

Computation of forces in quantum Monte Carlo

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In order to find the equilibrium geometries of molecules and solids and to perform ab initio molecular dynamics, it is necessary to calculate the forces on the nuclei. We present a correlated sampling method to efficiently calculate numerical forces and potential energy surfaces in diffusion Monte Carlo. It employs a novel coordinate transformation, earlier used in variational Monte Carlo, to greatly reduce the statistical error. Results are presented for first-row diatomic molecules.

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