Abstract Submitted
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Improved Algorithm for Calculating Observables in Diffusion and Reptation Quantum Monte Carlo JEREMY MCMINIS, DAVID CEPERLEY, Dept. of Physics, University of Illinois at Urbana-Champaign, CARLO PIERLEONI, Physics Department, University of L'Aquila — By reformulating the calculation of observables using the Hellman-Feynman theorem we are able to reduce the bias on observables calculated in Diffusion and Reptation Monte Carlo. Unlike previous attempts [1], our technique assumes no knowledge about derivatives of the trial or exact ground state wavefunction with respect to the perturbation. We will outline the derivation of the operator and show examples for DMC by comparing to forward walking, and within RMC by showing faster convergence to the unbiased, ground state observable. [1]Assaraf and Caffarel, J. Chem. Phys. 119, 10536 (2003)

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