replacing MAR16-2015-007154 Abstract Submitted

for the MAR16 Meeting of
The American Physical Society

Many-body physics via machine learning[1] LOUIS-FRANCOIS ARSENAULT, Columbia Univ, O. ANATOLE VON LILIENFELD, Basel Univ, ANDREW J. MILLIS, Columbia Univ — We demonstrate a method for the use of machine learning (ML) to solve the equations of many-body physics, which are functional equations linking a bare to an interacting Greens function (or self-energy) offering transferable power of prediction for physical quantities for both the forward and the reverse engineering problem of materials. Functions are represented by coefficients in an orthogonal polynomial expansion and kernel ridge regression is used. The method is demonstrated using as an example a database built from Dynamical Mean Field theory (DMFT) calculations on the three dimensional Hubbard model. We discuss the extension to a database for real materials. We also discuss some new area of investigation concerning high throughput predictions for real materials by offering a perspective of how our scheme is general enough for applications to other problems involving the inversion of integral equations from the integrated knowledge such as the analytical continuation of the Greens function and the reconstruction of lattice structures from X-ray spectra.

[1]Office of Science of the U.S. Department of Energy under Subcontract DOE No. 3F-3138 and FG-ER04169

Louis-Francois Arsenault
Columbia Univ

Date submitted: 06 Nov 2015 Electronic form version 1.4