AFQMC for challenging problems

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Obtaining a solution to the many-electron Schrödinger equation stands as one of the grand challenges in chemistry and physics. Highly accurate solutions are achievable for materials containing elements from the first two rows of the periodic table, enabling us to predict the energies and properties, sometimes even achieving accuracy on par with experimental results. However, the predictive power diminishes significantly when attempting to study the properties of transition metal-containing clusters or transition states. In this presentation, I will describe a promising new method known as Auxiliary Field Quantum Monte Carlo (AFMQC), which has the potential to address many of the challenges that conventional quantum chemistry methods face. Nevertheless, this method encounters three significant challenges: (a) it is relatively expensive, (b) obtaining properties beyond energy values can be challenging, and (c) systematically improving its accuracy can also be costly. It's worth noting that some of these challenges are not unique to AFQMC but afflict many other quantum Monte Carlo methods. During this talk, I will introduce novel techniques that have allowed us to overcome these three challenges. I will demonstrate that with the help of these developments, we have been able to tackle chemical problems that were previously inaccessible or exceptionally demanding. I will argue that AFQMC can be used in a plug-and-play manner, even by experimentalists.