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**Lattice regularized diffusion Monte Carlo method**[1]

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We introduce a lattice regularization scheme for quantum Monte Carlo calculations of realistic electronic systems[1]. Our method is based on the discretization of a projection operator (Green's function), constructed upon an effective regularized Hamiltonian[2]. In particular, its 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 one to take into account efficiently the different length scales in the system. Another advantage 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. However, we have recently shown[3] that also the standard diffusion Monte Carlo algorithm can be made stable and variational even in the presence of non-local pseudopotentials, by including a non-local discrete process in the diffusion operator. This work can open the route for even more reliable and accurate electronic ground state calculations using diffusion Monte Carlo methods.

[1] M. Casula, C. Filippi, and S. Sorella, Phys. Rev. Lett. **95**, 100201 (2005).
[2] S. Sorella, cond-mat/0201388.
[3] M. Casula, Phys. Rev. B **74**, 161102(R) (2006).

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