Contribution ID: **291** Type: **Talk**

Simulating the Hubbard Model with Normalizing Flows

Tuesday, 30 July 2024 16:15 (20 minutes)

Generative models, in particular normalizing flows, have demonstrated exceptional performance in learning probability distributions across various domains of physics, including statistical mechanics, collider physics, and lattice field theory. In lattice field theory, using normalizing flows for accurately learning the Boltzmann distribution has been applied to a wide range of tasks, such as the direct estimation of thermodynamic observables and the sampling of independent and identically distributed (i.i.d.) configurations.

In this work, for the first time, we provide a proof-of-concept demonstration that normalizing flows can be used to learn the Boltzmann distribution for the Hubbard model. This model is extensively used to study the electronic structure of graphene and other carbon nanomaterials. State-of-the-art numerical simulations of the Hubbard model, such as obtained with Hamiltonian Monte Carlo (HMC) methods, often suffer from ergodicity issues and thus lead to biased estimates of physical observables. Leveraging i.i.d. sampling from the normalizing flow, our numerical experiments demonstrate that generative models successfully overcome these issues.

Primary authors: SCHUH, Dominic; KREIT, Janik; BERKOWITZ, Evan (Forschungszentrum Jülich); FUNCKE, Lena (University of Bonn); LUU, Thomas (Forschungszentrum Jülich / University of Bonn); Dr NICOLI, Kim A. (knicoli@uni-bonn.de); RODEKAMP, Marcel (Forschungszentrum Jülich)

Presenter: SCHUH, Dominic

Session Classification: Applications outside particle physics

Track Classification: Applications Outside Particle Physics