When nothing really matters: finding the zeros of the fermionic many-body wave function.

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The emergence of parallel computing has altered the cost-benefit balance of the numerical methods used to study numerically the electronic structure of real materials. Sequential algorithms flourished during the 80s and 90s with single processors machines. However, they now suffer heavily from communication bottle necks in large parallel supercomputers. This is typically the case of methods based on density functional theory. Statistical methods, while dormant during many decades, are now taking over the front of electronic structure research since they can be easily distributed with a minimum of communication involved. Diffusion quantum Monte Carlo (DMC) is the many- body method of choice to study ab-initio systems with more than 12 electrons and has been used up to a few thousands. DMC is based on an analogy between the Schrödinger equation at imaginary time and the diffusion equation. DMC finds statistically the ground state energy of any many-body system without approximations. The ground state energy of most Hamiltonians is, however, the bosonic solution. For electronic problems one must first provide the exact surface where the many-body wave function changes sign (the node). Any error in the node increases the energy of the ground state found with DMC. Finding an approximation to the node belongs to the family of problems known as sign problems. In this talk we will outline a method that is able to find the node for electronic problems. The cost of the method is linear in the number degrees of freedom of the wave function. This method is not only able to find the node but also the many-body wave function itself. Applications to molecules and small clusters will be presented.