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Hamiltonian-driven modeling using image-recognition-based neural networks in rare-earth spin systems

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Neutron scattering technique is an ideal tool to observe spin orders and dynamics, primarily governed by the exchange Hamiltonian. Modeling neutron scattering data involves optimizing the Hamiltonian. Traditionally, forward calculations with a proposed Hamiltonian are used to model inelastic or diffuse neutron scattering data, which is achieved by directly fitting the energy and intensity information of selected one-dimensional (1D) slice-cut data from the measured 4D data space. A standard chi square loss function is usually used. However, the efficient and accuracy of this method is highly dependent on the specific magnetic system. Here, we demonstrate the capability of convolutional based encoding-decoding neural networks to model 3D diffuse scattering and 4D inelastic neutron scattering data and directly extract the exchange parameters of Hamiltonian that best fit the experimental data. Specifically, a variational auto-encoder is built to project an inelastic neutron scattering data to a low-dimensional latent space, and a fully connected neural network is coupled with the autoencoder to define a functional map between the parameters of the Hamiltonian and the latent variables of the autoencoder. The antoencoder and the fully connected neural networks are then jointly trained on the synthetic data. After training, the ML model can directly map an inelastic measurement to the corresponding parameters of the Hamiltonian. We selected the rare-earth spin systems for this demonstration due to its complex magnetic interaction matrices.

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