Comment on "Feynman-Kac Path-Integral Calculation of the Ground-State Energies of Atoms"

In a recent Letter [1], Korzeniowski, Fry, Orr, and Fazleev (KFOF) showed how to use a Monte Carlo method to evaluate Feynman-Kac path integrals and hence obtain accurate ground-state energies of many electron systems. In particular, they suggested that they had found a simple solution to the sign problem which plagues all other fermion quantum Monte Carlo methods. Unfortunately, I believe that their approach is almost equivalent to an extremely inefficient implementation of the familiar diffusion quantum Monte Carlo (DQMC) method, and that their proposed solution to the sign problem is just the well-known fixed node approximation [2]. This gives a variational upper bound on the ground-state energy but is only exact if the zeros of the full many electron wave function are known exactly.

Both the Feynman-Kac and DQMC techniques use a simulation method to solve the N electron imaginary time Schrödinger equation. This equation may be interpreted as describing walkers (not single electrons) diffusing in $3N$ dimensional phase space while dying (being removed from the simulation) or multiplying (producing copies of themselves) at a rate determined by the value of $-V(\mathbf{R})$. Here $V(\mathbf{R})$ is the total potential (including electron-electron interactions) at point $\mathbf{R}=(\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_N)$ in the $3N$ dimensional phase space. In the DQMC method the copies produced when a walker multiplies are allowed to propagate independently, but there is no fundamental reason why they should not all be "glued" to the original walker. The simulation method then amounts to walkers diffusing without branching but with a weight which depends on the regions of phase space they sample. The weight associated with a particular diffusion path is $\exp[-\int_0 V(\mathbf{R}(s))ds]$ and so this algorithm is exactly the one used by KFOF. In fact, DQMC methods usually use a combination of both algorithms, with the costly branching process only carried out now and again using weights accumulated over a number of diffusion steps. At the heart of most DQMC programs (without importance sampling) there is therefore a section which codes *exactly* the same algorithm as that used by KFOF. Equation (7) of KFOF is also used in DQMC calculations, where it is known as the growth estimate of the energy. The variance of this estimate can be enormously decreased by using importance sampling to increase the efficiency of the phase space sampling and similar improvements should be obtainable in the KFOF method [3]. The fact that the KFOF diffusion paths do not branch probably decreases their phase space sampling efficiency still further, but has the advantage that it makes the method very suitable for massive parallelization.

The sign problem arises because the fermion ground-state component of the starting state becomes exponentially damped relative to the lower energy boson ground-state component as the simulation progresses. The fixed node approximation circumvents the problem by starting with a good guess (usually from a Hartree-Fock calculation) at the nodal surface (the $3N-1$ dimensional surface of zeros) of the many electron wave function. A Monte Carlo algorithm is then used to sample the ground states in each of the nodal regions separately, with the boundary condition that the wave function vanishes on the nodal surface. The method gives approximate antisymmetric ground-state wave functions and variational energy estimates which become exact if the guessed nodal surface is exact.

The boundary conditions on the nodal surfaces are imposed by annihilating any walkers which cross those surfaces, which is equivalent to the KFOF procedure of assigning zero weight to diffusion paths crossing nodes. The instructions required to code the KFOF algorithm parallel those in a standard fixed node DQMC calculation exactly, and so the two methods are the same. The results obtained are variational but cannot be exact unless the assumed nodal surface is also exact. Since no general method for finding the nodal surfaces of many fermion wave functions is known [4] (symmetry arguments alone are not usually sufficient), this is unlikely to be the case.

In summary, the method described by KFOF is little different from the fixed node DQMC method without importance sampling and is not exact. The introduction of importance sampling would make the method much more efficient.

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