1139-81-426   **James D Whitfield***, Dartmouth College, 6127 Wilder Laboratory, Hanover, NH 03755, and **Sahil Gulania**, University of Southern California. *Exploiting wave function symmetries in quantum simulation.* Preliminary report.

In order to advance the state of the art in quantum simulation, we must update standard approaches in electronic structure. Our particular interest here is exploiting symmetry of the wave function including both point group symmetries and space-spin symmetries. In our previous work, we analyzed how to project first and second quantizated wave functions into particular irreducible representation of the symmetry group being exploited. Presently, we return to this effort to consider how to construct the Hamiltonian within a single irreducible representation. The recent efforts of several other research teams help inform our research. However, their works have focused on specific aspects whereas we will build a general mathematical framework based on projection operators. The ultimate goal is creating black box quantum simulations by constructing the Hamiltonian only within a single irreducible representation and we will report on our recent progress in this direction. (Received February 18, 2018)