Comment on "Gaussian Quantum Monte Carlo Methods for Fermions and Bosons"

In a recent Letter, Corney and Drummond propose a Gaussian quantum Monte Carlo method (GQMC) based on a Gaussian expansion of the density operator [1]. They claim that their method is able to solve bosonic and fermionic problems without encountering a "sign error." They present their method as a continuous diffusion process in configuration space. However, any practical implementation will have to resort to discrete time steps, where care has to be taken to include all relevant terms. When using the correct discrete-time propagation, one finds that GQMC is equivalent to the auxiliary-field quantum Monte Carlo method (AFQMC) [2–5] and hence must have the same sign problems [6,7]. To substantiate my claim I will show how the expressions for the repulsive fermionic Hubbard model given by Corney and Drummond can be derived in the framework of the AFQMC [8]. The discussion can easily be generalized to continuous-time [3], fermionic pair [4], and bosonic [5] versions of AFQMC.

AFQMC is based on the decomposition of the many-body density operator as a weighted average over an ensemble of exponentials of one-body operators, $e^{-\tau\hat{H}} = \int P_\tau(X)\exp[-\tau\hat{h}(X)]dX$. This permits to express grand-canonical expectation values in terms of the single-particle basis matrix representations h of the operators $\hat{h}$, e.g., the expectation value of the operator $a_j^\dagger a_i$ is given by $n_{ij}(\tau, X) = [e^{-\tau h(X)}/(1 + e^{-\tau h(X)})]_{ij}$. To arrive at such a decomposition, one splits the imaginary-time interval $[0, \tau]$ into a number of time slices and applies the Hubbard-Stratonovich transformation [9], $e^{-\epsilon\hat{H}} \propto \int e^{-\epsilon/2\xi^2} e^{\epsilon\hat{\Delta}(\xi)} d\xi + \mathcal{O}(\epsilon^2)$, with the one-body operator $\hat{\Delta}(\xi) = -\hat{H}_0 - \sum_{j=1}^m \xi_j \hat{A}_j$, and $\hat{H} = \hat{H}_0 - \frac{1}{2}\sum_{j=1}^m \hat{A}_j^2$. This leaves considerable freedom in the choice of operators $\hat{A}_j$ and auxiliary fields ξ. A way to optimize this *stochastic gauge* is given by the shifted-contour AFQMC [10], which consists in redefining the auxiliary field $\xi_j = \bar{\xi}_j - \langle\hat{A}_j\rangle_{\tau,X}$. The resulting operator $\Delta(\bar{\xi})$ is the one given by the expression below Eq. (9) in Ref. [1], if one takes into account that the imaginary-time correlation $\delta(\tau' - \tau)$ for the auxiliary fields translates in a factor $(2\epsilon)^{-1}$ when using discrete time steps.

Consider an infinitesimal step in imaginary time, $\tau' = \tau + 2\epsilon$, by multiplying each of the elements of the ensemble to the left and to the right with a propagator $\exp(-\epsilon\hat{H})$, decomposed using auxiliary fields $\bar{\xi}_l$ and $\bar{\xi}_r$. The one-body density matrix $n(\tau, X)$ will then evolve as $n(\tau', X') = n + \epsilon[(1 - n)\Delta(\bar{\xi}_l)n + n\Delta(\bar{\xi}_r) \times (1 - n)] + \mathcal{O}(\epsilon^2\Delta^2)$. If one draws the auxiliary fields $\bar{\xi}_{l,r}$ from a Gaussian distribution then one has to update only the non-Gaussian part of the weight, $\Omega(\tau', X') = \Omega(\tau, X)[1 - 2\epsilon\langle\hat{H}_0\rangle_{\tau,X} + \epsilon\sum_j\langle A_j\rangle_{\tau,X}^2] + \mathcal{O}(\epsilon^2\Delta^2)$. The formal limit $\epsilon \to 0$ would lead to the expressions in Ref. [1]. However, because the auxiliary fields $\bar{\xi}_{l,r}$ are of order $\epsilon^{-1/2}$, the $\mathcal{O}(\epsilon^2\Delta^2)$ terms have to be included. Otherwise the propagation will deviate from the exact solution already at leading order in ϵ, as is easily demonstrated for a one-site model [8]. Furthermore, this is also the place where the *sign problem* shows up: it is not guaranteed that the weights remain positive, even for very small values of ϵ [7]. In conclusion, if GQMC is implemented correctly then it is equivalent to AFQMC and hence it should have the same sign properties. Otherwise it provides only approximate results that might be improved upon by symmetry projections [11].

L. Pollet, K. Van Houcke, and M. Troyer are kindly acknowledged for the interesting discussions and the Fund for Scientific Research—Flanders for financial support.

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Received 11 November 2005; published 8 May 2006
DOI: 10.1103/PhysRevLett.96.188901
PACS numbers: 03.75.Ss, 02.70.Tt, 03.65.Ca, 42.50.Lc

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