MAR07-2006-007424

Abstract for an Invited Paper
for the MAR07 Meeting of
the American Physical Society

QMC simulations using backflow correlated wave functions

RICHARD NEEDS, University of Cambridge

An inhomogeneous backflow transformation for many-particle wave functions is presented and applied to electrons in atoms, molecules, and solids. Backflow transformations are compact parametrizations, by which we mean that the number of parameters required to retrieve a given fraction of the correlation energy increases only slowly with system size. We report variational and diffusion quantum Monte Carlo (VMC and DMC) energies for a number of systems and study the computational cost of using backflow wave functions. Backflow transformations alter the nodal surface of the wave function and can therefore be used to reduce the fixed-node error in DMC calculations. Applications to the homogeneous electron gas, the all-electron lithium atom and dimer, and carbon atom and dimer, and pseudopotential calculations for the carbon atom and dimer and carbon diamond are presented. When the initial nodal surface is reasonably accurate, backflow appears to do an excellent job in improving the VMC energy and correcting the remaining errors in the nodal surface. When the initial nodal surface is poor, however, backflow is apparently incapable of making the gross changes to the nodal surface required to correct the flaws, although it still normally lowers both the VMC and DMC energies significantly. Overall, we find that inhomogeneous backflow transformations can provide a substantial increase in the amount of correlation energy retrieved within VMC and DMC calculations. This approach is of considerable generality as it is successful in metals and in insulators, and in large and small systems. Backflow transformations can readily be used with pairing wave functions, and this approach could yield significant improvements when a wave function consisting of a single determinant of one-particle orbitals is a poor starting point.