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The quantum Monte Carlo method—electron correlation from random numbers

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Abstract
The fixed-node diffusion quantum Monte Carlo (DMC) method is the most accurate method known for calculating the energies of large many-particle quantum systems. The key element of the method is the development of accurate trial many-body wavefunctions which control the statistical efficiency of the calculations and the accuracy obtained. Accurate wavefunctions can be obtained by building correlation effects on top of mean field descriptions such as density functional theory. The wavefunctions can be improved by introducing multi-determinants, pairing functions, and backflow transformations. The calculations are expensive, but the method scales well with system size and calculations on 1000 particles are possible. Some recent applications of the DMC method to atoms, molecules and solids will be presented.

