Recent progress with the Lattice Regularized Diffusion Monte Carlo

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We review the recent approach proposed in Ref[1], the so called Lattice regularized Monte Carlo. In this method the basic ingredient is an Hamiltonian H^a that is an accurate rapresentation of the realistic Hamiltonian H, and maintains the basic properties of lattice Hamiltonians. Indeed H^a contains electron hoppings of minimum length a, and converges to the exact Hamiltonian in the limit $a \to 0$. Once the lattice space a is chosen the imaginary time propagation, used to project the ground state energy of H^a, can be implemented exactly with known and well established quantum Monte Carlo techniques. Moreover the so called Fixed node approximation, required to avoid the "fermion sign problem", is generally applicable, even in presence of non-local pseudopotentials. In the original formulation, two hopping lengths a and a' were introduced to sample the continuous space with a'/a equal to an irrational number. Here we show that this complication is unnecessary and a single hopping is sufficient and actually much more efficient for light atoms. A double mesh with appropriate value of a'/a is instead necessary only when ions of large atomic number, such as Iron, are present in the numerical simulation. Finally we show that it is possible to improve substantially the convergence of the ground state energy in the limit $a \to 0$ by using a different discretization close to the nodal region, where the wavefunction vanishes. This simple generalization is indeed important when schemes more accurate than the standard Fixed node approximation are implemented.

We present some examples of recent interest with Carbon based compounds, starting from the simplest Carbon atom up to the graphite layers.

[1] M. Casula, C. Filippi and S. Sorella *Diffusion Monte Carlo with lattice regularization*, Phys. Rev. Letters, **95**, 100201 (2005).