Relationship between Hirsch-Fye and weak-coupling diagrammatic quantum Monte Carlo methods

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Two weak-coupling continuous time quantum Monte Carlo (CTQMC) methods are shown to be equivalent for Hubbard-type interactions. A relation between these CTQMC methods and the Hirsch-Fye quantum Monte Carlo (HFQMC) method is established, identifying the latter as an approximation within CTQMC and providing a diagrammatic interpretation. Both HFQMC and CTQMC are shown to be equivalent when the number of time slices in HFQMC becomes infinite, implying the same degree of fermion sign problem in this limit.

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I. INTRODUCTION

Hirsch-Fye quantum Monte Carlo (HFQMC) is a standard method for the simulation of quantum lattice models [1–5]. However, during the past decade, new quantum Monte Carlo (QMC) methods have emerged, which are based on stochastic sampling of diagrams in a perturbative expansion [6]. These new methods avoid systematic errors due to finite discretization in the imaginary time and are commonly referred to as "continuous time quantum Monte Carlo" (CTQMC). With new variants of CTQMC appearing, a comparison of these formalisms becomes important. In this work, we consider two seemingly different CTQMC methods proposed by Rombouts *et al.* [7] and Rubtsov *et al.* [8] based on the expansion of the interaction term of Hamiltonian in the perturbation series, also known as "weak-coupling" CTQMC. We show that for Hubbard-type interactions these methods are equivalent. We also show that HFQMC can be interpreted as a summation of a specific subset of diagrams present in CTQMC.

II. EQUIVALENCE OF CTQMC ALGORITHMS BY ROMBOUTS *et al.* AND RUBTSOV *et al.*

These methods consider the perturbative expansion of the partition function in powers of the interaction and then sample the resulting series of multidimensional integrals stochastically. We will use a path integral formalism to illustrate this. Here, the partition function is written as an integral over the Grassman variables η, η^*: $Z = \int \mathcal{D}\eta^* \mathcal{D}\eta e^{-S(\eta^*, \eta)}$, with the action

$$S(\eta^*, \eta) = S_0(\eta^*, \eta) - \int_0^\beta d\tau V[\eta^*(\tau), \eta(\tau)], \qquad (1)$$

where S_0 is the bare part of S and V is the interacting part of the Hamiltonian H. For the purposes of discussion we consider Hubbard-type repulsive interaction [9],

$$V = U \sum_{j=1}^{N_c} \left[n_{j\uparrow} n_{j\downarrow} - \frac{1}{2}(n_{j\uparrow} + n_{j\downarrow}) \right]. \qquad (2)$$

In the Rombouts method [7], a constant K is introduced to shift the reference free energy and the resulting series expansion for the partition function can be written as

$$Z = e^{-K} \int_{\eta^*, \eta} e^{-S_0} \sum_{k=0}^\infty \left(\frac{K}{\beta}\right)^k \int_0^\beta d\tau_1 \cdots \int_0^{\tau_{k-1}}$$
$$\times d\tau_k \left[1 - \frac{\beta}{K} V(\tau_1) \right] \cdots \left[1 - \frac{\beta}{K} V(\tau_k) \right]. \qquad (3)$$

The following identity is then used to decouple the interaction terms and introduce an auxiliary field s,

$$\left(1 - \frac{\beta}{K} V \right) = \frac{1}{2N_c} \sum_{j=1}^{N_c} \sum_{s_j = \pm 1} e^{\gamma s_j(n_{j\uparrow} - n_{j\downarrow})}, \qquad (4)$$

where $\cosh \gamma = 1 + \frac{\beta U N_c}{2K}$. The resulting series for the partition function is

$$Z = e^{-K} \int_{\eta^*, \eta} e^{-S_0} \sum_{kj\tau s} \left(\frac{K}{2\beta N_c}\right)^k$$
$$\times e^{\gamma s_1[n_{j_1\uparrow}(\tau_1) - n_{j_1\downarrow}(\tau_1)]} \cdots e^{\gamma s_k[n_{j_k\uparrow}(\tau_k) - n_{j_k\downarrow}(\tau_k)]}, \qquad (5)$$

where multiple sums and integrals are denoted as

$$\sum_{kj\tau s} = \sum_{k=0}^\infty \int_0^\beta d\tau_1 \sum_{j_1=1}^{N_c} \sum_{s_1} \cdots \int_0^{\tau_{k-1}} d\tau_k \sum_{j_k=1}^{N_c} \sum_{s_k}. \qquad (6)$$

The fermion degrees of freedom can now be integrated out, and the partition function can be rewritten as [10]

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$$Z = \frac{Z_0}{e^K} \sum_{kj\tau s} \left(\frac{K}{2\beta N_c} \right)^k \prod_\sigma \det \mathcal{G}_\sigma^0 \cdot \det [G_\sigma^{\{s_i\}}]^{-1}, \qquad (7)$$

where $G_\sigma^{\{s_i\}}$ is the Green's function for a particular configuration of auxiliary fields and is related to the noninteracting Green's function $\mathcal{G}_\sigma^0$ by a Dyson's equation,

$$[G_\sigma^{\{s_i\}}]^{-1} e^{-\gamma W_\sigma^{\{s_i\}}} - e^{-\gamma W_\sigma^{\{s_i\}}} = [\mathcal{G}_\sigma^0]^{-1} - \mathrm{I}, \qquad (8)$$

with $W_\sigma^{\{s_i\}} = \mathrm{diag}(\sigma s_i)$ and $[\mathcal{G}_\sigma^0]_{pq} = \mathcal{G}_\sigma^0(j_p, \tau_p; j_q, \tau_q)$ being $k \times k$ matrices. Finally, QMC is used to perform the multidimensional sum [Eq. (6)] over different expansion orders and configurations of the auxiliary fields. For this, a Markov process is set up, which samples the configurations of random auxiliary fields $\{s_i\}$ with weight given by the product of determinants in Eq. (7).

In the Rubtsov method [8,11], the interaction is first rewritten as

$$V' = \frac{U}{2} \sum_{j=1}^{N_c} \sum_{\tilde{s}_j = \pm 1} \left(n_{j\uparrow} - \frac{1}{2} - \alpha \tilde{s}_j \right) \left(n_{j\downarrow} - \frac{1}{2} + \alpha \tilde{s}_j \right), \qquad (9)$$

thereby introducing auxiliary fields $\tilde{s}$. This amounts to introducing a shift in the free energy,

$$\frac{K}{\beta} = U N_c \left(\alpha^2 - \frac{1}{4} \right). \qquad (10)$$

The auxiliary fields $\tilde{s}$ suppress the oscillating sign of the integrand in the perturbative expansion [8] as follows:

$$Z = e^{-K} \int_{\eta^*, \eta} e^{-S_0} \sum_{kj\tau s} \left(\frac{-U}{2} \right)^k \prod_\sigma$$
$$\times \left[n_{j_1 \sigma}(\tau_1) - \frac{1}{2} - \alpha \sigma \tilde{s}_1 \right] \cdots \left[n_{j_k \sigma}(\tau_k) - \frac{1}{2} - \alpha \sigma \tilde{s}_k \right]. \qquad (11)$$

The fermion degrees of freedom can be integrated out, and the partition function becomes [11] as follows:

$$Z = \frac{Z_0}{e^K} \sum_{kj\tau s} \left(\frac{-U}{2} \right)^k \prod_\sigma \det \left(\mathcal{G}_\sigma^0 - \frac{1}{2} - \alpha W_\sigma^{\{\tilde{s}_i\}} \right). \qquad (12)$$

Again, the product of determinants in Eq. (12) gives the weight in QMC to evaluate the multidimensional sum over the configurations of auxiliary fields $\{\tilde{s}_i\}$.

We now show that the two expansions, Eqs. (7) and (12), are equivalent (term by term) and that the auxiliary fields $\{s_i\}$ and $\{\tilde{s}_i\}$ are equivalent as well. Using Eq. (8), the inverse Green's function $G_\sigma^{\{s_i\}-1}$ can be rewritten as

$$G_\sigma^{\{s_i\}-1} = \mathcal{G}_\sigma^{0-1} \left[\mathcal{G}_\sigma^0 - \frac{\mathrm{I}}{2} - \alpha^* W_\sigma^{\{s_i\}} \right] (\mathrm{I} - e^{\gamma W_\sigma^{\{s_i\}}}), \qquad (13)$$

where $\alpha^* = [2 \tanh \frac{\gamma}{2}]^{-1}$. Using this, and the fact that $\prod_\sigma (1 - e^{\gamma \sigma s_i}) = 2 - 2 \cosh \gamma = -\frac{\beta U N_c}{K}$, the integrand of Eq. (7) can be rewritten as

$$\left(\frac{K}{2\beta N_c} \right)^k \prod_\sigma \det \mathcal{G}_\sigma^0 \cdot \det [G_\sigma^{\{s_i\}}]^{-1}$$
$$= \left(-\frac{U}{2} \right)^k \prod_\sigma \det \left(\mathcal{G}_\sigma^0 - \frac{1}{2} - \alpha^* W_\sigma^{\{s_i\}} \right) \qquad (14)$$

from which we deduce that both algorithms are equivalent if $\alpha = \alpha^*$, which is the same as requiring that Eq. (10) holds for freely adjustable parameters K and α in these methods. Both algorithms must have the same degree of sign problem and statistics of measurements (such as autocorrelation time), as long as the above-mentioned condition for the parameters K and α is satisfied.

III. RELATION BETWEEN HFQMC AND CTQMC

The derivation of the Hirsch-Fye algorithm involves breaking up the partition function using a Trotter decomposition and decoupling the quartic part of the Hamiltonian with the transformation [2,12] as follows:

$$e^{-\Delta \tau U [n_\uparrow n_\downarrow - 1/2(n_\uparrow + n_\downarrow)]} = \frac{1}{2} \sum_{s = \pm 1} e^{\lambda s (n_\uparrow - n_\downarrow)}, \qquad (15)$$

where $\cosh \lambda = e^{\Delta \tau U/2}$. The resulting partition function takes the well-known form [1,2] as follows:

$$Z = \sum_{\{s_j\}} \int_{\eta^*, \eta} e^{-\sum_{ij\sigma} \eta_{i\sigma}^* [(\mathcal{G}_\sigma^{0-1} - \mathrm{I}) e^{\lambda W_\sigma^{\{s_i\}}} + \mathrm{I}] \eta_{j\sigma}}, \qquad (16)$$

$$= \sum_{\{s_j\}} \prod_{\sigma = \pm 1} \det [G_\sigma^{\{s_j\}}]^{-1}, \qquad (17)$$

where $G_\sigma^{\{s_j\}}$ is the Green's function for a particular configuration of auxiliary fields $\{s_j\}$,

$$[G_\sigma^{\{s_j\}}]^{-1} = \mathcal{G}_\sigma^{0-1} e^{\lambda W_\sigma^{\{s_j\}}} - e^{\lambda W_\sigma^{\{s_j\}}} + \mathrm{I}. \qquad (18)$$

The product of determinants [Eq. (17)] yields a sampling weight for a corresponding configuration of the auxiliary fields $\{s_j\}$. It is very similar to the sampling weight in CTQMC [Eq. (7)], as are the transformations employed [Eqs. (4) and (15)] and the update formulas [Eq. (8) and (18)]. The only difference is that in HFQMC, the number of the auxiliary fields is fixed to $k_{HF} = \beta N_c / \Delta \tau$, and they are distributed evenly in the imaginary time. In addition, the parameter λ plays the same role as the parameter γ in CTQMC to couple the auxiliary fields to the fermion spin. In fact, one can formulate a set of restrictions, under which CTQMC reduces to HFQMC:

(1) restrict the expansion order k in CTQMC equal to the number of the auxiliary fields k_{HF} in the HFQMC and distribute them evenly in the imaginary time interval $(0 \ldots \beta)$;

(2) set the strength of the auxiliary field in CTQMC: $\gamma = \lambda$. In terms of CTQMC parameters K or α, this condition is equivalent to

$$K = \frac{\beta U N_c}{2 \sinh^2 \frac{\lambda}{2}} = \frac{\beta U N_c}{2(e^{\Delta \tau U/2} - 1)}, \qquad (19)$$
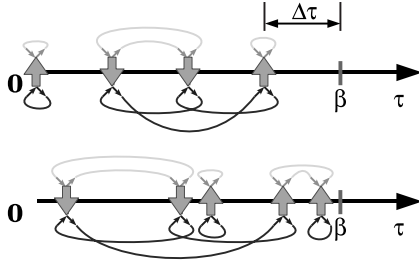
FIG. 1. Example of the diagrams sampled in HFQMC (top) and CTQMC (bottom). The light and dark lines denote propagation of spin-up and spin-down fermions, respectively. The block arrows represent the auxiliary field, associated with an interaction vertex. These vertices are distributed evenly in HFQMC, with interval $\Delta\tau$, while the distribution, the positions, and the number of vertices are arbitrary in the CTQMC. Note that both connected and disconnected diagrams are sampled in both methods. In fact, product of determinants [Eqs. (12) and (17)] accounts for all $(k!)^2$ possible diagrams for a particular set of vertices.

$$\alpha = \frac{1}{2\tanh\frac{\lambda}{2}} = \frac{1}{2\sqrt{\tanh\frac{\Delta\tau U}{4}}}. \tag{20}$$

(3) Restrict the Monte Carlo moves to flipping the auxiliary fields associated with the interaction vertices; shifting vertices in imaginary time is not allowed.

These restrictions imply that only a subset of diagrams with fixed expansion order and equidistant auxiliary fields are sampled in HFQMC, whereas in CTQMC, all diagrams of variable order and all possible sets of auxiliary field configurations contribute (see Fig. 1).

The relation between CTQMC and HFQMC persists for the attractive Hubbard model ($U<0$). Here, a different discrete Hubbard Stratonovich transformation is used,

$$e^{\Delta\tau|U|[n_\uparrow n_\downarrow - 1/2(n_\uparrow + n_\downarrow - 1)]} = \frac{1}{2}\sum_{s=\pm 1} e^{\lambda s(n_\uparrow + n_\downarrow - 1)}, \tag{21}$$

with $\cosh\lambda = e^{\Delta\tau|U|/2}$. The corresponding form for the interaction in CTQMC also has to be modified as

$$V' = \frac{U}{2}\sum_{j=1}^{N_c}\sum_{\tilde{s}_j=\pm 1}\left(n_{j\uparrow} - \frac{1}{2} + \alpha\tilde{s}_j\right)\left(n_{j\downarrow} - \frac{1}{2} + \alpha\tilde{s}_j\right). \tag{22}$$

Since the attractive Hubbard model has no sign problem, the parameter α can be set equal to zero. However, for $\alpha>0$, the relation to HFQMC is again given by the same set of restrictions as defined above [including Eqs. (19) and (20)]. Similarly, the relation between CTQMC and HFQMC is preserved in case of nonlocal density-density interactions.

IV. SMALL $\Delta\tau$ LIMIT

When $\Delta\tau\to 0$, systematic errors in HFQMC are eliminated and in this sense HFQMC and CTQMC are equivalent. The relationship described above will also hold for $\alpha\to\infty$ [see Eq. (20)]. In the discussion above, HFQMC is interpreted as sampling just one order in series expansion. To understand this, we need to revisit the sampling and mea-
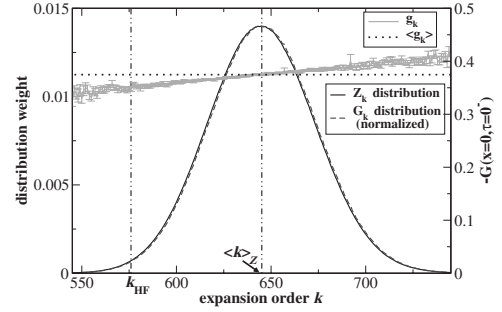

FIG. 2. The distribution of the contributions $Z_k(G_k)$ to the partition function (Green's function) vs the expansion order k for the two-dimensional (2D) Hubbard model with $N_c=16$ sites, $U=W$ (bandwidth), filling $f=0.75$, $\beta=4.5$, and $\alpha=1.01$. Note that the distributions almost perfectly overlap, and their ratio (proportional to g_k) varies very little with k. Restricting diagrams to one order $k=k_{HF}$ and restricting vertices to discrete imaginary time grid result in the Hircsh-Fye algorithm with $\Delta\tau=0.125$.

surement procedure in the CTQMC. The expectation value of any operator can be written as a series expansion,

$$G = \frac{1}{Z}\sum_k G_k = \frac{1}{Z}\sum_k \frac{G_k}{Z_k}Z_k = \frac{1}{Z}\sum_k g_k Z_k. \tag{23}$$

In both variants of CTQMC the evaluation of this sum is done with importance sampling, and the weight (or the "guiding function") is taken to be equal to the corresponding contribution to the partition function Z_k, with $g_k=\frac{G_k}{Z_k}$ being the Monte Carlo estimator for a fixed order of expansion. Of course, Z_k depends on the configuration of the auxiliary fields $\{s_k\}$, so the actual estimator is $g_k^{\{s_k\}}=\frac{G_k^{\{s_k\}}}{Z_k^{\{s_k\}}}$. However, for this discussion, we are only interested in how this estimator depends on the expansion order, so we assume that the auxiliary fields are already summed.

The series expansion for the partition function [Eq. (11)] defines a distribution (see Fig. 2) with mean value [11],

$$\langle k\rangle_Z = -\int_0^\beta d\tau\langle V(\tau)\rangle. \tag{24}$$

This can be generalized for higher factorial moments as follows:

$$\langle (k)_n\rangle_Z = \langle k(k-1)\cdots(k-n+1)\rangle_Z$$
$$= (-1)^n\int_0^\beta d\tau_1\cdots\int_0^\beta d\tau_n\langle T_\tau V(\tau_1)\cdots V(\tau_n)\rangle. \tag{25}$$

For the Hubbard model with sufficiently large α, these moments scale as

$$\lim_{\alpha\to\infty}\langle (k)_n\rangle_Z = (\beta U N_c\alpha^2)^n = \rho^n, \tag{26}$$

which is a property of Poisson distribution $P_\rho(k)=\frac{\rho^k e^{-\rho}}{k!}$ with parameter $\rho=\beta U N_c\alpha^2$. Of course, for large ρ, the Poisson distribution approximates a normal distribution (see Fig. 2).

In a similar way as the series expansion for the partition function defines its distribution, the expansion for the Green's function (or any measurable quantity) defines another distribution,

$$G(\tau_i, \tau_j) = \sum_k G_k(\tau_i, \tau_j) = \sum_k \frac{(-1)^k}{k!} \int_0^\beta d\tau_1 \cdots \int_0^\beta \\ \times d\tau_k \langle T_\tau c(\tau_i) c^\dagger(\tau_j) V(\tau_1) \cdots V(\tau_k) \rangle, \qquad (27)$$

which is characterized by its factorial moments as follows:

$$\langle (k)_n \rangle_{G_{ij}} = \frac{(-1)^n}{G(\tau_i, \tau_j)} \int_0^\beta d\tau_1 \cdots \int_0^\beta \\ \times d\tau_n \langle T_\tau c(\tau_i) c^\dagger(\tau_j) V(\tau_1) \cdots V(\tau_n) \rangle. \qquad (28)$$

In general, this distribution is different from the one defined by the expansion of the partition function. However, in the limit when $\alpha \to \infty$, the factorial moments of Green's function distribution scale as

$$\lim_{\alpha \to \infty} \langle (k)_n \rangle_G = (\beta U N_c \alpha^2)^n = \lim_{\alpha \to \infty} \langle (k)_n \rangle_Z. \qquad (29)$$

Since all the moments for both distributions are the same, the distributions are the same as well in this limit and the estimator g_k becomes a constant, independent of the expansion order k (see Fig. 2). Thus, the sum over all expansion orders k can be replaced by any single term corresponding to a fixed value of $k = k_{HF}$. That explains why sampling just one single order in the expansion for the partition function (as is done in HFQMC) gives the same exact result when $\Delta \tau \to 0$.

V. COMPUTATIONAL IMPLICATIONS

When the product of determinants [Eqs. (7), (12), and (17)] is not positive definite, its absolute value is taken as a weight in QMC. This approach fails if the average sign of the product of determinants becomes small. This is the infamous fermion sign problem, the main limitation in any fermion QMC method. From the discussion above, it follows that both HFQMC and CTQMC have the same degree of sign problem when $\alpha \to \infty$ and $\Delta \tau \to 0$. For typical finite values of $\Delta \tau$ and α, the difference in average sign is still small (see Fig. 3) and depends on model parameters. Altogether, we find that neither of the methods has a definite advantage in
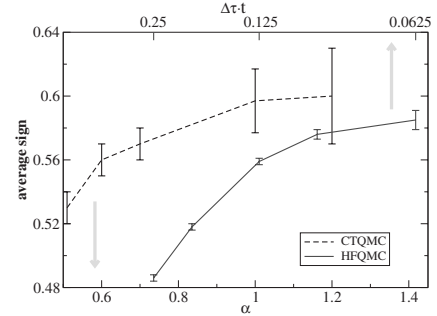

FIG. 3. Comparison of the average sign for the 2D Hubbard model with $N_c = 24E$, $U = 8t$, filling $= 0.95$, and $\beta t = 4.5$. In CTQMC, the average sign depends on parameter α (lower horizontal axis), while in HFQMC, it depends on the size of the time slice $\Delta \tau t$ (upper horizontal axis). Marks on both axes are related by Eq. (20).

terms of the degree of the sign problem. Also, the auxiliary fields enter the same way in both methods, and correlations in these fields give information about the spin and charge correlations in the repulsive and attractive Hubbard models, respectively. Thus, optimization strategies developed for HFQMC can be applied to CTQMC.

VI. CONCLUSIONS

We have investigated two weak-coupling CTQMC methods proposed by Rombouts *et al.* [7] and Rubtsov *et al.* [8] and shown that they are equivalent for a certain choice of freely adjustable parameters in these methods. We also established the relation between the CTQMC methods and HFQMC method and identified the latter as an approximation within CTQMC where the Monte Carlo sum is restricted to a certain subset of diagrams. We have shown that this approximation becomes exact in the limit when an infinite number of time slices is taken in HFQMC, implying that both methods have the same degree of the sign problem in this limit.

[1] J. E. Hirsch and R. M. Fye, Phys. Rev. Lett. **56**, 2521 (1986).

[2] R. M. Fye and J. E. Hirsch, Phys. Rev. B **38**, 433 (1988).

[3] A. Georges, G. Kotliar, W. Krauth, and M. J. Rozenberg, Rev. Mod. Phys. **68**, 13 (1996).

[4] F. F. Assaad, in *Quantum Simulations of Complex Many-Body Systems: From Theory to Algorithms*, NIC Series Vol. 10 edited by J. Grotendorst, D. Marx, and A. Muramatsu (John von Neumann Institute for Computing, Jülich, 2002), pp. 99–156.

[5] R. R. dos Santos, Braz. J. Phys. **33**, 36 (2003).

[6] N. V. Prokof'ev, B. V. Svistunov, and I. S. Tupitsyn, JETP Lett. **64**, 911 (1996).

[7] S. M. A. Rombouts, K. Heyde, and N. Jachowicz, Phys. Rev. Lett. **82**, 4155 (1999).

[8] A. N. Rubtsov, V. V. Savkin, and A. I. Lichtenstein, Phys. Rev. B **72**, 035122 (2005).

[9] J. Hubbard, Proc. R. Soc. London, Ser. A **276**, 238 (1963); M. C. Gutzwiller, Phys. Rev. Lett. **10**, 159 (1963); J. Kanamori, Prog. Theor. Phys. **30**, 275 (1963).

[10] E. Gull, P. Werner, O. Parcollet, and M. Troyer, Europhys. Lett. **82**, 57003 (2008).

[11] F. F. Assaad and T. C. Lang, Phys. Rev. B **76**, 035116 (2007).

[12] J. E. Hirsch, Phys. Rev. B **28**, 4059 (1983).