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Accurate energy differences with Quantum Monte Carlo SIMONE CHIESA, DAVID CEPERLEY, JEONGNIM KIM, RICHARD MARTIN, UIUC — Computation of accurate energy differences is of primary importance in the study of transformations as those occurring in solid to solid phase transitions or chemical reactions. In stochastic quantum simulations this can be done efficiently, employing correlated sampling techniques whereby fluctuations cancel with each other leading to results with a much smaller statistical error. Although correlated sampling is very effective for variational Monte Carlo such is not the case for diffusion Monte Carlo where branching and different nodal structures force the introduction of uncontrolled approximations. Here we describe the use of reptation Monte Carlo as a method that maintains a single path for both systems and leads to energies which are exact within the fixed node approximation. We show how to combine umbrella sampling with coordinate transformations to give a simple and efficient algorithm to compute small energy differences. Application to dissociation reaction paths and weakly bound systems are presented.

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