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Ab initio molecular dynamics with noisy and cheap quantum Monte Carlo forces: accurate calculation of vibrational frequencies YE LUO, SANDRO SORELLA, Scuola Internazionale Superiore di Studi Avanzati (SISSA) — We introduce a general and efficient method for the calculation of vibrational frequencies of electronic systems, ranging from molecules to solids. By performing damped molecular dynamics with ab initio forces, we show that quantum vibrational frequencies can be evaluated by diagonalizing the time averaged position-position or force-force correlation matrices, although the ionic motion is treated on the classical level within the Born-Oppenheimer approximation. The novelty of our approach is to evaluate atomic forces with QMC by means of a highly accurate and correlated variational wave function which is optimized simultaneously during the dynamics. QMC is an accurate and promising many-body technique for electronic structure calculation thanks to massively parallel computers. However, since infinite statistics is not feasible, property evaluation may be affected by large noise that is difficult to harness. Our approach controls the QMC stochastic bias systematically and gives very accurate results with moderate computational effort, namely even with noisy forces. We prove the accuracy and efficiency of our method on the water monomer[A. Zen et al., JCTC 9 (2013) 4332] and dimer. We are currently working on the challenging problem of simulating liquid water at ambient conditions.

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