Abstract Submitted
for the DAMOP19 Meeting of
The American Physical Society

Transfer matrix theory of surface spin-echo experiments with molecules[1] JOSHUA T. CANTIN, University of British Columbia, GIL ALEXANDROWICZ, Swansea University, ROMAN V. KREMS, University of British Columbia — ^{3}He spin-echo experiments have been used to study surface morphology, atomic surface diffusion, and phase transitions of ionic liquids. By replacing ^{3}He atoms with molecules, one may be able to exploit additional molecular degrees of freedom, such as rotation, to provide even more insight into surface dynamics. Indeed, a recent experiment used *ortho*-hydrogen to probe the orientation of a Cu(115) surface [1]. However, the large manifold of molecular states and magnetic field-induced couplings between these states preclude a semi-classical description for these new experiments. Here, we build an efficient, fully quantum mechanical theoretical framework that connects the experimental signal to the elements of the molecule-surface scattering matrix. To do this, we derive a one-dimensional transfer matrix method that includes the molecular hyperfine degrees of freedom. We apply our framework to the case of *ortho*-hydrogen, show that the calculated experimental signal is sensitive to the scattering matrix elements, and present a preliminary comparison to experiment. This work sets the stage for machine learning techniques to determine the details of molecule-surface interactions from experimental data. [1] Godsi et al., Nat. Comm. **8**, 15357 (2017).

[1]This work was funded by NSERC of Canada and the Horizon 2020 Research and Innovation Programme grant 772228.

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Date submitted: 01 Feb 2019 Electronic form version 1.4