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Displaced path integral formulation for the momentum distribution of quantum particles LIN LIN, Princeton University, JOSEPH MORRONE, Columbia University, ROBERTO CAR, Princeton University, MICHELE PARRINELLO, ETH Zurich — The proton momentum distribution, accessible by deep inelastic neutron scattering, is a very sensitive probe of the potential of mean force experienced by the protons in hydrogen-bonded systems. In this work we introduce a novel estimator for the end-to-end distribution of the Feynman paths, i.e. the Fourier transform of the momentum distribution. In this formulation, free particle and environmental contributions factorize. Moreover, the environmental contribution has a natural analogy to a free energy surface in statistical mechanics, facilitating the interpretation of experiments. The new formulation is not only conceptually but also computationally advantageous, because the displaced path distribution can be sampled accurately with thermodynamic integration techniques. We illustrate the method with applications to one-dimensional model systems and to an empirical water model.

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