Forces and Response Functions in QMC

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We will discuss two different subjects, physically related but very far from each other in terms of technical development in quantum Monte Carlo (QMC).

One is a Nudged Elastic Band (NEB) calculation of minimum energy paths for a few chemical reactions between small molecules –a structural optimization problem which is carried out using QMC forces. It is aimed at showing that routine use of forces is becoming feasible in QMC. Interestingly, the accuracy on the transition states' geometries and energies is much better than using DFT with GGA functionals (adopted in the vast majority of NEB calculations for catalysis problems), and even slightly better than using DFT with highly parameterized hybrid functionals (which include the studied reactions in their learning data sets).

The other one, a more explorative effort, is an attempt at exploiting imaginary-time correlation functions for spectral properties of Fermions. We will show (i) an example in liquid 3He where the nodal constraint used in QMC to avoid the sign problem can be in part relaxed to good effect, and (ii) an assessment of accuracy for the imaginary time evolution for the jellium model, obtained by Auxiliary Field Monte Carlo in the phaseless approximation.