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QUANTUM MONTE CARLO: SUCCESSES AND CHALLENGES

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Over the last three decades, the use of Monte Carlo methods to solve some mathematical problems that arise in Quantum Many-body Theory have become widely used. The applications are very broad, to nuclear and condensed-matter physics, to quantum chemistry, to dilute gases at ultra-low temperatures, and to nanosystems. In essence, it is required to solve a partial differential equation in 3N dimensions to treat an N-body system. Direct solution of the equations by random-walk methods as well as variational methods are used. That this is possible in a scalable way that can attain the accuracy needed for chemistry is a consequence of the exponential growth of computing power and of increasing algorithmic understanding. Standard techniques of transport Monte Carlo: importance sampling, creation of efficient estimators, and correlation methods all turn out to be crucial. I will explain the mathematical context, some of the methodologies, and show some striking examples of the predictive power of these methods. For many-fermion systems, computational methods that have no uncontrolled approximations are inhibited by a "sign problem" in which negative estimators can asymptotically destroy the signal to noise ratio.

Recent progress in solving that problem will be described. Our approach is to work in the larger space of two walkers that carry opposite signs, to use an importance function that distinguishes between positive and negative walkers, to correlate the moves of opposite walkers to bring then together in the large dimensional space, and to cancel close pairs.