Lattice regularized diffusion Monte Carlo

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We introduce an efficient lattice regularization scheme for quantum Monte Carlo calculations of realistic electronic systems. The Laplacian is discretized with two incommensurate mesh sizes, a and a', where a'/a is a fixed irrational number, and the regularized Hamiltonian goes to the continuous limit for $a \to 0$. The use of the double mesh improves significantly the convergence to the $a \to 0$ limit, and allows to take into account the different length scales in the system, with an efficiency gain which becomes more and more relevant as the atomic number increases. One of the main advantages of this framework is the possibility to include non-local potentials in a consistent variational scheme, substantially improving both the accuracy and the computational stability upon previous non-variational diffusion Monte Carlo approaches. We present some applications of our method to cases involving transition metal elements.