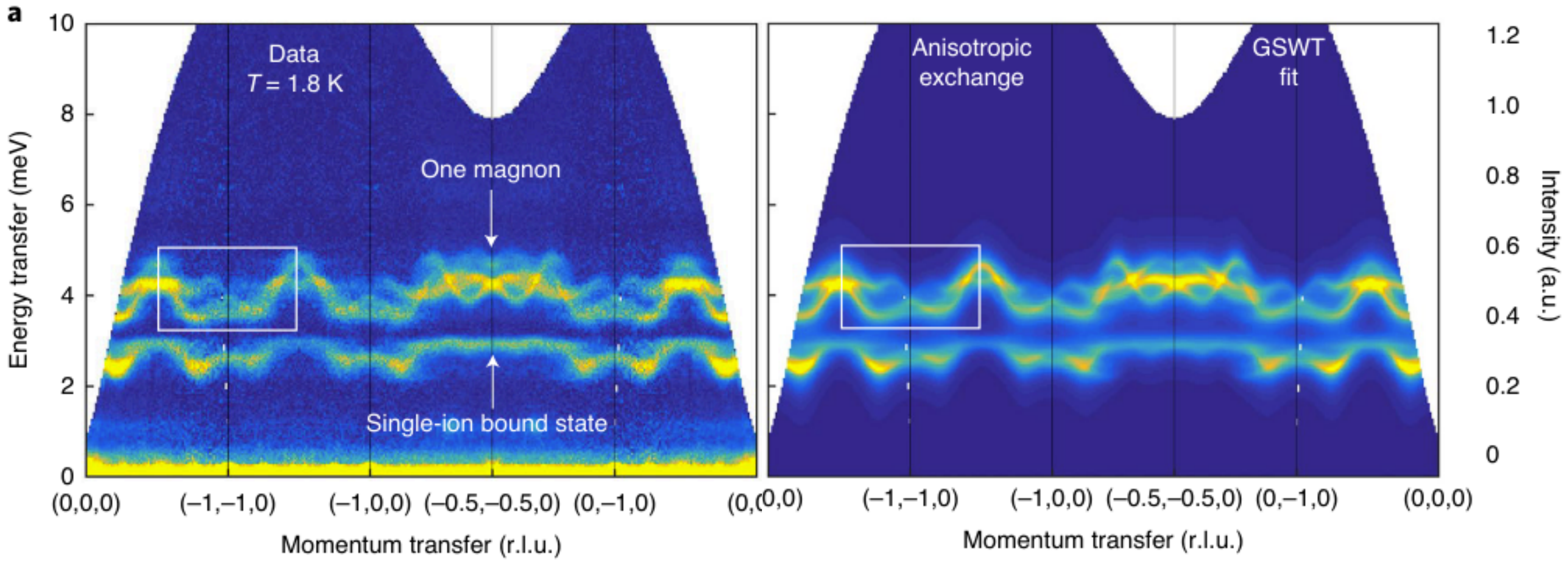
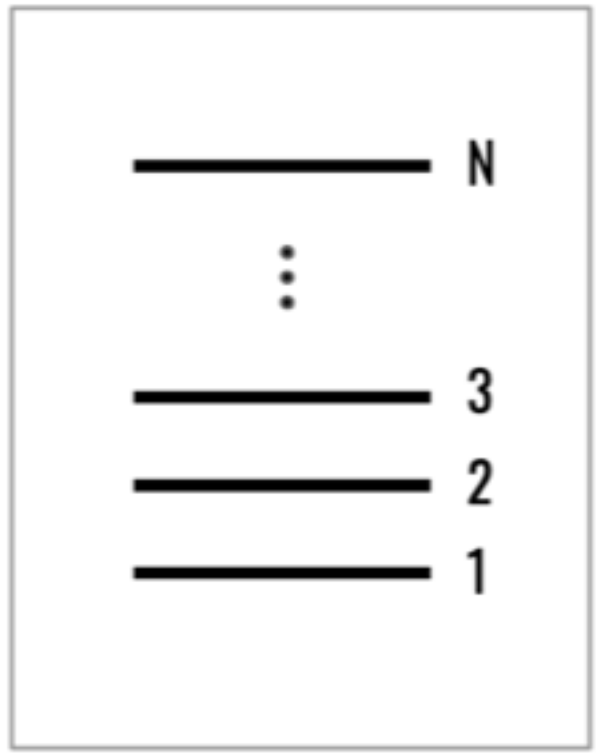


Xiaojian Bai et al. “Hybridized quadrupolar excitations…”, Nature Physics (2021).

What else can go in the box?

- No reason the local Hilbert space must be interpreted as a big spin.
- No reason local Hamiltonian has to be constructed from spin (or higher order multipole) operators alone.
- Can put whatever quantum mechanical system at each box.

$\mathfrak{H}_i$

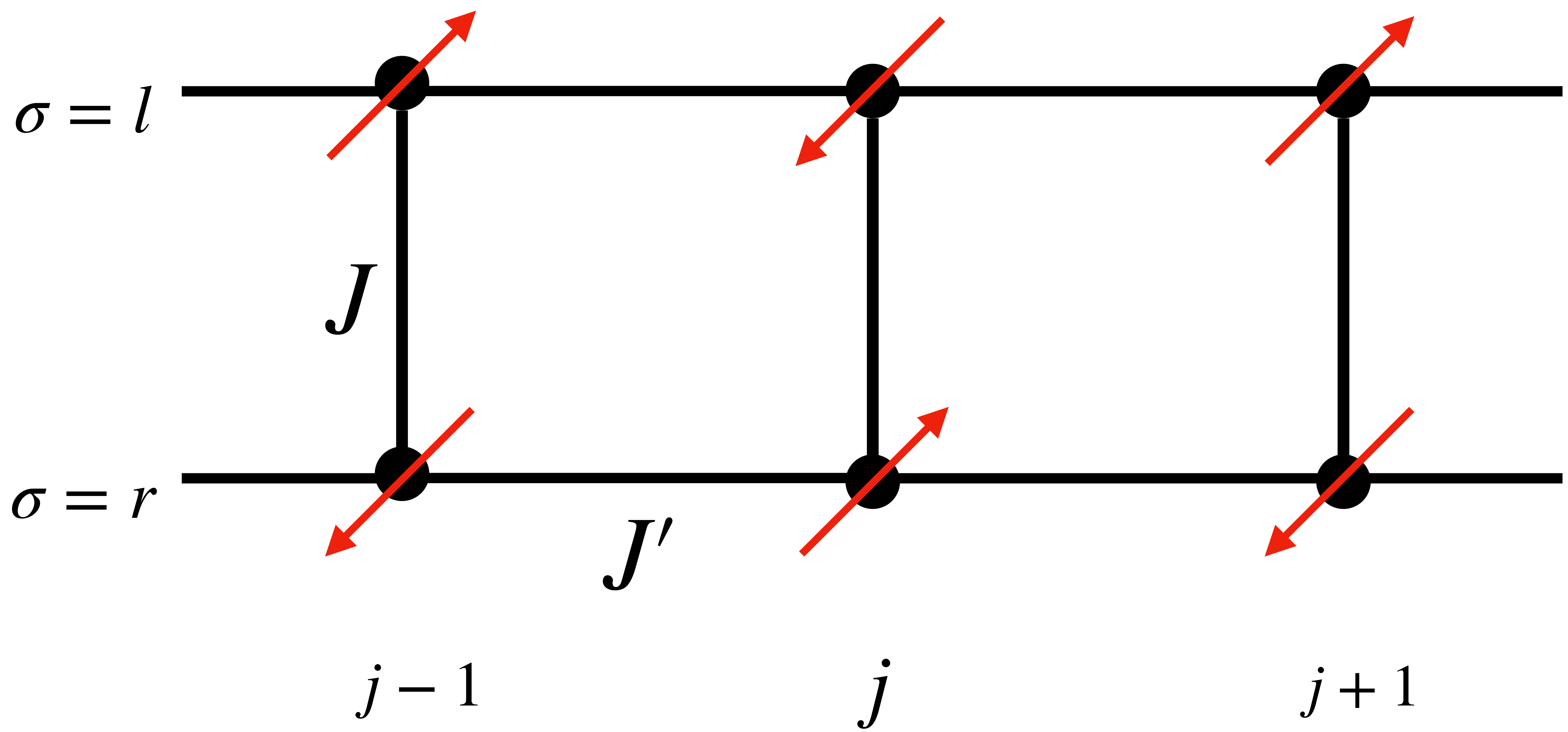


Strong-rung S=1/2 ladder

Modeling localized entanglement

- AFM $S = 1/2$ spin ladder

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



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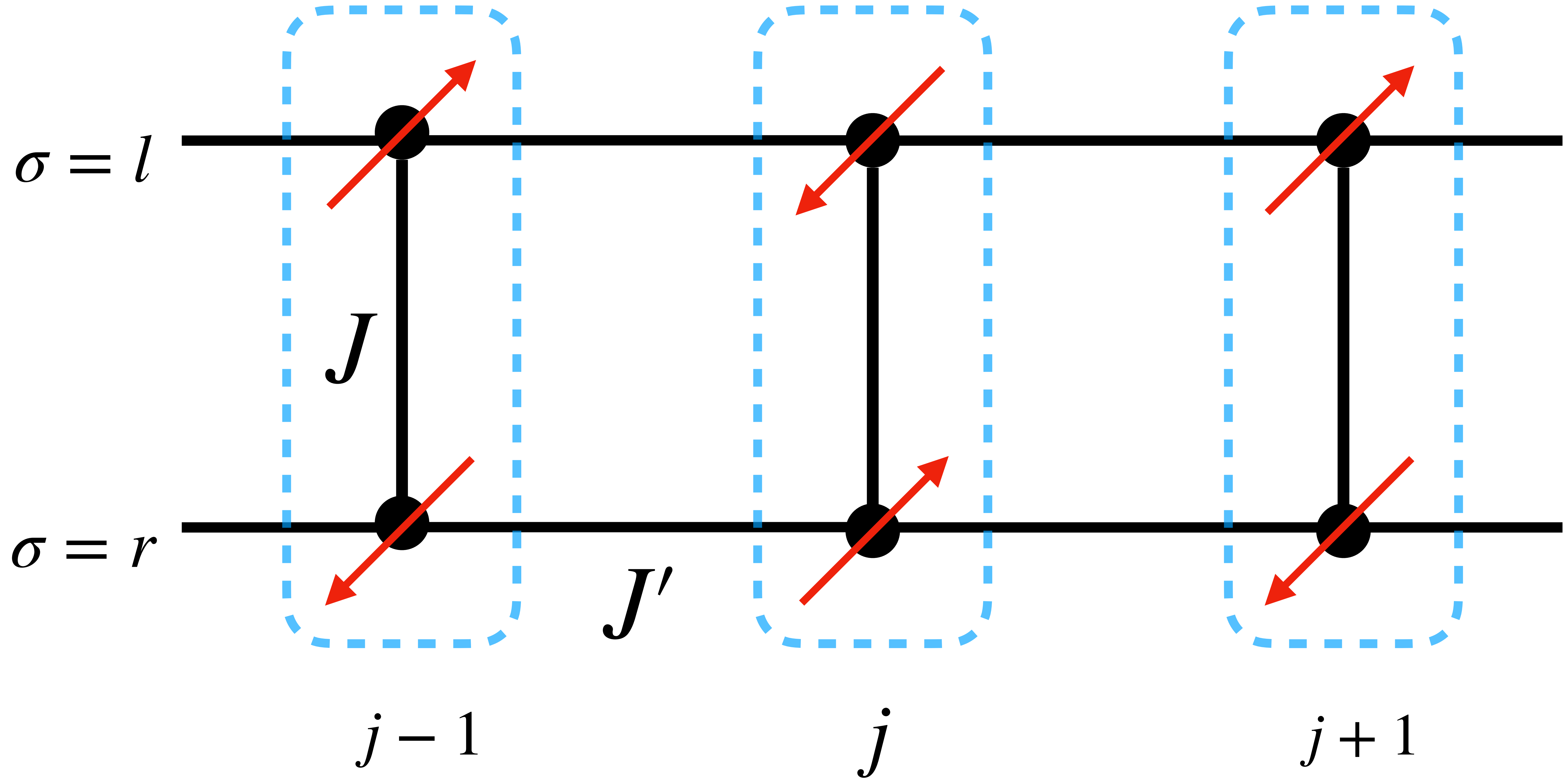
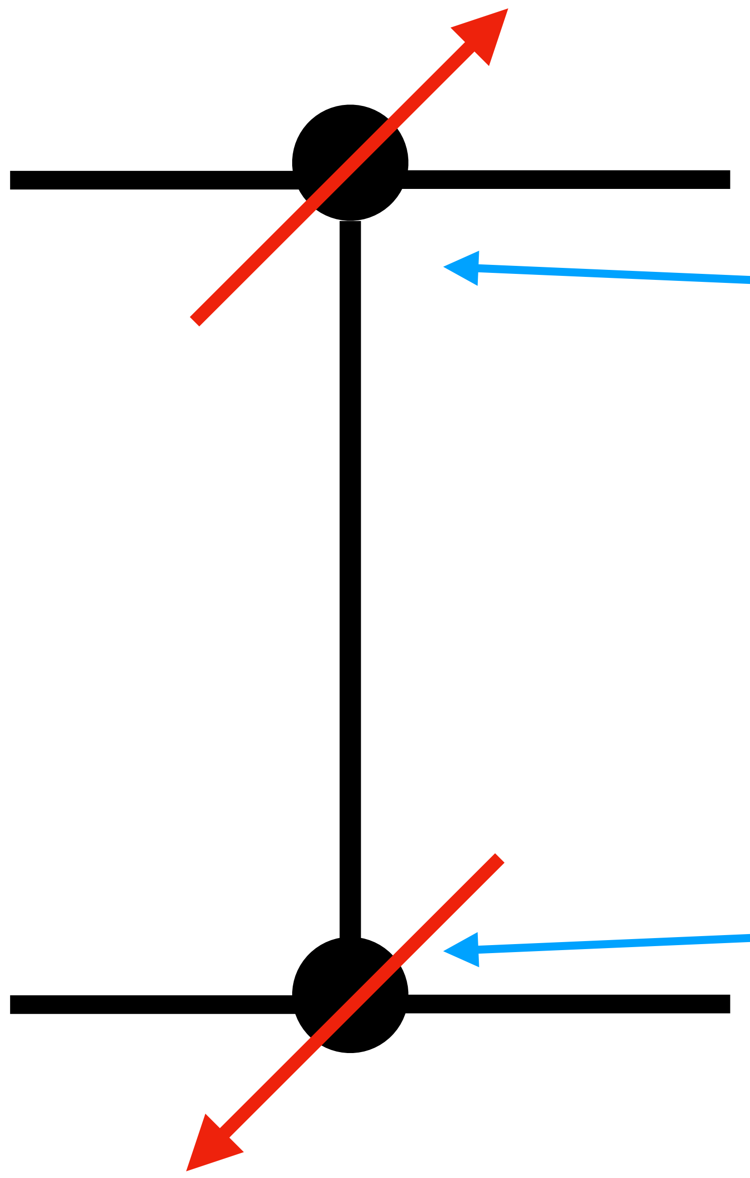


$J'/J < 0.5$

Strong-rung S=1/2 ladder

Choosing the "local Hilbert space"

- In the large S approach, the local Hilbert space is 2 spin-1/2: $\mathbb{C}^2 \oplus \mathbb{C}^2$



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

SU(2) CS

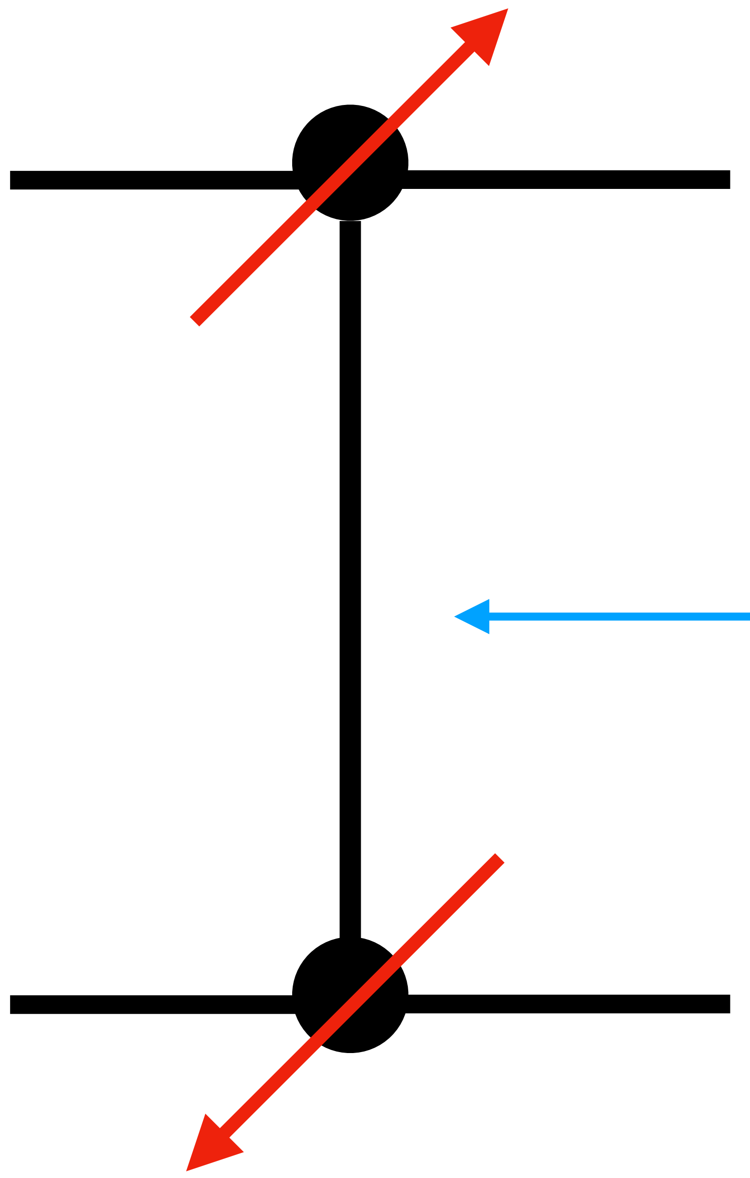
$$\begin{pmatrix} \alpha_{j,r} \\ \beta_{j,r} \end{pmatrix} = \alpha_{j,r} | \uparrow \rangle + \beta_{j,r} | \downarrow \rangle$$

SU(2) CS

Strong-rung S=1/2 ladder

Choosing the "local Hilbert space"

- Here we instead choose the Hilbert space of bonds: $\mathbb{C}^2 \otimes \mathbb{C}^2 = \mathbb{C}^4$



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

SU(4) CS

Strong-rung S=1/2 ladder

Choosing a "basis" of SU(4) generators

- We will work in the Heisenberg picture and select an explicit (and complete) set of observables:

$$
\begin{array}{lll}
\hat{T}^1 = \hat{S}_l^x & \hat{T}^2 = \hat{S}_l^y & \hat{T}^3 = \hat{S}_l^z \\
\hat{T}^4 = \hat{S}_r^x & \hat{T}^5 = \hat{S}_r^y & \hat{T}^6 = \hat{S}_r^z \\
\hat{T}^7 = 2\hat{S}_l^x \hat{S}_r^x & \hat{T}^8 = 2\hat{S}_l^y \hat{S}_r^y & \hat{T}^9 = 2\hat{S}_l^z \hat{S}_r^z \\
\hat{T}^{10} = 2\hat{S}_l^y \hat{S}_r^z & \hat{T}^{11} = 2\hat{S}_l^z \hat{S}_r^y & \hat{T}^{12} = 2\hat{S}_l^z \hat{S}_r^x \\
\hat{T}^{13} = 2\hat{S}_l^x \hat{S}_r^z & \hat{T}^{14} = 2\hat{S}_l^x \hat{S}_r^y & \hat{T}^{15} = 2\hat{S}_l^y \hat{S}_r^x
\end{array}
$$

Strong-rung S=1/2 ladder

Choosing a "basis" of SU(4) generators

- These observables are "complete" in the sense that any Hermitian operator acting on $\mathbb{C}^4$ may be written as a linear combination in terms of them:

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

- And they orthonormal in that,

$$\mathrm{tr}\hat{T}^\alpha \hat{T}^\beta = \delta_{\alpha\beta}$$

Strong-rung S=1/2 ladder

Choosing a “basis” of SU(4) generators

- Finally, they satisfy the commutation relations,

$$\left[\hat{T}^{\alpha}, \hat{T}^{\beta}\right] = i f_{\alpha\beta\gamma} \hat{T}^{\gamma}$$

- With the structure constants,

$$\begin{gathered}
f_{1,2,3} = f_{1,8,11} = f_{2,9,13} = f_{2,11,14} = f_{3,7,15} = 1 \\
f_{1,9,10} = f_{1,12,15} = f_{2,7,12} = f_{3,8,14} = f_{3,10,13} = -1 \\
f_{4,5,6} = f_{4,8,10} = f_{5,9,12} = f_{5,10,15} = f_{6,7,14} = 1 \\
f_{4,9,11} = f_{4,13,14} = f_{5,7,13} = f_{6,8,15} = f_{6,11,12} = -1.
\end{gathered}$$

Strong-rung S=1/2 ladder

Classical limit

- We now have all the pieces necessary to derive the generalized Landau-Lifshitz equations for this problem.

- Given a product of SU(4) coherent states: $$|\Psi\rangle = \bigotimes_j |\Psi_j\rangle$$

- Define our "classical" variables: $$n_j^\alpha = \left\langle \Psi \left| \hat{T}^\alpha \right| \Psi \right\rangle$$

Strong-rung S=1/2 ladder

Classical limit

- Replace operators in the Hamiltonian with respect to the expectation values in this product state

- Formally in the $M \to \infty$ limit, but Hamiltonian is linear in $\hat{T}^{\alpha}$ by construction

$$\hat{\mathcal{H}} = J\sum_j \hat{S}^{\beta}_{j,l}\hat{S}^{\beta}_{j,r} + J'\sum_j \left(\hat{S}^{\beta}_{j,l}\hat{S}^{\beta}_{j+1,l} + \hat{S}^{\beta}_{j,r}\hat{S}^{\beta}_{j+1,r}\right) \longrightarrow \begin{aligned} \mathcal{H}_{\mathrm{SU(4)}} &= \langle\Psi\,|\hat{\mathcal{H}}|\,\Psi\rangle \\ &= \frac{J}{2}\sum_j \left(n_j^7 + n_j^8 + n_j^9\right) \\ &+ J'\sum_j \left(n_j^1 n_{j+1}^1 + n_j^2 n_{j+1}^2 + n_j^3 n_{j+1}^3\right) \\ &+ J'\sum_j \left(n_j^4 n_{j+1}^4 + n_j^5 n_{j+1}^5 + n_j^6 n_{j+1}^6\right) \end{aligned}$$

Strong-rung S=1/2 ladder

Classical limit

- Now have all the components necessary to specify the dynamical equations:

$$\frac{dn_j^\alpha}{dt} = f_{\alpha\beta\gamma}\frac{\partial \mathcal{H}_{\mathrm{SU}(4)}}{\partial n_j^\beta} n_j^\gamma$$

- This is a set of 15 coupled, nonlinear differential equations evolving the expected values of

$$\begin{array}{lll}
\hat{T}^1 = \hat{S}_l^x & \hat{T}^2 = \hat{S}_l^y & \hat{T}^3 = \hat{S}_l^z \\
\hat{T}^4 = \hat{S}_r^x & \hat{T}^5 = \hat{S}_r^y & \hat{T}^6 = \hat{S}_r^z \\
\hat{T}^7 = 2\hat{S}_l^x\hat{S}_r^x & \hat{T}^8 = 2\hat{S}_l^y\hat{S}_r^y & \hat{T}^9 = 2\hat{S}_l^z\hat{S}_r^z \\
\hat{T}^{10} = 2\hat{S}_l^y\hat{S}_r^z & \hat{T}^{11} = 2\hat{S}_l^z\hat{S}_r^y & \hat{T}^{12} = 2\hat{S}_l^z\hat{S}_r^x \\
\hat{T}^{13} = 2\hat{S}_l^x\hat{S}_r^z & \hat{T}^{14} = 2\hat{S}_l^x\hat{S}_r^y & \hat{T}^{15} = 2\hat{S}_l^y\hat{S}_r^x
\end{array}$$

Strong-rung S=1/2 ladder

Multiflavor SWT calculation

- We just showed how to derive the classical equations in the $M \to \infty$ limit.
- One can use this classical Hamiltonian to find the ground state for a corresponding multi-flavor SWT calculation organized as an expansion in M.
- Recall that and $SU(4)$ coherent state may be uniquely specified with $2(N-1) = 6$ angles, which corresponds to 3 modes.
- So we will need 4 bosons, yielding, after condensation, 3 modes per site.

Strong-rung S=1/2 ladder

Multiflavor SWT calculation

- Rewrite our Hamiltonian in terms of the SU(4) generators defined to derive the classical limit.

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

$$\downarrow$$

$$\hat{\mathcal{H}} = \frac{1}{2}\sum_j \left[J\sum_{\alpha=7}^{9} \hat{T}^{\alpha}_j + J'\sum_{\delta=\pm1}\sum_{\beta=1}^{6} \hat{T}^{\beta}_j \hat{T}^{\beta}_{j+\delta} \right]$$

$$\boxed{\begin{array}{lll}
\hat{T}^1 = \hat{S}^x_l & \hat{T}^2 = \hat{S}^y_l & \hat{T}^3 = \hat{S}^z_l \\
\hat{T}^4 = \hat{S}^x_r & \hat{T}^5 = \hat{S}^y_r & \hat{T}^6 = \hat{S}^z_r \\
\hat{T}^7 = 2\hat{S}^x_l\hat{S}^x_r & \hat{T}^8 = 2\hat{S}^y_l\hat{S}^y_r & \hat{T}^9 = 2\hat{S}^z_l\hat{S}^z_r \\
\hat{T}^{10} = 2\hat{S}^y_l\hat{S}^z_r & \hat{T}^{11} = 2\hat{S}^z_l\hat{S}^y_r & \hat{T}^{12} = 2\hat{S}^z_l\hat{S}^x_r \\
\hat{T}^{13} = 2\hat{S}^x_l\hat{S}^z_r & \hat{T}^{14} = 2\hat{S}^x_l\hat{S}^y_r & \hat{T}^{15} = 2\hat{S}^y_l\hat{S}^x_r
\end{array}}$$

Strong-rung S=1/2 ladder

Multiflavor SWT calculation

- Our goal is to bosonize the Hamiltonian in terms of 4 flavors of boson for each site j

$$\left\{ b_{j,0}, b_{j,1}, b_{j,2}, b_{j,3} \right\}$$

- To make a representation of $SU(4)$ generators, these must be subject to the constraint.

$$\sum_{m=0}^{3} b^{\dagger}_{j,m} b_{j,m} = M$$

Strong-rung S=1/2 ladder

Multiflavor SWT calculation

- Note that, when $M = 1$, pairs of bosons can be naturally associated with matrix elements of the generators.

- Bosonization therefore follows a simple recipe:

$$\hat{T}_j^{\alpha} \to \mathbf{b}_j^{\dagger} \hat{T}_j^{\alpha} \mathbf{b}_j \qquad \mathbf{b}_j = \begin{pmatrix} b_{j,0} \\ b_{j,1} \\ b_{j,2} \\ b_{j,3} \end{pmatrix}$$

Strong-rung S=1/2 ladder

Multiflavor SWT calculation

- However, we want our “condensed” boson to have the effect of creating the ground (singlet) state. So define transformed bosons:

$$\tilde{\mathbf{b}}_j = U_j \mathbf{b}_j, \quad \tilde{\mathbf{b}}_j^\dagger = \mathbf{b}_j^\dagger U_j^\dagger$$

- Here U_j is an $SU(4)$ group action moving the “fully polarized” state to the singlet state $|\Psi_j\rangle = \big(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\big)/\sqrt{2}$ (the ground state).

$$|\Psi_j\rangle = \tilde{b}_{j,0}^\dagger |\varnothing\rangle$$

Strong-rung S=1/2 ladder

Multiflavor SWT calculation

- We can then rewrite the Hamiltonian in terms of these transformed bosons.

$$\hat{\mathcal{H}} = \frac{1}{2}\sum_j \left[J \sum_{\alpha=7}^{9} \hat{T}_j^{\alpha} + J' \sum_{\delta=\pm 1} \sum_{\beta=1}^{6} \hat{T}_j^{\beta} \hat{T}_{j+\delta}^{\beta} \right]$$

$$\downarrow$$

$$\hat{\mathcal{H}} = \frac{J}{2} \sum_{j;\alpha=7,9} \tilde{\mathbf{b}}_j^{\dagger} \tilde{T}_j^{\alpha} \tilde{\mathbf{b}}_j^{\dagger} + \frac{J'}{2} \sum_{\substack{j;\beta=1,6 \\ \delta=\pm 1}} \tilde{\mathbf{b}}_j^{\dagger} \tilde{T}_j^{\beta} \tilde{\mathbf{b}}_j \tilde{\mathbf{b}}_j^{\dagger} \tilde{T}_{j+\delta}^{\beta} \tilde{\mathbf{b}}_j$$

$$\tilde{T}_j^{\alpha} = U_j \hat{T}_j^{\alpha} U_j^{\dagger}$$

Strong-rung S=1/2 ladder

Multiflavor SWT calculation

- This can be multiplied out to get a sum of boson pairs.
- We next wish to condense out the singlet state — i.e., make the assumption that we are close to the ground state.
- This is achieved with a generalized Holstein-Primakoff transformation:

$$\tilde{b}^{\dagger}_{j,0} = \tilde{b}_{j,0} = \sqrt{M}\sqrt{1 - \frac{1}{M}\sum_{m=1}^{3} \tilde{b}^{\dagger}_{j,m}\tilde{b}_{j,m}}$$

Strong-rung S=1/2 ladder

Multiflavor SWT calculation

- Finally, we expand the square root in the (three) number operators and collect terms of order M

$$
\begin{aligned}
\hat{\mathcal{H}}^{(2)} &= J \sum_{j} \sum_{m=1}^{3} \tilde{b}^{\dagger}_{j,m} \tilde{b}_{j,m} \\
&+ \frac{J'}{2} \sum_{j,\delta} \sum_{m=1}^{3} \left[\tilde{b}^{\dagger}_{j,m} \tilde{b}_{j+\delta,m} + h.c. \right] \\
&+ \frac{J'}{2} \sum_{j,\delta} \sum_{m=1}^{3} \left[\sigma(m) \tilde{b}_{j,m} \tilde{b}_{j+\delta,m} + h.c. \right]
\end{aligned}
$$

Strong-rung S=1/2 ladder

Multiflavor SWT calculation

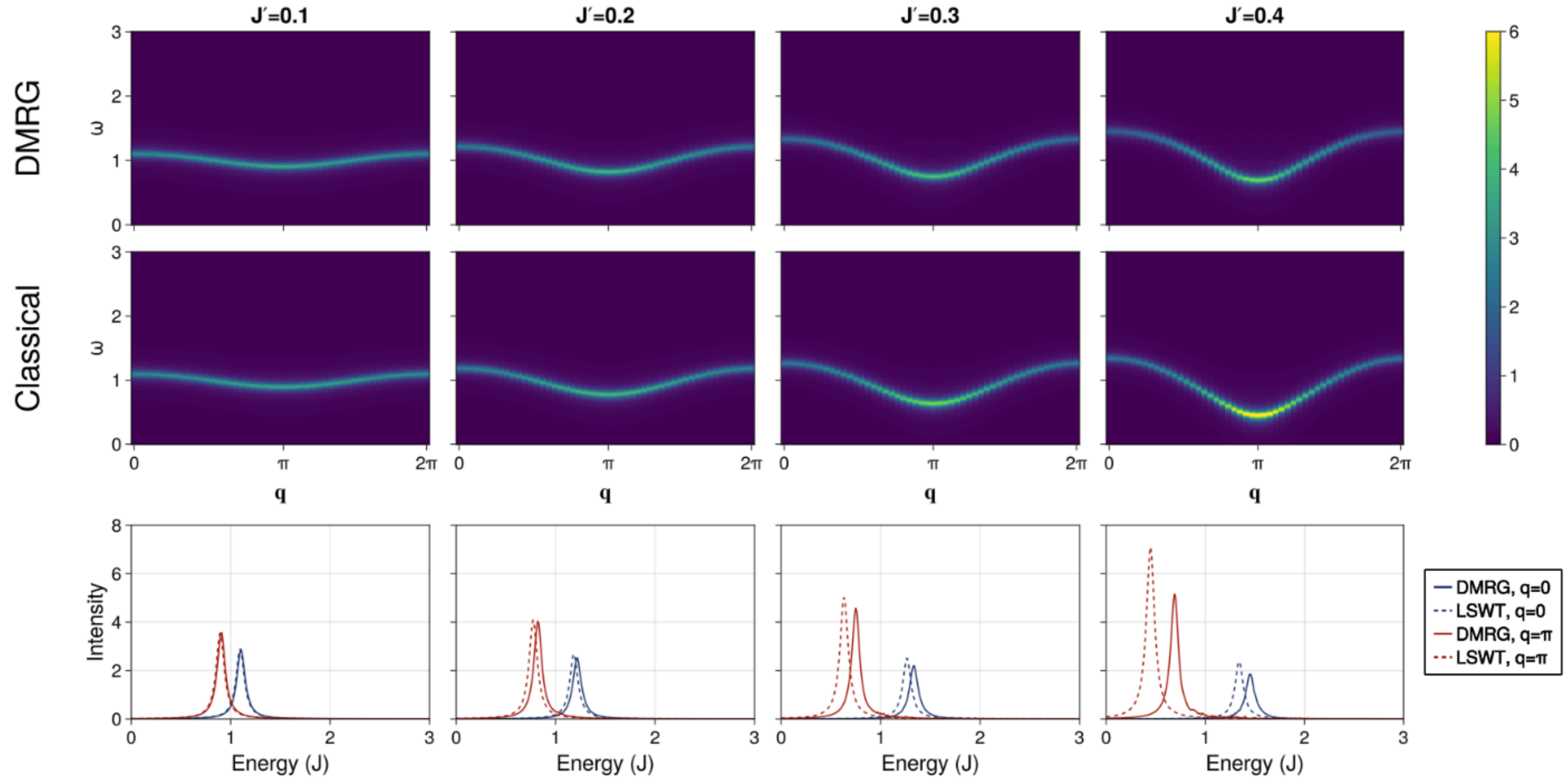
- We can diagonalize this by Fourier transforming and applying a Bogoliubov transformation, yielding three degenerate dispersion relations for each triplon mode.

$$\boxed{\omega_m(k) = \pm J\sqrt{1 + \frac{2J'}{J}\cos(k)}}$$

- Gives a sense where this approximation fails. But where is it "good"?
- Test against DMRG…

Strong-rung S=1/2 ladder

Multiflavor SWT calculation



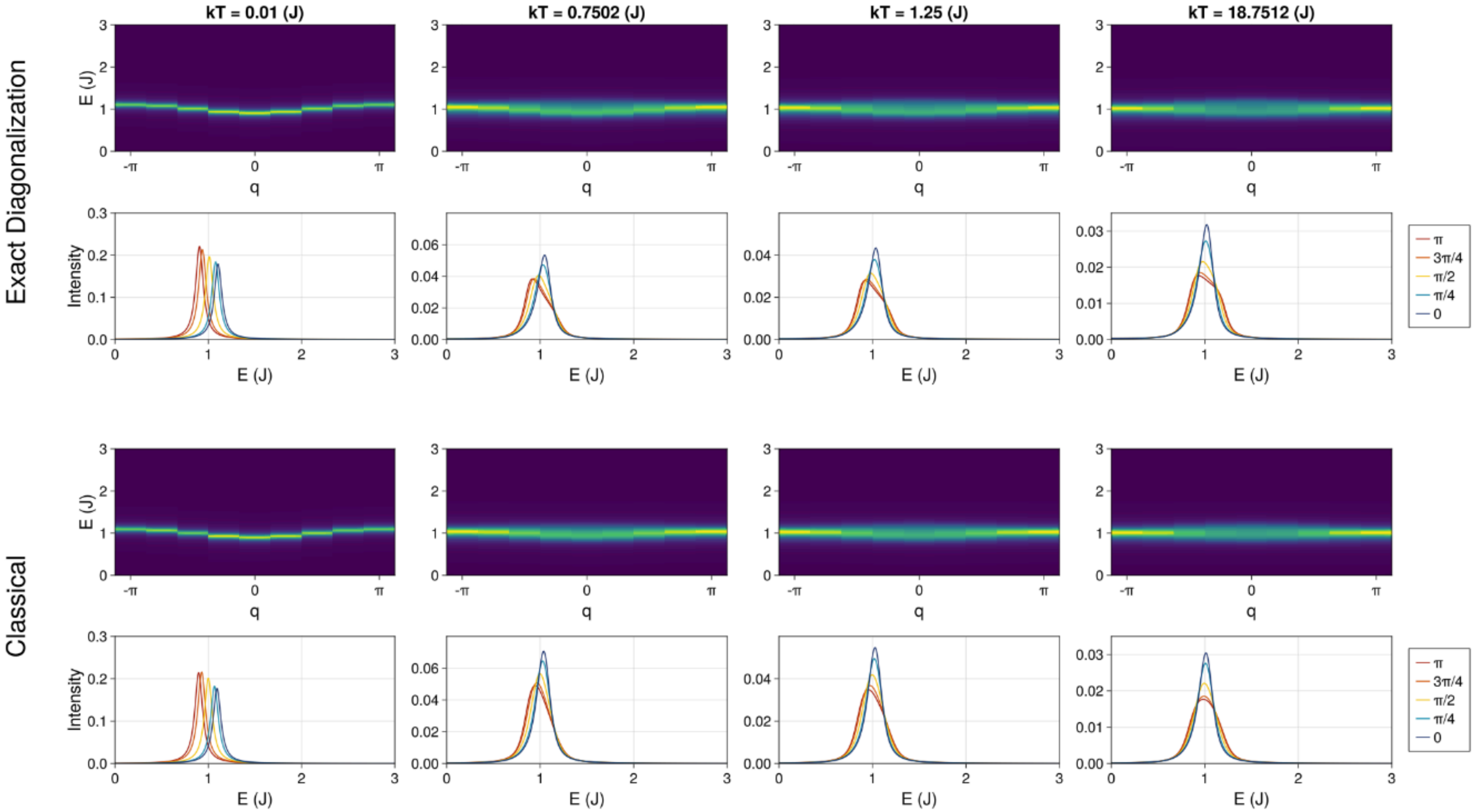
Strong-rung S=1/2 ladder

Finite-T classical calculations

- Because we have the corresponding classical theory, we can also investigate the behavior at elevated temperatures.
- Test against exact diagonalization…

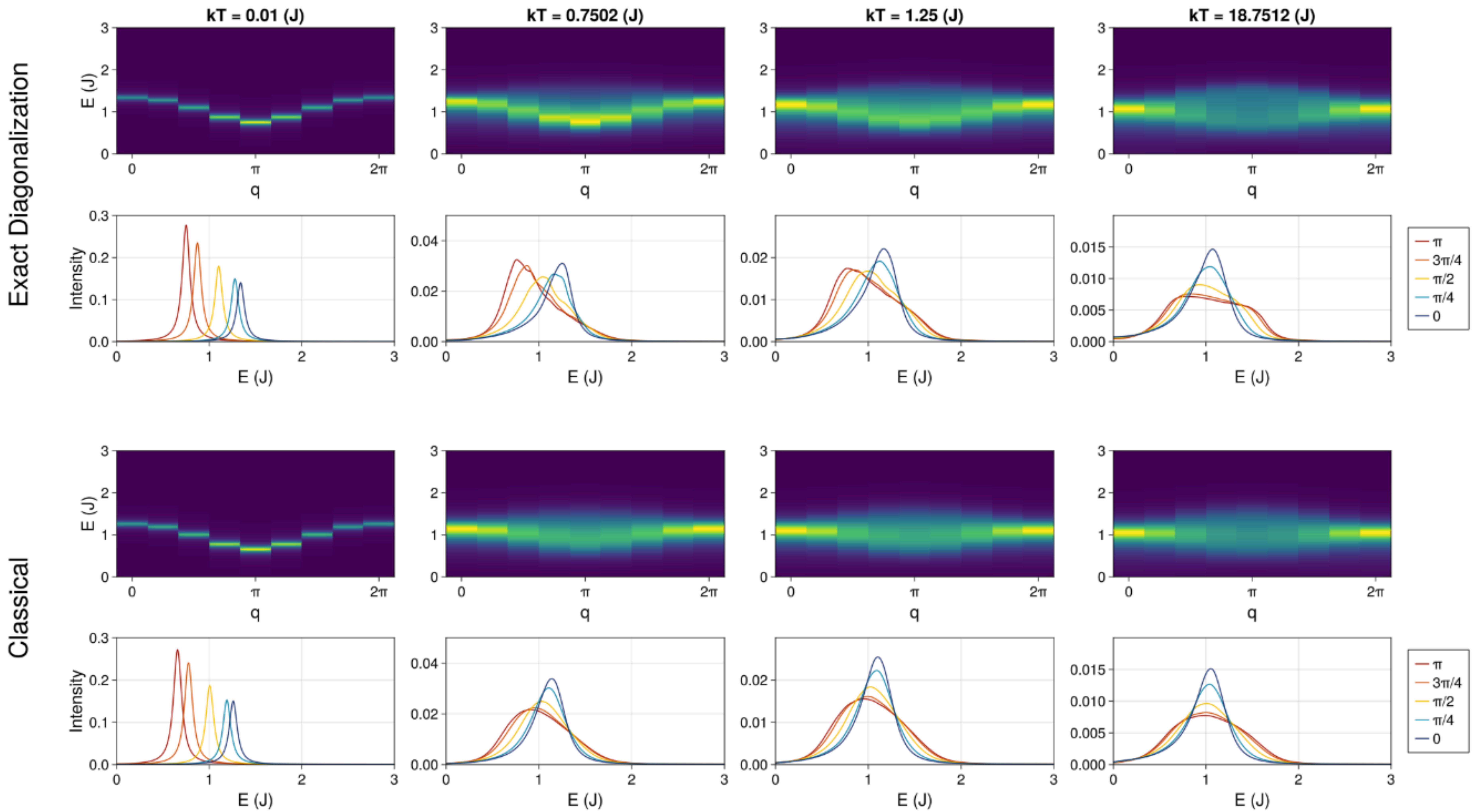
Strong-rung S=1/2 ladder

Finite-T classical calculations



Strong-rung S=1/2 ladder

Finite-T classical calculations



Strong-rung S=1/2 ladder

Conclusions

- This model represents a stringent test for the approach: small S, low coordination number.
- Works extremely well when $J' < 0.4$.
- Approach not limited to dimers — any entangled unit compatible with lattice symmetries.
- Importantly, you do not need to do all the work we just went through: this is precisely what Sunny was designed for.

Entangled units in a real material

$Ba_3Mn_2O_8$ (Sunny example)

PRL **100,** 237201 (2008) PHYSICAL REVIEW LETTERS week ending 13 JUNE 2008

Singlet-Triplet Dispersion Reveals Additional Frustration in the Triangular-Lattice Dimer Compound $Ba_3Mn_2O_8$

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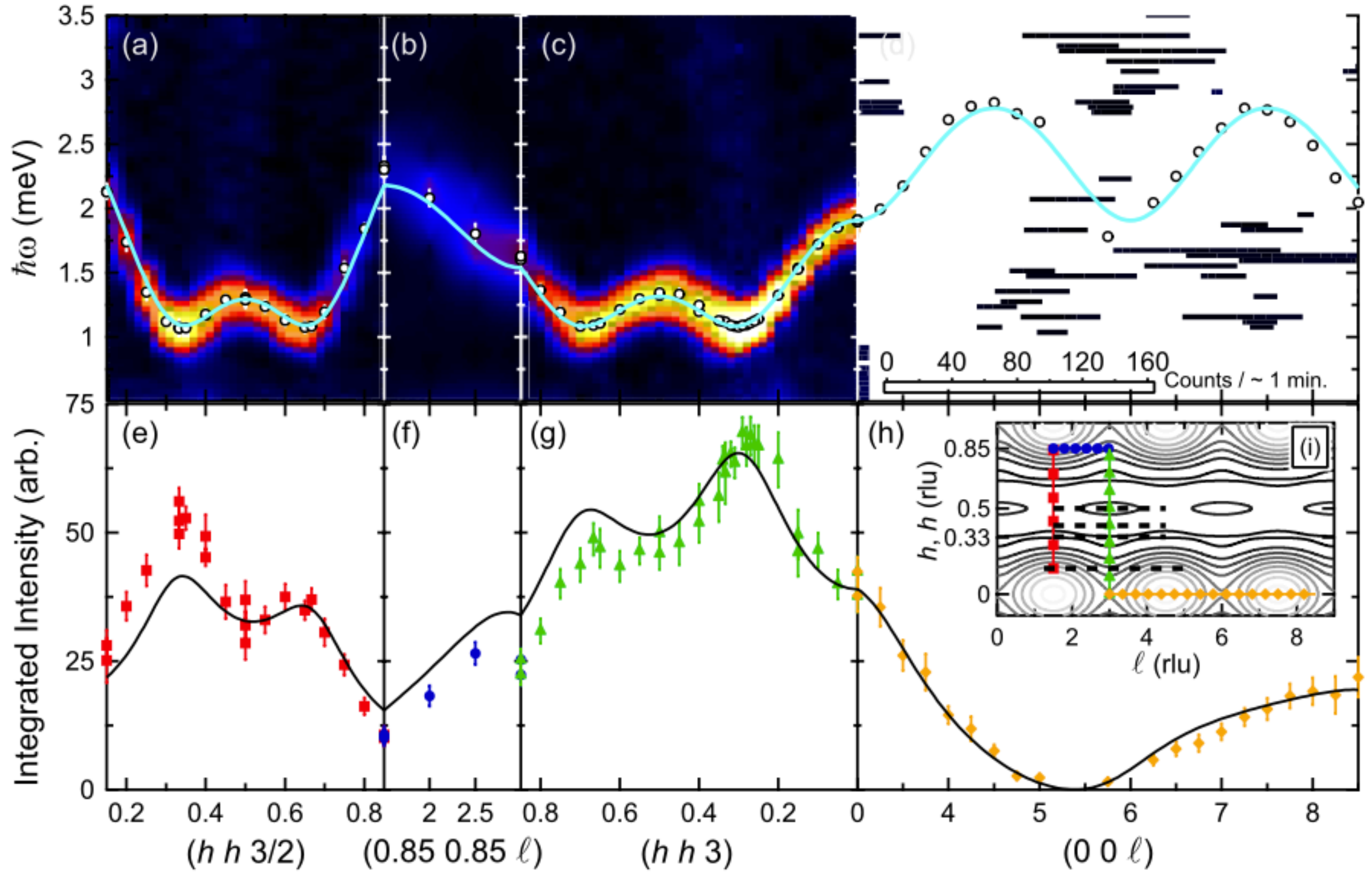
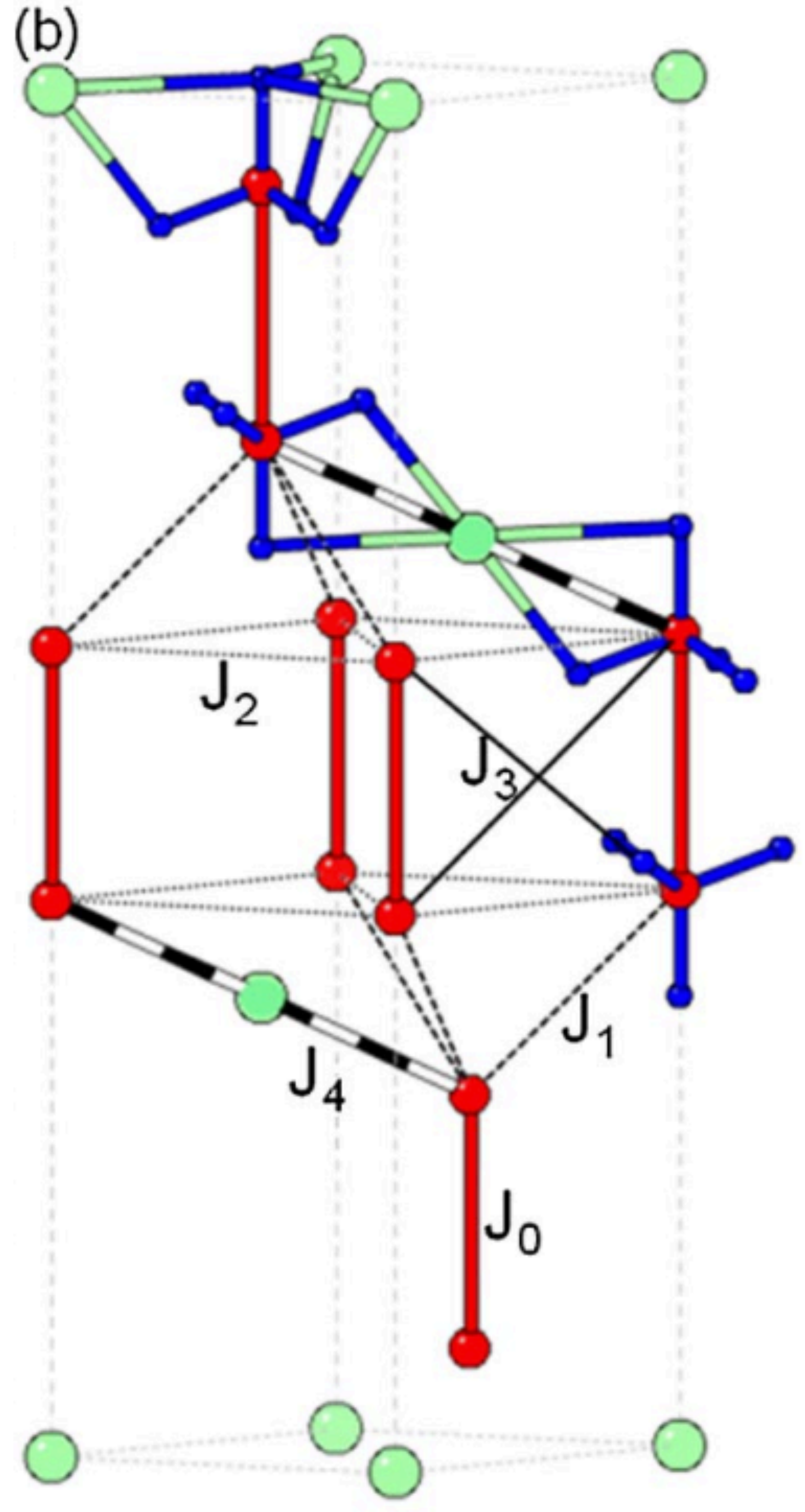




Takeaways

- The $SU(N)$ approach generalizes the traditional $SU(2)$ approach by giving a general N-level "container" (local Hilbert space) on each site, not just a dipole.
- This local Hilbert space completely captures the local degrees of freedom.
- Sunny allows you to use this formalism simply by specifying a lattice, local Hilbert space properties, and the interactions of the Hamiltonian.

Ideas behind Sunny.jl

Lecture 3: Deriving renormalizations with classical limits

David Dahlbom (ORNL) & Cristian Batista (UTK, LANL, ORNL) — April 17th, 2024

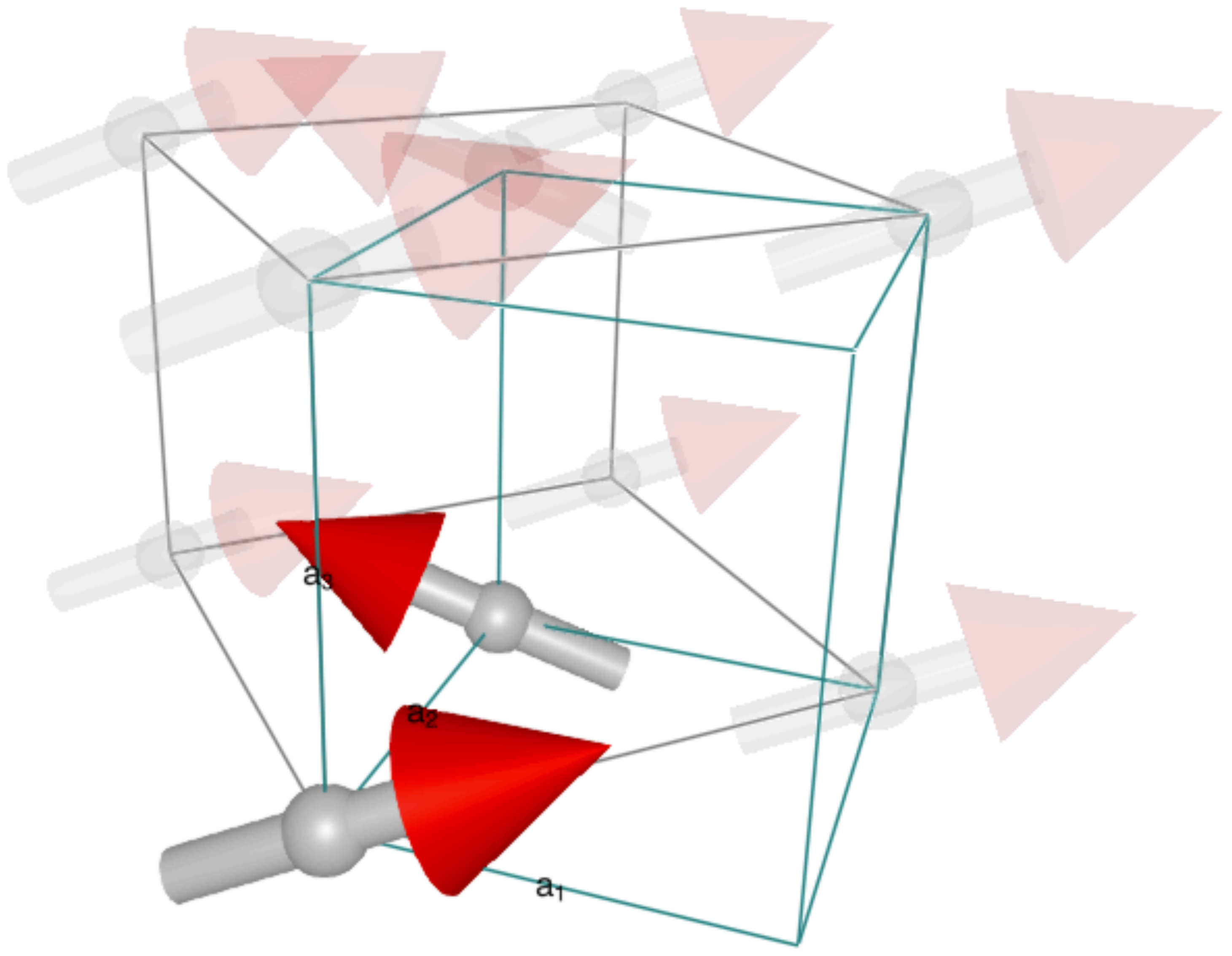
Renormalized classical theory

Motivating problem

- Consider a simple S=1 Hamiltonian

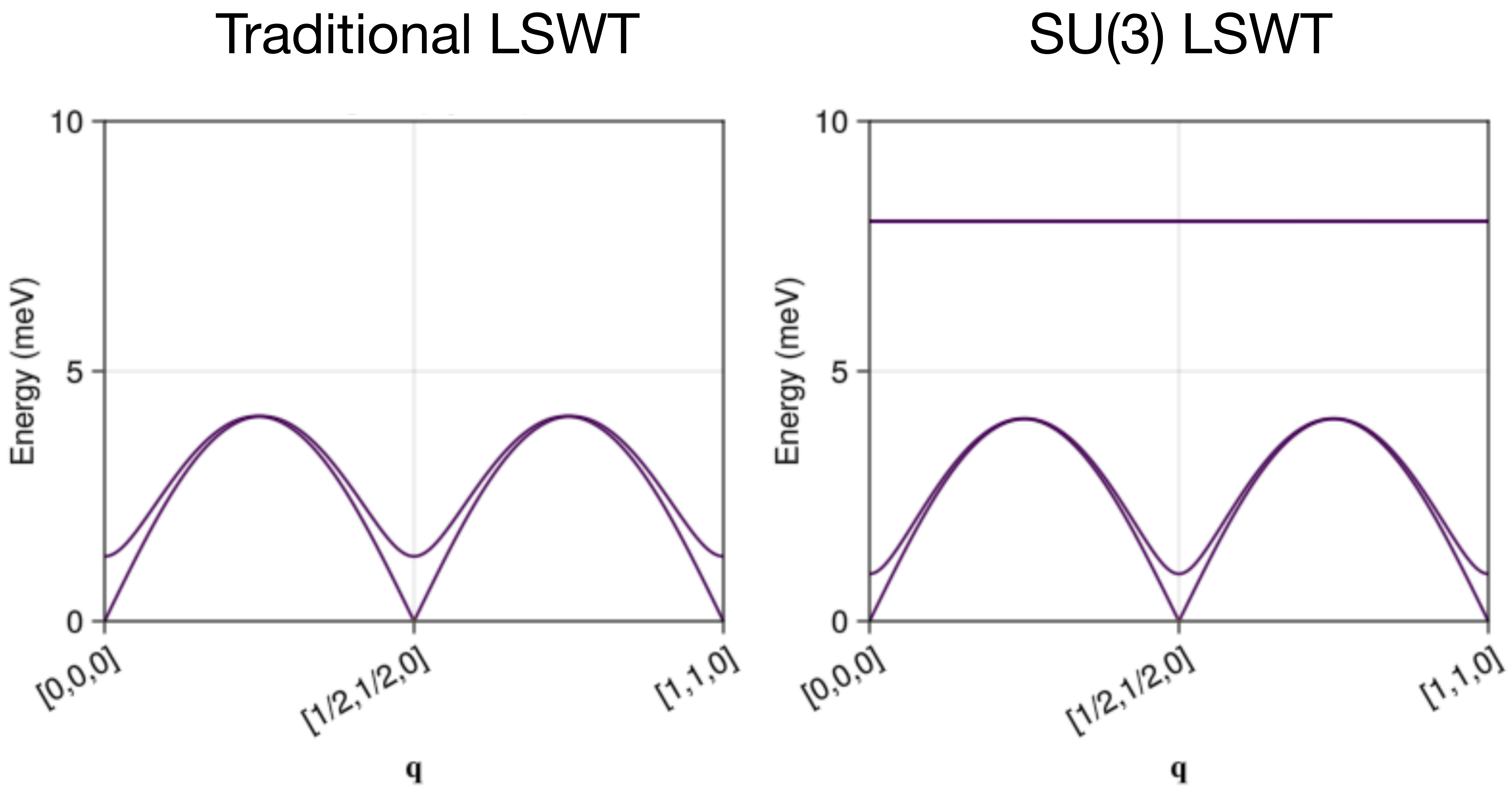
$$\mathcal{H} = J\sum_{\langle i,j\rangle} \mathbf{S}_i \cdot \mathbf{S}_j + D\sum_i (S_i^z)^2 - h\sum_i S_i^z$$

  - Antiferromagnetic $J < 0$
  - D “easy-plane” and $|J| \gg |D|$
  - External magnetic field
  - Square lattice



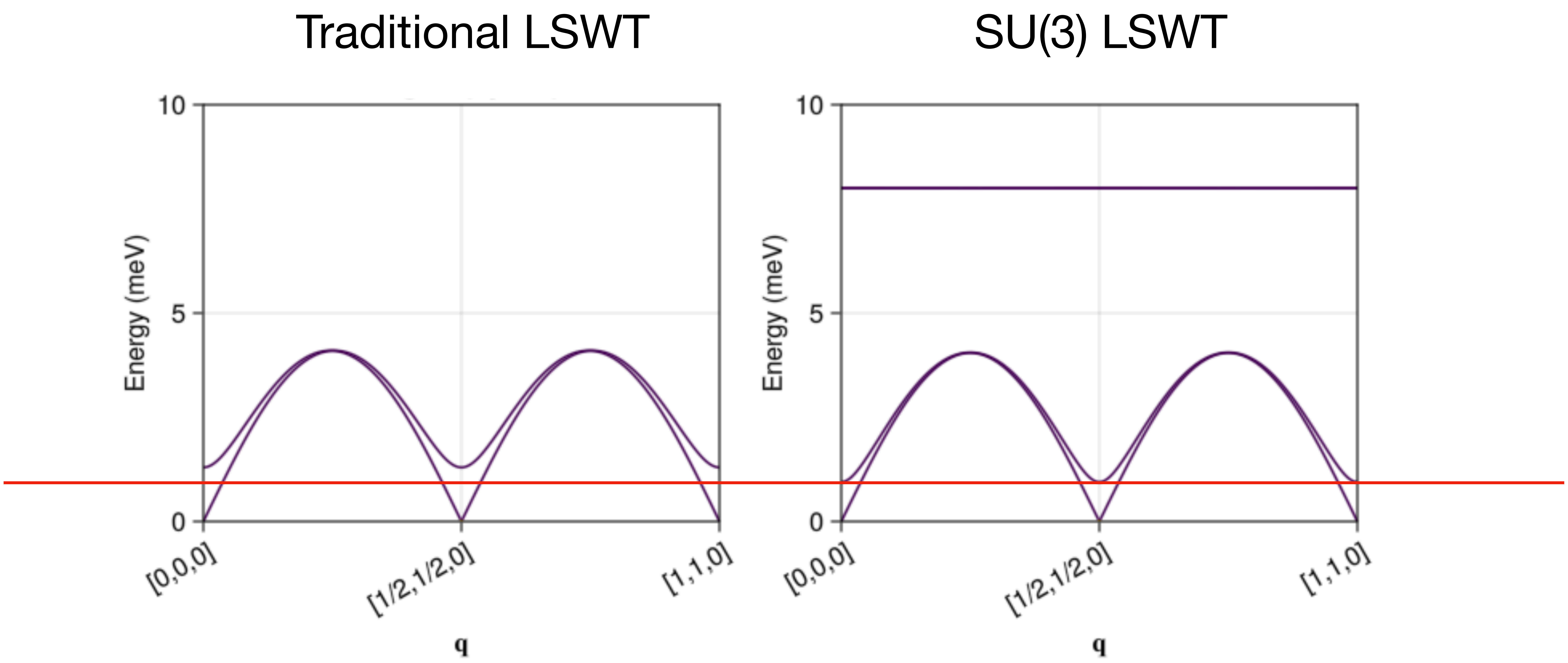
Renormalized classical theory

Dispersions from two methods



Renormalized classical theory

Dispersions from two methods



Renormalized classical theory

Renormalizations in the literature

- The source of the problem is the “nonlinear” term: $\left(\hat{S}^z\right)^2$
- Known problem. There is an extensive literature deriving renormalizations of such terms by applying higher-order corrections to LSWT

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Renormalized classical theory

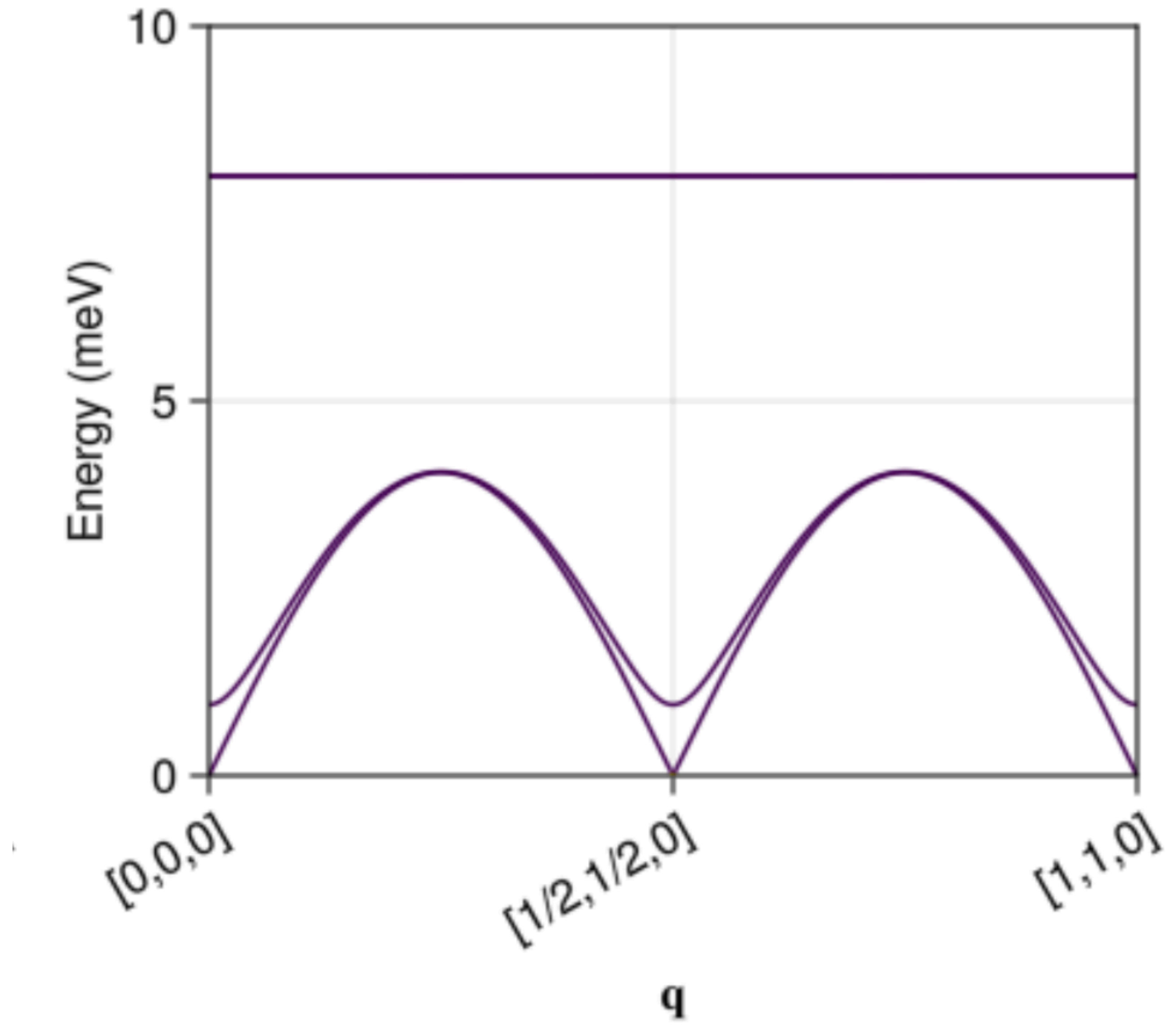
Renormalizations in the literature

- These approaches involve including “higher-order corrections” ($\frac{1}{S}$ etc.)
- This is difficult and typically done on a case-by-case basis
- If one attempts to just pick the “relevant” terms in an expansion, one may break symmetries of the Hamiltonian
- Moreover, the renormalization must be applied *before* bosonization in order to get the correct rotated reference frame (i.e., in order to bosonize the Hamiltonian correctly).

Renormalized classical theory

SU(N) result

- The $SU(3)$ theory reproduces the effect of these renormalizations at the classical level (and hence at the linear level of SWT).
- But the $SU(3)$ theory produces an "extra" mode.
- Moreover, this "extra" mode will typically be over-damped in the 2-magnon continuum



Renormalized classical theory

SU(N) result

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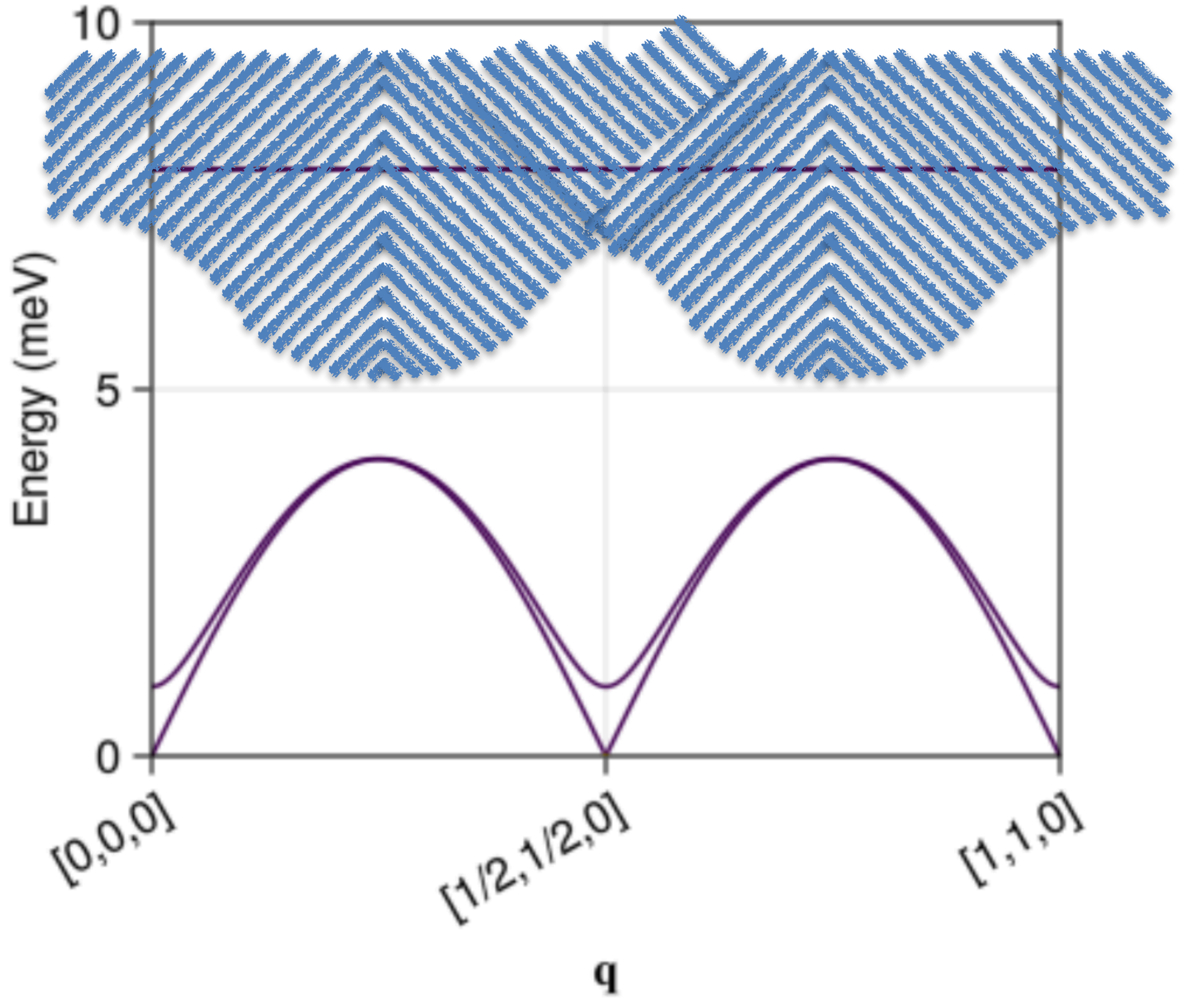
- Moreover, this “extra” mode will typically be over-damped in the 2-magnon continuum



Renormalized classical theory

- We can capture the renormalization by using the $SU(N)$ approach while *constraining* the theory to purely dipolar states.
- Recall that for any $SU(2)$ coherent state $\left|\Omega\left(\theta, \phi\right)\right\rangle$, the expectation value of the vector of dipole operators will be constant.

$$\left|\left(\left\langle \hat{S}^x \right\rangle, \left\langle \hat{S}^y \right\rangle, \left\langle \hat{S}^z \right\rangle, \right)\right| = S$$

Renormalized classical theory

- These states always exist as a submanifold of $SU(N)$ coherent states, where $N > 2$.
- For example, $SU(3)$ coherent states are equivalent to the space of all pure states in a 3-level system.
- Clearly, the $SU(2)$ coherent states in the $S = 1$ representation are a subset in the space of all pure 3-level states:

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

Renormalized classical theory

Evaluating expectation values in the classical limit: SU(2)

- Spin operators (SU(2) algebra) are simply replaced with their expectation value:

$$\lim_{S\to\infty} \left\langle \hat{S}^{\alpha} \right\rangle = \left\langle \hat{S}^{\alpha} \right\rangle$$

- If, however, the operator is not in this algebra, as $\left(\hat{S}^{z}\right)^{2}$ is not, then we must apply the **factorization rule:**

$$\lim_{S\to\infty} \left\langle \hat{S}^{\alpha}\hat{S}^{\beta} \right\rangle = \left\langle \hat{S}^{\alpha} \right\rangle \left\langle \hat{S}^{\beta} \right\rangle$$

Renormalized classical theory

Evaluating expectation values in the classical limit

- The key point about the $SU(N)$ classical limit is that we choose our algebra (and resulting group) large enough that it is never necessary to apply the factorization rule.

- I.e., all operators in the Hamiltonian can be written as linear combinations of algebra elements

- The expectation value is always a normal expectation value — no factorization rule needed:

$$\lim_{M\to\infty} \left\langle (\hat{S}^z)^2 \right\rangle = \left\langle \sum_\alpha c_\alpha \hat{T}^\alpha \right\rangle = \sum_\alpha c_\alpha \left\langle \hat{T}^\alpha \right\rangle$$

Renormalized classical theory

Procedure

- To figure out renormalizations, we can simply compare the result of the $S \to \infty$ classical limit with the results of the $M \to \infty$ result when evaluated on dipolar states.
- These will only differ for terms that are "nonlinear" in the spin operators.
- A useful basis for such terms is the given by the Stevens operators

Renormalized classical theory

Stevens operators

- These operators provide a “basis” for nonlinear operators.
- They are often used to specify crystal field Hamiltonians.
- They transform according to irreps of $SO(3)$
- Consequently, so will their classical limits.
- Functions transforming to identical irreps must be proportional.

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

Renormalized classical theory

Stevens operators

- These operators provide a “basis” for nonlinear operators.
- They are often used to specify crystal field Hamiltonians.
- They transform according to irreps of $SO(3)$
- Consequently, so will their classical limits.
- Functions transforming to identical irreps must be proportional.

$$\boxed{\langle\Omega|\,\hat{O}_q^{(k)}\,|\Omega\rangle = c_k\left[\lim_{S\to\infty}\langle\Omega|\,\hat{O}_q^{(k)}\,|\Omega\rangle\right]}$$

Renormalized classical theory

Example calculation: $\mathcal{O}_0^{(2)}$

$$\hat{O}_0^{(2)} = 3\left(\hat{S}^z\right)^2 - \mathbf{S}^2$$

Renormalized classical theory

Example calculation: $\mathscr{O}_0^{(2)}$

$$\hat{O}_0^{(2)} = 3\left(\hat{S}^z\right)^2 - \mathbf{S}^2$$

$$M \to \infty$$

$$\begin{aligned}\langle S|\,\hat{O}_0^{(2)}\,|S\rangle &= 3\langle S|\left(\hat{S}^z\right)^2|S\rangle - \langle S|\mathbf{S}^2|S\rangle \\ &= 3S^2 - S(S+1)\end{aligned}$$

Renormalized classical theory

Example calculation: $\mathcal{O}_0^{(2)}$

$$\hat{O}_0^{(2)} = 3\left(\hat{S}^z\right)^2 - \mathbf{S}^2$$

$M \to \infty$

$$\langle S|\,\hat{O}_0^{(2)}\,|S\rangle = 3\langle S|\left(\hat{S}^z\right)^2|S\rangle - \langle S|\mathbf{S}^2|S\rangle$$
$$= 3S^2 - S(S+1)$$

$S \to \infty$

$$\lim_{S\to\infty}\langle S|\,\hat{O}_0^{(2)}\,|S\rangle = 3\left\langle S\middle|\hat{S}^z\middle|S\right\rangle^2$$
$$-\left(\left\langle S\middle|\hat{S}^x\middle|S\right\rangle^2 + \left\langle S\middle|\hat{S}^y\middle|S\right\rangle^2 + \left\langle S\middle|\hat{S}^z\middle|S\right\rangle^2\right)$$
$$= 2S^2$$

Renormalized classical theory

Example calculation: $\mathcal{O}_0^{(2)}$

$$\hat{O}_0^{(2)} = 3\left(\hat{S}^z\right)^2 - \mathbf{S}^2$$

$M \to \infty$

$S \to \infty$

$$\begin{aligned}\langle S|\,\hat{O}_0^{(2)}\,|S\rangle &= 3\langle S|\left(\hat{S}^z\right)^2|S\rangle - \left\langle S\middle|\mathbf{S}^2\middle|S\right\rangle \\ &= 3S^2 - S(S+1)\end{aligned}$$

$$\begin{aligned}\lim_{S\to\infty}\langle S|\,\hat{O}_0^{(2)}\,|S\rangle &= 3\left\langle S\middle|\hat{S}^z\middle|S\right\rangle^2 \\ &\quad - \left(\left\langle S\middle|\hat{S}^x\middle|S\right\rangle^2 + \left\langle S\middle|\hat{S}^y\middle|S\right\rangle^2 + \left\langle S\middle|\hat{S}^z\middle|S\right\rangle^2\right) \\ &= 2S^2\end{aligned}$$

$$3S^2 - S(S+1) = c_2\left(2S^2\right)$$

Renormalized classical theory

Example calculation: $\mathcal{O}_0^{(2)}$

$$\hat{O}_0^{(2)} = 3\left(\hat{S}^z\right)^2 - \mathbf{S}^2$$

$M \to \infty$

$S \to \infty$

$$\begin{aligned}\langle S|\,\hat{O}_0^{(2)}\,|S\rangle &= 3\langle S|\left(\hat{S}^z\right)^2|S\rangle - \langle S|\mathbf{S}^2|S\rangle \\ &= 3S^2 - S(S+1)\end{aligned}$$

$$\begin{aligned}\lim_{S\to\infty}\langle S|\,\hat{O}_0^{(2)}\,|S\rangle &= 3\langle S|\hat{S}^z|S\rangle^2 \\ &\quad - \left(\langle S|\hat{S}^x|S\rangle^2 + \langle S|\hat{S}^y|S\rangle^2 + \langle S|\hat{S}^z|S\rangle^2\right) \\ &= 2S^2\end{aligned}$$

$$3S^2 - S(S+1) = c_2\left(2S^2\right) \implies \boxed{c_2 = 1 - \frac{1}{2S}}$$

Renormalized classical theory

General crystal field Hamiltonian

$$\hat{\mathcal{H}}^{\mathrm{A}} = \sum_{j,q,k} A_q^k \hat{O}_q^{(k)}(\hat{\mathbf{S}}_j) \quad \longrightarrow \quad \mathcal{H}^{\mathrm{A}} = \sum_{j,q,k} c_k A_q^k O_q^{(k)}(\mathbf{s}_j)$$

$$\boxed{\begin{aligned} c_2 &= 1 - \frac{1}{2}S^{-1} \\ c_4 &= 1 - 3S^{-1} + \frac{11}{4}S^{-2} - \frac{3}{4}S^{-3} \\ c_6 &= 1 - \frac{15}{2}S^{-1} + \frac{85}{4}S^{-2} - \frac{225}{8}S^{-3} + \frac{137}{8}S^{-4} - \frac{15}{4}S^{-5} \end{aligned}}$$

Renormalized classical theory

Biquadratic interactions

$$\hat{\mathcal{H}}^{\mathrm{Biq}} = \frac{1}{2}\sum_{i\neq j}\mathcal{K}_{ij}(\hat{S}_i\cdot\hat{S}_j)^2 \longrightarrow \tilde{\mathcal{H}}^{\mathrm{Biq}}_{\mathrm{cl}} = \frac{1}{2}\sum_{i\neq j}\mathcal{K}_{ij}\left[r(\vec{\Omega}_1\cdot\vec{\Omega}_2)^2 - \frac{1}{2}\vec{\Omega}_1\cdot\vec{\Omega}_2 + S^3 + \frac{S^2}{4}\right]$$

$$\boxed{r = \left(1 - \tfrac{1}{S} + \tfrac{1}{4S^2}\right)}$$

Key points

Theoretical

- These proportionality constants are polynomials in $\frac{1}{S}$, but S was never used to organize an expansion.
- Instead, they emerge simply the proportionality constants between two different classical limits.
- Specifically, they tell us how to recover the renormalizations that occur naturally in the $SU(N)$ theory by simply renormalizing the traditional $S \to \infty$ theory.

Key points

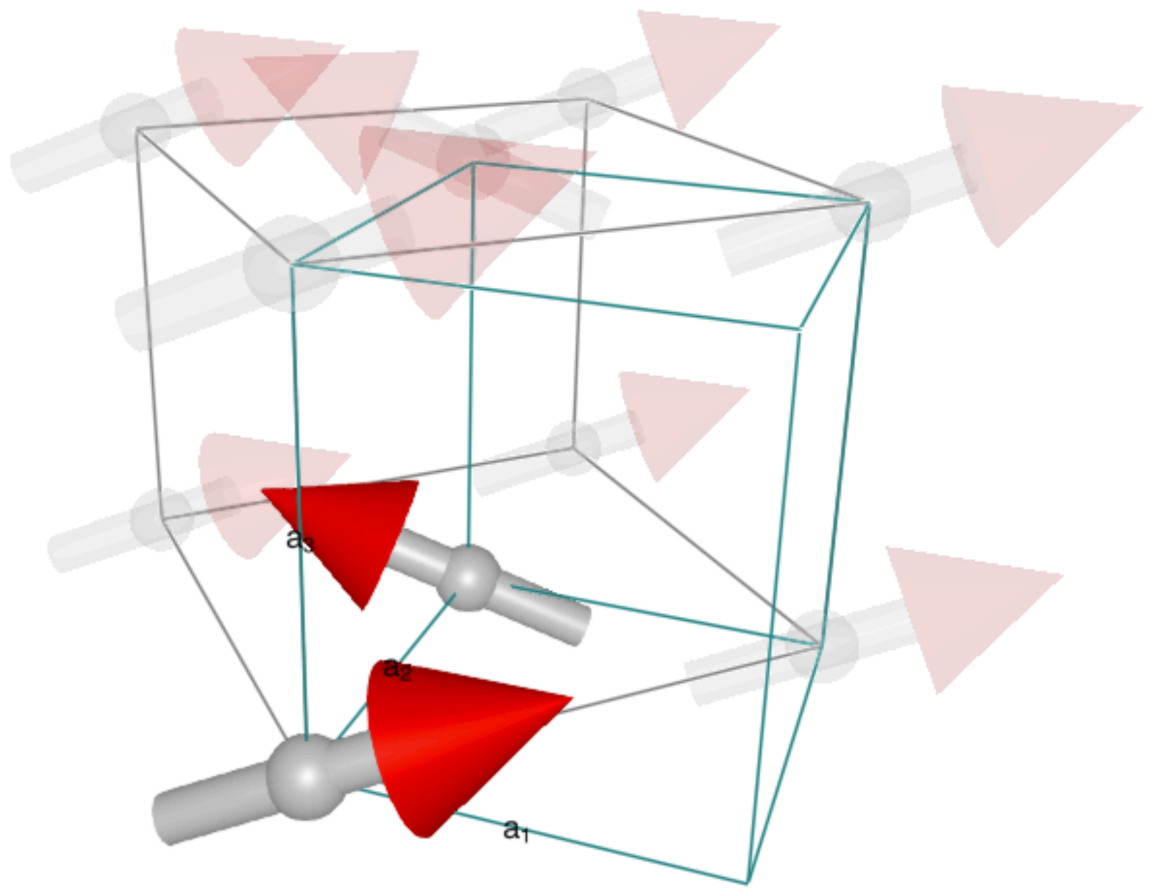
Theoretical

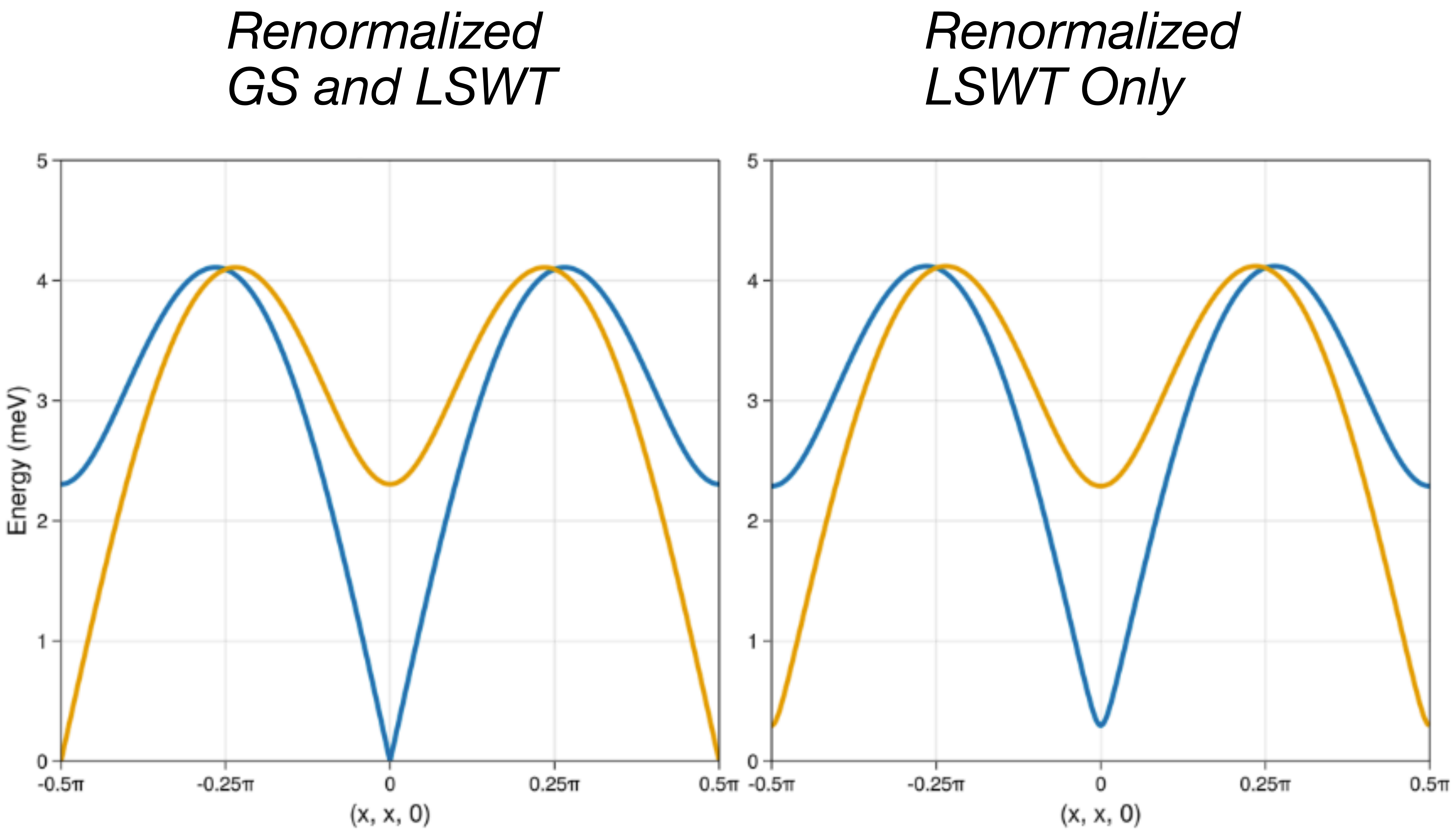
- If doing LSWT, these renormalizations *must* be applied when finding the classical ground state.
- Recall the classical ground state determines rotated reference frames used for bosonization.
- If no renormalization is used for finding the classical ground state, but the renormalization is applied to the bosonic Hamiltonian, this can lead to imaginary eigenvalues or broken symmetries.

Key points

Dangers of inconsistent application of renormalizations

$$\mathcal{H} = J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j + D \sum_i (S_i^z)^2 - h \sum_i S_i^z$$





Key points

Dangers of inconsistent application of renormalizations

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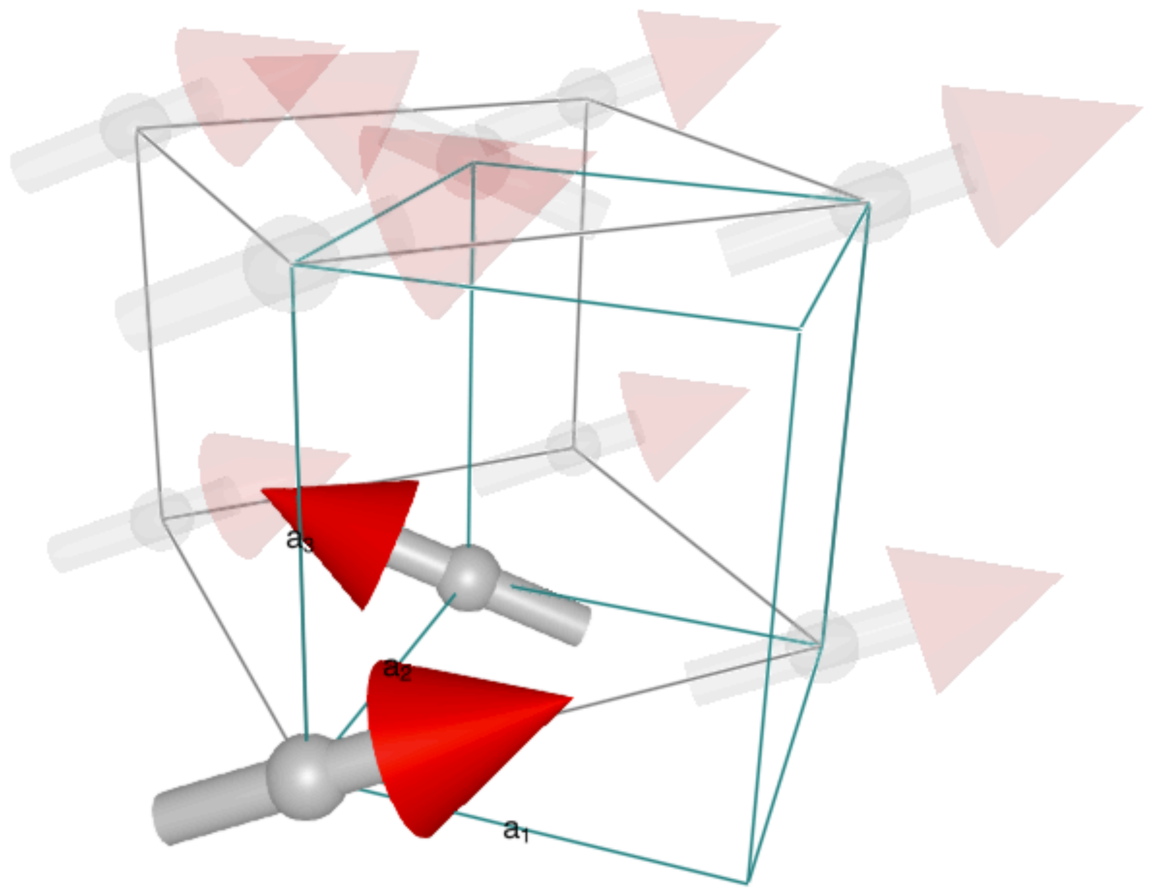
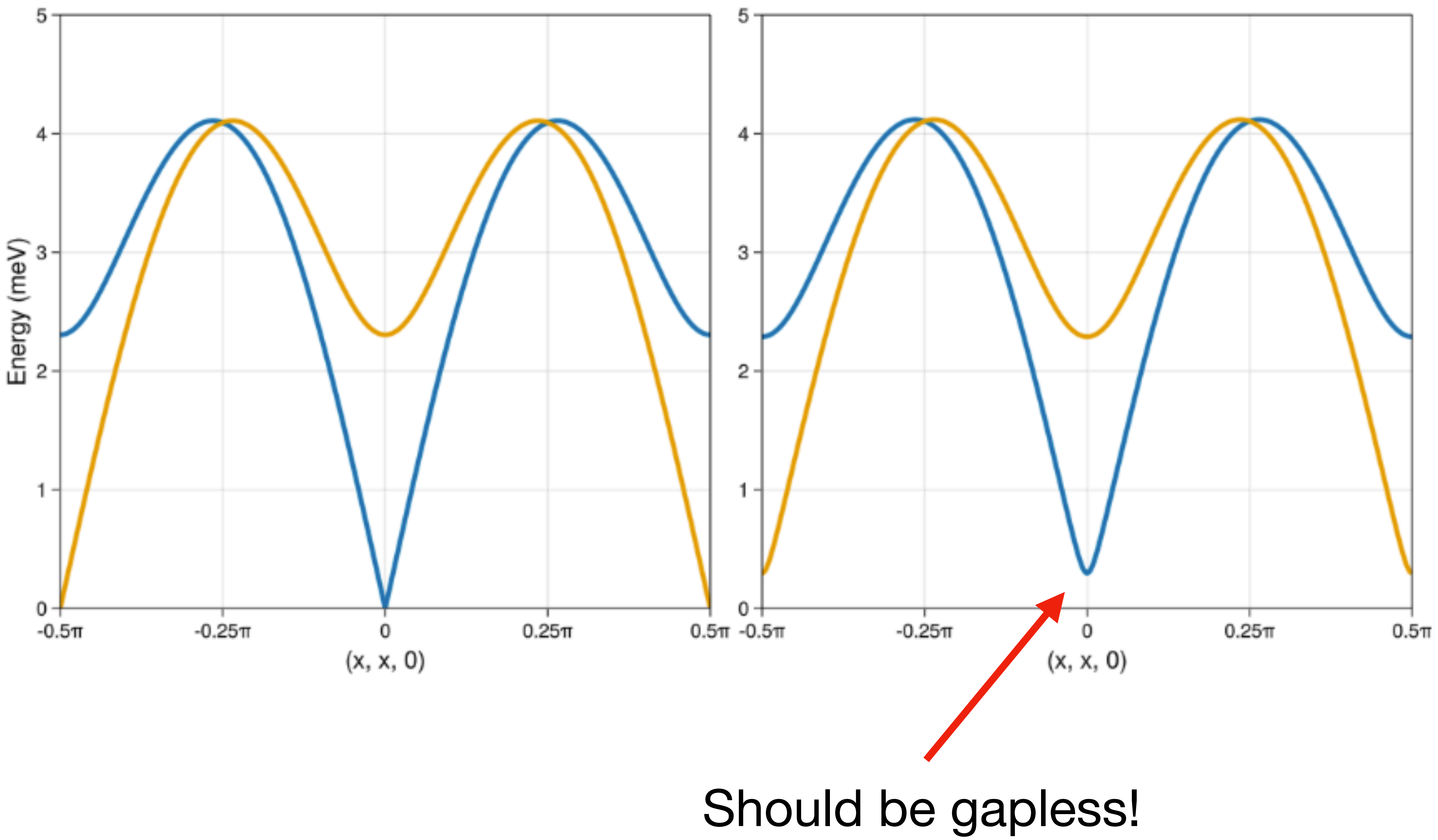


Renormalized GS and LSWT

Renormalized LSWT Only



Key points

In relation to Sunny

- These renormalizations are automatically applied in `:dipole` mode
- To recover the behavior of SpinW, use `:dipole_large_S`

Final takeaways (the big ideas)
SU(N) theory

- The theory is useful whenever you have large spins and “nonlinear” operators in your Hamiltonian (4d-5d, 4f-5f and some 3d materials).
- It also facilitates the modeling of “localized” entanglement (dimers, trimers, tetramers, etc.).
- More abstractly, the $SU(N)$ theory is useful whenever you want to capture the full structure (all degrees of freedom) of a local Hilbert space.
- For a given N, one captures the structure of an N-level local Hilbert space and generates $(N-1)$ modes per “site.”
- The $SU(N)$ theory also gives an approach to deriving renormalizations in a simple way.

Summary of Sunny “modes”

What the modes are

- `: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.

Research outlook

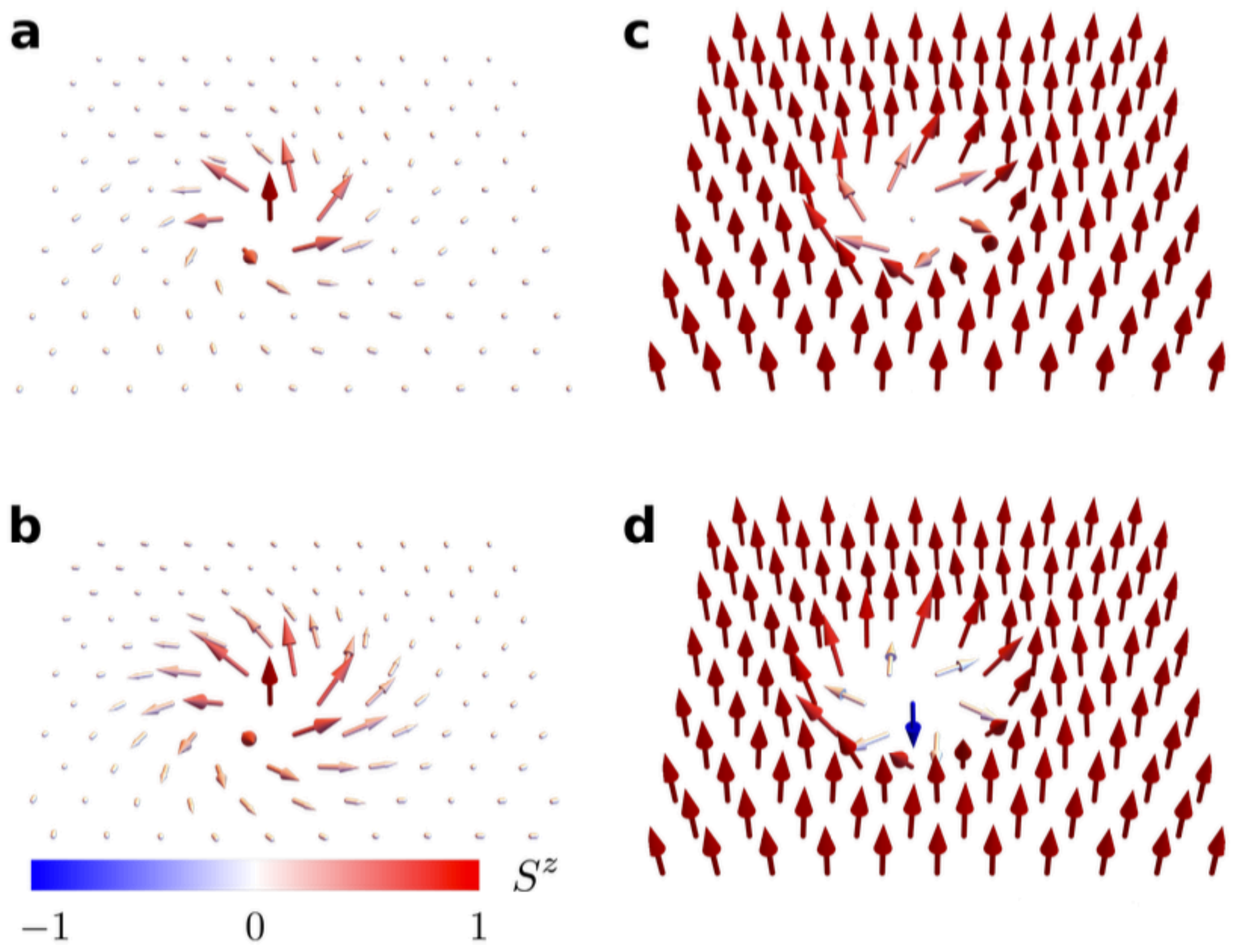
- Most obvious applications involve modeling "exotic" ground states and excitations.
  - Non-magnetic ground states
  - Hybridized dipolar-quadrupolar excitations
  - Singlet-triplet excitations

Research outlook

- Many opportunities for exploring novel spin textures and their excitations, for example, new types of skyrmions.

$$\boxed{\hat{\mathcal{H}} = \sum_{\langle i,j \rangle} J_{ij} \left(\hat{S}_i^x \hat{S}_j^x + \hat{S}_i^y \hat{S}_j^y + \Delta \hat{S}_i^z \hat{S}_j^z \right) - h \sum_i \hat{S}_i^z + D \sum_i \left(\hat{S}_i^z \right)^2}$$

$S = 1$ triangular lattice with competing exchange interactions and both exchange and single-site anisotropy.



H. Zhang, Z. Wang, **DD**, K. Barros, C.D. Batista, “Hybridized quadrupolar excitations”, Nature Communications (2021).