Quantum Monte Carlo Methods

It is a paramount goal of nuclear physics to describe the collision of two nuclei in terms of the dynamics of all of the neutrons and protons involved. Thus, the collision of a 3H nucleus and a neutron is fundamentally a four-body problem. The complexity of the nuclear interaction and the fermionic many-body nature of nuclear systems has however greatly restricted the range of such 'ab initio' reaction models to a small number of favorable cases, often with simplified interactions. The variational Monte Carlo (VMC) and Green's function Monte Carlo (GFMC) -- collectively, quantum Monte Carlo (QMC), which achieved important early successes in reproducing discrete nuclear states and constraining the three-nucleon interaction. Single-channel scattering of neutrons from 4He has been successfully described with the QMC methods, but eventual application to reactions requires development of 'coupled channel' methods suitable for reactions that alter the colliding projectiles. As a first example of coupled channels, we are studying neutron scattering from tritium, in which the final states can have different total spin or orbital angular momentum from the initial state. As an initial step, we are computing wave functions and phase shifts using nuclear VMC wave functions (which will also be needed as starting points for GFMC calculations). Our calculation uses both two- and three- body terms of a nuclear Hamiltonian that describes hydrogen and helium isotopes accurately. Our solution strategy is to impose particle-in-a-box boundary conditions and use VMC/GFMC to find the energy and wave function of the lowest state in the box. Then the energy, surface boundary conditions, and amplitudes at the box surface can be matched onto scattering solutions outside the box. The main challenge for coupled channels is to generate pairs of linearly independent solutions with the same energy but different boundary conditions and read out their surface amplitudes accurately. To guide the choice of boundary conditions we constructed a phenomenological two-body potential of neutron-triton scattering to guide our variational minimization. Through VMC we will build the four-body wave functions, these wave functions will then be the first step toward extracting reaction properties using GFMC. Since the mass-four systems are computed accurately using the same Hamiltonian by other methods, this work will allow us to benchmark the accuracy of our results. It will pave the way for more complicated coupled-channels problems in which the colliding nuclei exchange particles.

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