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Analyzing collective excitations using implicit neural representations

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Understanding collective excitations in materials is important for developing the next generation of spintronic devices for information transfer and storage. Excitations are often characterized via the dynamical structure factor, $S(\mathbf{Q}, \omega)$, which can be measured using inelastic neutron or x-ray scattering techniques. Real-time analysis during an experiment is challenging due to the high dimensionality of datasets and the slow nature of theoretical simulations. We present a data-driven tool using 'neural implicit representations' for efficient parameter extraction from inelastic neutron scattering data. By training the tool with linear spin wave theory simulations, we achieve precise Hamiltonian parameter extraction for the square-lattice spin-1 antiferromagnet La_2NiO_4, highlighting automatic refinement possibilities for ordered magnetic systems [1].

[1] Chitturi, Sathya R., et al. "Capturing dynamical correlations using implicit neural representations." Nature Communications 14.1 (2023): 5852.

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