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Bridging the momentum distribution and the potential energy surface of protons in hydrogen bonds JOSEPH MORRONE, Columbia University, LIN LIN, ROBERTO CAR, Princeton University, MICHELE PARRINELLO, ETH Zurich — Open path integral Car-Parrinello molecular dynamics studies have uncovered the proton momentum distribution in various phases of ice [1,2]. These systems exhibit a wide range of behavior, including symmetric hydrogen bonds and quantum tunneling. In this work, we provide an in-depth statistical analysis of the simulation results. This analysis reveals a direct relation between the open path formalism of quantum particles and their underlying potential energy surface. Application of this analysis to ice systems provides quantitative information about the principle axes of the potential energy surface that the proton experiences, and indicates that the oxygen-oxygen distance is a proper reaction coordinate for such systems. Our analysis also facilitates a direct observation of anharmonic effects along the principle axes. [1] J. A. Morrone and R. Car, Phys. Rev. Lett. 101, 17801, 2008. [2] J. A. Morrone, L. Lin and R. Car, J. Chem. Phys. 130, 204511, 2009.

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