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**Backflow transformations in inhomogeneous systems** PABLO LOPEZ RIOS, ANDREA MA, NEIL D. DRUMMOND, RICHARD J. NEEDS, TCM Group, University of Cambridge — The quality of trial wave-functions, and of their nodal surface in particular, determines the accuracy of the results obtained within the Fixed-Node Diffusion Monte Carlo (DMC) method. Backflow transformations have been proven capable of improving the nodal surface of Slater-Jastrow (SJ) wave-functions in homogeneous systems. In this work we will present the extension of backflow to inhomogeneous systems, along with DMC results for atoms, molecules and solids which show the improved accuracy of this form of trial wave-function. We will also discuss the advantages of using electron-by-electron algorithms to enhance the computational efficiency of QMC with backflow wave-functions.

Pablo Lopez Rios  
TCM group, University of Cambridge

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