Efficient calculation of forces by quantum Monte Carlo

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The computational cost for the calculation of forces by quantum Monte Carlo can be dramatically reduced by using the so called "Algorithmic Differentiations"[1], that allow us to compute the forces acting on all atoms of a complex electronic system with a computational time comparable to the one for evaluating the total energy. Several applications will be discussed, the accurate calculations of the vibrational modes in the water molecule and dimer, the structural optimization of large molecules, and, finally, a first attempt of an ab-initio molecular dynamics[2] for water at ambient conditions.

[1] S. Sorella and Luca Capriotti, J. Chem. Phys. **133**, 234111 (2010).

[2] C. Attaccalite and S. Sorella, Phys. Rev. Lett. **100**, 114501 (2008).