Derivatives of the fixed−−node energy

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The fixed−node ground state energy of a many−fermion system can be expressed in a path integral representation which lends itself naturally to a fairly efficient Monte Carlo sampling.

In principle, through analytic derivatives of this explicit expression for the total energy, a single ground state simulation gives access to several quantities of physical interest such as forces and susceptibilities.

We discuss the practical implementation of these ideas for the cases of the Lithium dimer and the Fermi gas.
