

Corney and Drummond Reply: Rombouts' Comment [1] on our Letter [2] raises two issues that require clarification. The first is how to correctly implement the Gaussian quantum Monte Carlo (GQMC) method. We agree with Rombouts that this requires some care, especially with regard to the type of stochastic calculus employed. The second is whether GQMC is equivalent to the auxiliary field quantum Monte Carlo (AFQMC) method. In regard to the latter, we find that the evidence presented in the Comment to support the claim that they are equivalent is inconclusive, and so this question remains open.

GQMC is based on a mapping of the evolution of the density operator onto a continuous Markov process in a generalized phase space. It leads to a set of weighted stochastic differential equations that must be implemented numerically. As with any numerical solution of continuous equations (stochastic or deterministic), the corresponding discretized equations must converge to the differential equation in the limit that the step size ϵ goes to zero. There are two commonly used formulations of stochastic calculus: Itô and Stratonovich, which correspond to *different* discretized equations. Our GQMC equations in [2] for the Hubbard model are identified as Stratonovich equations, and must be solved with a numerical algorithm that is consistent with Stratonovich calculus, such as a semi-implicit approach [3]. In contrast, the difference equations quoted in [1] correspond to an explicit Euler algorithm, with an update based on values at the beginning of the time step, and thus converge to Itô stochastic equations. Even though these difference equations appear similar to ours (after truncation), the changed stochastic calculus makes them inequivalent. Nevertheless, there is a well-defined procedure for transforming between the two [see, e.g., [4]].

The figures in the auxiliary material [5] from the preceding Comment show incorrect results obtained from solving the truncated Ito equations. If the simulations are to be regarded as an implementation of the Stratonovich equations in [2], then the resulting discrepancies have nothing to do with any approximations in GQMC, or sampling issues [6], or possible boundary terms, but merely to do with an inconsistent choice of numerical algorithm. To solve the GQMC equations, we use a semi-implicit method, which gives correct answers for the one-site Hubbard model, as was demonstrated in [2]. In order to use a Euler (or Milstein) algorithm, as Rombouts does, one must first transform our equations to an Itô form, which for Eq. (9) in [2] means redefining the propagation matrix to be $\Delta_{ij\sigma}^{(r)} \equiv t_{ij} - \delta_{ij}(Un_{jj,-\sigma} - \mu + f\xi_j^{(r)})$. The GQMC equations are therefore clearly different to the truncated and approximate equations that Rombouts has simulated. Thus the figures in [5] are a clear demonstration

of the consequences of using an Euler algorithm to solve a Stratonovich equation, but they shed no light on the relationship between AFQMC and GQMC.

To substantiate the claim that GQMC is equivalent to AFQMC, one could try to prove that any equation that can be derived in GQMC corresponds to a well-defined limit of an AFQMC equation. This is not proved in the Comment or the auxiliary material. Instead, Rombouts focuses on the specific equations given in [2] for the Hubbard model, and seeks to derive AFQMC equations that are equivalent.

From AFQMC, Rombouts derives Euler difference equations for the correlation matrix n and the weight Ω . The statement that the formal limit $\epsilon \rightarrow 0$ would lead to the equations in [2] cannot be proved by a direct comparison involving the AFQMC equations as they are written in the Comment. First, one must explicitly evaluate the unspecified terms denoted $\mathcal{O}(\epsilon^2\Delta^2)$, since, as Rombouts points out, they are actually of first order in ϵ . Second, the resulting formal limit needs careful attention, since it would lead to an Itô equation, and cannot be compared directly with our Stratonovich equation without further corrections. Even if the formal limit were the same, there appear to be clear differences in the numerical implementation, as is evident, for example, in [6].

Finally, we emphasize that just because the two approaches apparently lead to two different numerical implementations does not mean that either is incorrect. Rather, it means that there is a choice of methods, with different sampling and numerical efficiencies, that require further investigation.

J. F. Corney and P. D. Drummond

ARC Centre of Excellence for Quantum-Atom Optics
The University of Queensland
Brisbane, Qld 4072, Australia

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