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# Characterizing quantum materials with scattering experiments and machine learning

*Monday 8 April 2024 11:00 (30 minutes)*

The past few years have witnessed booming research in machine learning in chemistry and materials sciences. New pharmaceutical molecules and new energy materials have been identified by machine learning, leading to a paradigm shift in research and industry. Quantum materials, on the other hand, despite constant new reports in using machine learning, have experienced significant challenge due to the complex interplay between the charge, spin, orbital, and lattice degrees of freedom, and the often-met out-of-distribution (OOD) problem.

In this talk, we introduce our recent efforts in connecting machine learning to various quantum materials with various experimental scattering and spectroscopic techniques. For topological materials with band topology, since "topology"itself is not measurable, seeking the experimental manifestation becomes critical. We introduce our recent effort, to use machine learning to improve neutron measurement resolution [1], and to use x-ray absorption to detect topology with 90% accuracy [2]. For collective excitations of phonons, measurable by inelastic scattering, we show how 3D symmetry can be encoded into a neural network that could lead to efficient property predictions [3], and beyond that how to encode the Brillouin zone into real-space graph neural network to predict complex materials [4]. We present our most recent work on machine learning to classify Majorana bound state from tunneling conductance data, even the OOD problem is severe [5]. We conclude by presenting a few more examples showing the increasingly important role machine learning may play in a variety of quantum many-body and scattering experiments even with scarcity of data and challenges in computation.

[1] NA, ZC, ML, Appl. Phys. Rev. 9, 011421 (2022)
[2] NA, ML Advanced Materials 34, 202204113 (2022)
[3] ZC, NA, ML. Adv. Sci. 8, 2004214 (2021), ZC, XS, ML, Advanced Materials 35, 2206997 (2023)
[4] RO, AC, ML, arXiv:2301.02197 (2023).
[5] MC, RO, AC, ML, arXiv:2310.18439 (2023).

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