Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

**Deep learning and the electronic structure problem** KYLE MILLS, University of Ontario Institute of Technology, MICHAEL SPANNER, National Research Council of Canada, ISAAC TAMBLYN, University of Ontario Institute of Technology & National Research Council of Canada — In the past decade, the fields of artificial intelligence and computer vision have progressed remarkably. Supported by the enthusiasm of large tech companies, as well as significant hardware advances and the utilization of graphical processing units to accelerate computations, deep neural networks (DNN) are gaining momentum as a robust choice for many diverse machine learning applications. We have demonstrated the ability of a DNN to solve a quantum mechanical eigenvalue equation directly, without the need to compute a wavefunction, and without knowledge of the underlying physics. We have trained a convolutional neural network to predict the total energy of an electron in a confining, 2-dimensional electrostatic potential. We numerically solved the one-electron Schrödinger equation for millions of electrostatic potentials, and used this as training data for our neural network. Four classes of potentials were assessed: the canonical cases of the harmonic oscillator and infinite well, and two types of randomly generated potentials for which no analytic solution is known. We compare the performance of the neural network and consider how these results could lead to future advances in electronic structure theory.

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Date submitted: 10 Nov 2016 Electronic form version 1.4