Gaussian quantum Monte Carlo and its relation to Auxiliary-field quantum Monte Carlo: detailed derivations (auxiliary material)

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This paper explains in detail how the expressions for the Gaussian quantum Monte Carlo method of Corney and Drummond can be derived in the framework of auxiliary-field quantum Monte Carlo.

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I. INTRODUCTION

Recently, Corney and Drummond have proposed a Gaussian quantum Monte Carlo method (GQMC) based on a Gaussian expansion of the system density operator [1]. In this paper it is shown in full detail how the GQMC arises naturally in the framework of auxiliary-field quantum Monte Carlo (AFQMC). Therefore, if it is implemented correctly, GQMC has the same sign problems as AFQMC.

II. AUXILIARY FIELD MONTE CARLO

Like most QMC methods [2], the auxiliary field quantum Monte Carlo algorithm (AFQMC) [3–10] starts from a decomposition of the imaginary-time propagator $\exp(-\tau\hat{H})$ into parts that can be handled more easily. In the case of AFQMC those parts are exponentials of one-body operators [6]. They can be considered as (non-Hermitian) Hamiltonians of non-interacting systems. Because non-interacting particles propagate independently, these operators are easy to deal with. I will use a *hat* to denote the operator $\hat{h}$ related to a matrix h by $\hat{h} = \sum_{ij} h_{ij}\hat{a}_i^\dagger\hat{a}_j$. In the grand canonical ensemble the following relations hold (for a temperature $T = 1/(k\tau)$ and assuming that the chemical potential is included in $\hat{h}$):

$$\mathrm{Tr}\left[e^{-\tau\hat{h}}\right] = \det\left(1+\theta e^{-\tau h}\right)^{\theta}, \tag{1}$$

$$\langle\hat{a}_j^\dagger\hat{a}_i\rangle_{\tau,h} = \frac{\mathrm{Tr}\left[\hat{a}_j^\dagger\hat{a}_i e^{-\tau\hat{h}}\right]}{\mathrm{Tr}\left[e^{-\tau\hat{h}}\right]} = \left[\frac{e^{-\tau h}}{1+\theta e^{-\tau h}}\right]_{ij}, \tag{2}$$

with $\theta = +1$ for fermions and $\theta = -1$ for bosons. These expressions are readily verified by expressing them in a basis in which the matrix h is diagonal. This means that properties of exponentials of one-body operators can be expressed in terms of matrices $\exp(-\tau h)$, which have the dimension of the one-body space.

A standard trick to decompose the full propagator into independent particle propagators is to divide the imaginary-time interval $[0,\tau]$ into a series of imaginary-time slices of length $\epsilon = \tau/N_t$,

$$e^{-\tau\hat{H}} = \left(e^{-\epsilon\hat{H}}\right)^{N_t}, \tag{3}$$

and to reduce in each time slice the interacting propagator $\exp(-\epsilon\hat{H})$ to an integral over non-interacting propagators by means of the Hubbard-Stratonovich decomposition [11]:

$$e^{-\epsilon\hat{H}} = (2\pi/\epsilon)^{-m/2}\int e^{-\frac{\epsilon}{2}\xi^2}e^{\epsilon\hat{\Delta}(\xi)}d\xi + \mathcal{O}(\epsilon^2), \tag{4}$$

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with the one-body operator $\hat{\Delta}(\xi) = -\hat{H}_0 - \sum_{j=1}^{m} \xi_j \hat{A}_j$, and where the operators $\hat{H}_0$ and $\hat{A}_j$ are such that $\hat{H} = \hat{H}_0 - \frac{1}{2}\sum_{j=1}^{m} \hat{A}_j^2$. m is the number of auxiliary fields needed per time slice. In this way the exponential of a two-body operator is reduced to a (continuous) sum over exponentials of one-body operators. For fermions, more efficient discrete decompositions can be devised [12, 13].

Suppose now that one has an ensemble of one-body exponentials that represent the full many-body propagator at a given imaginary time τ,

$$e^{\tau \hat{H}} = \int P(X) e^{-\tau \hat{h}(X)} dX. \tag{5}$$

Then one can write that

$$\langle \hat{a}_j^\dagger \hat{a}_i \rangle_{\tau,H} = \frac{\mathrm{Tr}\left[\hat{a}_j^\dagger \hat{a}_i e^{-\tau \hat{H}}\right]}{\mathrm{Tr}\left[e^{-\tau \hat{H}}\right]} = \frac{\int P(X) \mathrm{Tr}\left[\hat{a}_j^\dagger \hat{a}_i e^{-\tau \hat{h}(X)}\right] dX}{\int P(X) \mathrm{Tr}\left[e^{-\tau \hat{h}(X)}\right] dX} \tag{6}$$

$$= \frac{\int P(X) \det\left[1 + \theta e^{-\tau h(X)}\right]^\theta n(\tau, X)_{ij} dX}{\int P(X) \det\left[1 + \theta e^{-\tau h(X)}\right]^\theta dX}, \tag{7}$$

with

$$n(\tau, X) = \frac{e^{-\tau h(X)}}{1 + \theta e^{-\tau h(X)}}. \tag{8}$$

Hence, if one can generate a sample of configurations $\{X_1, X_2, \ldots, X_M\}$ proportional to the weight

$$W(\tau, X) = P(X) \det\left[1 + \theta e^{-\tau h(X)}\right]^\theta, \tag{9}$$

then the one-body reduced density matrix can be estimated as

$$\langle \hat{a}_j^\dagger \hat{a}_i \rangle_{\tau,H} \simeq \frac{1}{M} \sum_{m=1}^{M} n(\tau, X_m). \tag{10}$$

The standard way to evaluate the terms of the decomposition is the Metropolis-Hastings algorithm [14]. However, one can also use a diffusion process in configuration space, such as the walker+branching algorithm [15, 16]. In any case, the use of stochastic techniques requires that $\det\left[1 + \theta e^{-\tau h(X)}\right] > 0$, which is where the *sign problem* shows up in AFQMC [15, 17].

III. EVOLVING THE ENSEMBLE IN IMAGINARY TIME

The ensemble of Eq.(5) can be extended to 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 ξ_l and ξ_r:

$$e^{-\epsilon \hat{H}} = (2\pi/\epsilon)^{-m/2} \int e^{-\frac{\epsilon}{2}\xi^2} e^{\epsilon \hat{\Delta}(\xi)} d\xi, \tag{11}$$

$$e^{-\tau' \hat{H}} = (2\pi/\epsilon)^{-m} \int P(X) e^{-\frac{\epsilon}{2}\xi_l^2} e^{-\frac{\epsilon}{2}\xi_r^2} e^{\epsilon \hat{\Delta}(\xi_l)} e^{-\tau \hat{h}(X)} e^{\epsilon \hat{\Delta}(\xi_r)} dX d\xi_l d\xi_r. \tag{12}$$

The corresponding matrix representation for the configuration $X' = (\xi_l, X, \xi_r)$, would then evolve as

$$e^{-\tau' h(X')} = e^{\epsilon \Delta(\xi_l)} e^{-\tau h(X)} e^{\epsilon \Delta(\xi_r)}. \tag{13}$$

Now it is interesting to observe what happens with $n(\tau, X)$ as the ensemble is extended to τ' ($n(\tau, X)$, $\Delta(\xi_l)$, $\Delta(\xi_r)$ and $h(X)$ have been abbreviated to n, Δ_l, Δ_r and h respectively in order to ease the notation):

$$\begin{aligned}
n(\tau', X') &= \frac{e^{\epsilon\Delta_l}e^{-\tau h}e^{\epsilon\Delta_r}}{1+\theta e^{\epsilon\Delta_l}e^{-\tau h}e^{\epsilon\Delta_r}} \\
&= \frac{e^{-\tau h}+\epsilon\left(\Delta_l e^{-\tau h}+e^{-\tau h}\Delta_r\right)}{1+\theta e^{-\tau h}+\theta\epsilon\left(\Delta_l e^{-\tau h}+e^{-\tau h}\Delta_r\right)}+\mathcal{O}(\epsilon^2\Delta^2) \\
&= \frac{n+\epsilon\left((1-\theta n)\Delta_l e^{-\tau h}+n\Delta_r\right)}{1+\theta\epsilon\left((1-\theta n)\Delta_l e^{-\tau h}+n\Delta_r\right)}+\mathcal{O}(\epsilon^2\Delta^2) \\
&= n+\epsilon\left((1-\theta n)\Delta_l e^{-\tau h}+n\Delta_r\right)-\theta\epsilon\left((1-\theta n)\Delta_l e^{-\tau h}n+n\Delta_r n\right)+\mathcal{O}(\epsilon^2\Delta^2) \\
&= n+\epsilon\left((1-\theta n)\Delta_l e^{-\tau h}(1-\theta n)+n\Delta_r(1-\theta n)\right)+\mathcal{O}(\epsilon^2\Delta^2) \\
&= n+\epsilon\left((1-\theta n)\Delta_l n+n\Delta_r(1-\theta n)\right)+\mathcal{O}(\epsilon^2\Delta^2). \qquad (14)
\end{aligned}$$

It is tempting to take here the formal limit $\epsilon \to 0$, which would lead to

$$\frac{dn}{d\tau} = \frac{1}{2}\left\{(1-\theta n)\Delta_l n + n\Delta_r(1-\theta n)\right\}. \qquad (15)$$

This is exactly the same expression as Eq.(9) of Ref.[1]! However, the auxiliary fields arising from the Hubbard-Stratonovich decomposition are of order $\epsilon^{-1/2}$, because $\langle\xi^2\rangle = \epsilon^{-1}$. Therefore the operators $\epsilon\Delta_{l,r}$ will contain terms of order $\epsilon^{1/2}$. In the limit of $\epsilon \to 0$ this results in a δ-function normalization for the auxiliary fields ξ. The more practical way to update n for finite values of ϵ, is to compute the matrices $\exp(\epsilon\Delta_{l,r})$ explicitly such that all orders of ϵ are included.

At the same time one can evaluate how the weight of Eq.(9) evolves:

$$\begin{aligned}
W(\tau', X') &= (2\pi/\epsilon)^{-m}P(X)e^{-\frac{\epsilon}{2}\xi_l^2}e^{-\frac{\epsilon}{2}\xi_r^2}\det\left[1+\theta e^{\epsilon\Delta_l}e^{-\tau h}e^{\epsilon\Delta_r}\right]^\theta \\
&= (2\pi/\epsilon)^{-m}P(X)e^{-\frac{\epsilon}{2}\xi_l^2}e^{-\frac{\epsilon}{2}\xi_r^2}\det\left[1+\theta e^{-\tau h}e^{\epsilon\Delta_r}e^{\epsilon\Delta_l}\right]^\theta \\
&= (2\pi/\epsilon)^{-m}P(X)e^{-\frac{\epsilon}{2}\xi_l^2}e^{-\frac{\epsilon}{2}\xi_r^2}\det\left[1+\theta e^{-\tau h}+\theta e^{-\tau h}\left(e^{\epsilon\Delta_r}e^{\epsilon\Delta_l}-1\right)\right]^\theta \\
&= (2\pi/\epsilon)^{-m}P(X)e^{-\frac{\epsilon}{2}\xi_l^2}e^{-\frac{\epsilon}{2}\xi_r^2}\det\left[1+\theta e^{-\tau h}\right]^\theta\det\left[1+\theta n\left(e^{\epsilon\Delta_r}e^{\epsilon\Delta_l}-1\right)\right]^\theta \\
&= W(\tau,X)(2\pi/\epsilon)^{-m}e^{-\frac{\epsilon}{2}\xi_l^2}e^{-\frac{\epsilon}{2}\xi_r^2}\det\left[1+\theta n\left(e^{\epsilon\Delta_r}e^{\epsilon\Delta_l}-1\right)\right]^\theta \qquad (16)
\end{aligned}$$

IV. THE STOCHASTIC GAUGE

The Hubbard-Stratonovich decomposition leaves considerable freedom in the choice of operators $\hat{A}_j$ and auxiliary fields ξ used in the Monte Carlo process. Corney and Drummond coin the term 'stochastic gauge'. Let me restrict the discussion here to the minimal repulsive fermionic Hubbard-model. A natural choice for the Hubbard-Stratonovich decomposition is to take

$$\hat{A}_j = \sqrt{U}(\hat{a}^\dagger_{j,\uparrow}\hat{a}_{j,\uparrow} - \hat{a}^\dagger_{j,\downarrow}\hat{a}_{j,\downarrow}), \qquad (17)$$

with j an index referring to the lattice site.

A way to optimize the stochastic gauge is given by the shifted-contour AFQMC [18], which consists in redefining the auxiliary field $\xi_j = \bar{\xi}_j - \bar{a}_j$, with $\bar{a}_j = \langle\hat{A}_j\rangle_{\tau,X}$. Then one can write that

$$\begin{aligned}
e^{-\epsilon\hat{H}} &= (2\pi/\epsilon)^{-m/2}\int e^{-\frac{\epsilon}{2}\sum_j\xi_j^2}e^{-\epsilon\left[\hat{H}_0+\sum_j\xi_j\hat{A}_j\right]}d\xi+\mathcal{O}(\epsilon^2) \\
&= (2\pi/\epsilon)^{-m/2}\int e^{-\frac{\epsilon}{2}\sum_j(\bar{\xi}_j-\bar{a}_j)^2}e^{-\epsilon\left[\hat{H}_0+\sum_j(\bar{\xi}_j-\bar{a}_j)\hat{A}_j\right]}d\bar{\xi}+\mathcal{O}(\epsilon^2) \\
&= (2\pi/\epsilon)^{-m/2}\int e^{-\frac{\epsilon}{2}\sum_j\bar{\xi}_j^2}e^{-\frac{\epsilon}{2}\sum_j\bar{a}_j^2+\epsilon\sum_j\bar{\xi}_j\bar{a}_j}e^{-\epsilon\left[\hat{H}_0+\sum_j(\bar{\xi}_j-\bar{a}_j)\hat{A}_j\right]}d\bar{\xi}+\mathcal{O}(\epsilon^2) \qquad (18)
\end{aligned}$$

Working with these shifted auxiliary fields, one can define the operator

$$\hat{\Delta}(\bar{\xi}) = -\hat{H}_0 - \sum_j(\bar{\xi}_j-\bar{a}_j)\hat{A}_j, \qquad (19)$$

that can be used in Eq.(14). Its matrix representation is given by

$$\Delta_{ij,\sigma}(\bar{\xi}) = t_{ij} - \delta_{ij}\left[U(n_{jj,-\sigma} - n_{jj,\sigma} + \frac{1}{2}) + \sigma\sqrt{U}\bar{\xi}_j\right], \tag{20}$$

with $\sigma = +1$ or -1 for spin-up and spin-down respectively. Note the resemblance to the expression below Eq.(9) in Ref.[1]. However, there is a difference in the normalization of the auxiliary fields due to the discretization of the time step.

To complete the analysis, I want to evaluate also the weight in this stochastic gauge. If one samples the auxiliary fields $\bar{\xi}$ from a Gaussian distribution $\propto \exp(-\epsilon\bar{\xi}^2/2)$, one has to keep track only of the non-Gaussian part Ω of the weight W,

$$\Omega(\tau', X') = \Omega(\tau, X) e^{-\epsilon\sum_j \bar{a}_j^2 + \epsilon\sum_j(\bar{\xi}_{l,j}+\bar{\xi}_{r,j})\bar{a}_j} \det\left[1 + n(\tau, X)\left(e^{\epsilon\Delta(\bar{\xi}_r)}e^{\epsilon\Delta(\bar{\xi}_l)} - 1\right)\right]. \tag{21}$$

Expanding this expression up to order $\epsilon\Delta$, one finds

$$\begin{aligned}
\Omega(\tau', \bar{\xi}')/\Omega(\tau, X) &= e^{-\epsilon\sum_j \bar{a}_j^2 + \epsilon\sum_j(\bar{\xi}_{l,j}+\bar{\xi}_{r,j})\bar{a}_j} \det\left[1 + \epsilon n(\tau, X)\left(\Delta(\bar{\xi}_r) + \Delta(\bar{\xi}_l)\right)\right] + \mathcal{O}(\epsilon^2\Delta^2) \\
&= e^{-\epsilon\sum_j \bar{a}_j^2 + \epsilon\sum_j(\bar{\xi}_{l,j}+\bar{\xi}_{r,j})\bar{a}_j}\left(1 + \epsilon\mathrm{Tr}\left[n(\tau, X)\left(\Delta(\bar{\xi}_r) + \Delta(\bar{\xi}_l)\right)\right]\right) + \mathcal{O}(\epsilon^2\Delta^2) \\
&= e^{-\epsilon\sum_j \bar{a}_j^2 + \epsilon\sum_j(\bar{\xi}_{l,j}+\bar{\xi}_{r,j})\bar{a}_j}\left(1 + \epsilon\left\langle\Delta(\bar{\xi}_r) + \Delta(\bar{\xi}_l)\right\rangle_{\tau,X}\right) + \mathcal{O}(\epsilon^2\Delta^2) \\
&= e^{-\epsilon\sum_j \bar{a}_j^2 + \epsilon\sum_j(\bar{\xi}_{l,j}+\bar{\xi}_{r,j})\bar{a}_j} \\
&\quad \times\left[1 - 2\epsilon\langle\hat{H}_0\rangle_{\tau,X} - \epsilon\sum_j(\bar{\xi}_{r,j} - \bar{a}_j)\langle\hat{A}_j\rangle_{\tau,X} - \epsilon\sum_j(\bar{\xi}_{l,j} - \bar{a}_j)\langle\hat{A}_j\rangle_{\tau,X}\right] + \mathcal{O}(\epsilon^2\Delta^2) \\
&= \left(1 - \epsilon\sum_j \bar{a}_j^2 + \epsilon\sum_j(\bar{\xi}_{l,j} + \bar{\xi}_{r,j})\bar{a}_j\right)\left[1 - 2\epsilon\langle\hat{H}_0\rangle_{\tau,X} + 2\epsilon\sum_j \bar{a}_j^2 - \epsilon\sum_j(\bar{\xi}_{r,j} + \bar{\xi}_{l,j})\bar{a}_j\right] + \mathcal{O}(\epsilon^2\Delta^2) \\
&= 1 - 2\epsilon\langle\hat{H}_0\rangle_{\tau,X} + \epsilon\sum_j \bar{a}_j^2 + \mathcal{O}(\epsilon^2\Delta^2).
\end{aligned} \tag{22}$$

The formal limit $\epsilon \to 0$ would result in

$$\frac{d\Omega}{d\tau} = -\Omega\left(\langle H_0\rangle_{\tau,X} - \frac{1}{2}\sum_j\langle A_j\rangle_{\tau,X}^2\right), \tag{23}$$

similar to the expression seven lines below Eq.(9) in Ref.[1]. However, again one has to take into account that $\Delta(\xi)$ contains terms of the order $\epsilon^{-1/2}$. Therefore the terms $\mathcal{O}(\epsilon^2\Delta^2)$ do contain contributions of order ϵ not included in Eq.(23). This means that the update of the weight Ω does depend on the auxiliary fields ξ, and hence can become negative for values of ξ in the tails of the Gaussian distribution.

V. EXAMPLE: THE ONE-SITE HUBBARD MODEL

The importance of the terms of order $\epsilon^2\Delta^2$ is well illustrated by a simple example: a one-site fermionic Hubbard model $\hat{H} = -\mu n_\uparrow - \mu n_\downarrow + U n_\uparrow n_\downarrow$, and a one-body density matrix

$$n(\tau) = \begin{pmatrix} n_\uparrow & 0 \\ 0 & n_\downarrow \end{pmatrix}, \tag{24}$$

with weight $\Omega(\tau) = 1$. First order updates would result in

$$n(\tau + 2\epsilon, \bar{\xi}) = n + \epsilon\left[(1-n)\Delta(\bar{\xi}_l)n + n\Delta(\bar{\xi}_r)(1-n)\right], \tag{25}$$

$$\Omega(\tau + 2\epsilon, \bar{\xi}) = \Omega(\tau) - 2\epsilon\Omega(\tau)\left[-\mu n_\uparrow - \mu n_\downarrow + U n_\uparrow n_\downarrow\right], \tag{26}$$

with

$$\Delta_\sigma(\bar{\xi}) = \mu + \left[U(n_\sigma - n_{-\sigma} - \frac{1}{2}) - \sigma\sqrt{U}\bar{\xi}\right], \tag{27}$$

$$\bar{\xi}_{(l,r)} \propto e^{-\frac{\epsilon}{2}\bar{\xi}_{(l,r)}^2}, \tag{28}$$

and $\sigma = +1, -1$ for spin-up and spin-down respectively. Averaging over all resulting matrices $n(\tau + 2\epsilon, \bar{\xi})$, one finds

$$n_\sigma(\tau + 2\epsilon) \;=\; n_\sigma + 2\epsilon\mu(1 - n_\sigma)n_\sigma + 2\epsilon U(1 - n_\sigma)n_\sigma(n_\sigma - n_{-\sigma} - \frac{1}{2}). \tag{29}$$

On the other hand one can apply first-order perturbation theory with the full Hamiltonian, and use Wick's theorem (which is valid for the Gaussian operators of Ref.[1]) to evaluate higher-order expectation values, leading to

$$\begin{aligned} n_\sigma(\tau + 2\epsilon) &= \frac{n_\sigma(\tau) - 2\epsilon \left\langle \hat{a}_\sigma^\dagger \hat{a}_\sigma \hat{H} \right\rangle_\tau}{1 - 2\epsilon \left\langle \hat{H} \right\rangle_\tau} \\ &= \frac{n_\sigma + 2\epsilon\mu n_\sigma + 2\epsilon\mu n_\sigma n_{-\sigma} - 2\epsilon U n_\sigma n_{-\sigma}}{1 + 2\epsilon\mu n_\sigma + 2\epsilon\mu n_{-\sigma} - 2\epsilon U n_\sigma n_{-\sigma}} \\ &= n_\sigma + 2\epsilon\mu n_\sigma + 2\epsilon\mu n_\sigma n_{-\sigma} - 2\epsilon U n_\sigma n_{-\sigma} - 2\epsilon\mu n_\sigma n_\sigma - 2\epsilon\mu n_\sigma n_{-\sigma} + 2\epsilon U n_\sigma n_\sigma n_{-\sigma} \\ &= n_\sigma + 2\epsilon\mu(1 - n_\sigma)n_\sigma - 2\epsilon U(1 - n_\sigma)n_\sigma n_{-\sigma}. \end{aligned} \tag{30}$$

The difference between Eq.(29) and Eq.(30) amounts to

$$\epsilon U n_\sigma(1 - n_\sigma)(1 - 2n_\sigma). \tag{31}$$

This is a consequence of the fact that the derivation of Eq.(29) averages out the auxiliary fields $\bar{\xi}_{(l,r)}$ and is insensitive to the variance of $\bar{\xi}_{(l,r)}$. Therefore a term of the order $\epsilon \left\langle (\hat{a}_\sigma^\dagger \hat{a}_\sigma - n_\sigma)(\hat{A} - \bar{a})^2 \right\rangle_\tau$ is missing in Eq.(29).

A. numerical simulations

The above discussion highlights the problems related to a single discrete time step. Because the GQMC is formulated in the continuum limit, one should take the limit of infinitely many infinitesimal time steps, while the total imaginary time interval stays constant. To this end a numerical simulation of Eqs.(25,26) was implemented for the one-site repulsive Hubbard model [20]. Because there is no hopping term, one has to keep track of the diagonal elements of n only. The imaginary time β was divided in $N_t = 1, 2, 4, \ldots 128$ equally sized intervals. Eq.(26) was implemented as an update for $\log(\Omega)$, such that the weights remained positive all the time. Fig.(1) and Fig.(2) compares the densities for chemical potential $\mu = -1$ and interaction strength $U = 4$ and 8 with the exact results,

$$n_\sigma = \frac{e^{\beta\mu} + e^{\beta(2\mu - U)}}{1 + 2e^{\beta\mu} + e^{\beta(2\mu - U)}}. \tag{32}$$

One finds that the use of more intervals reduces the error from Eq.(31) to about half its value in the continuum limit. Still, this implementation of the GQMC fails to reproduce the exact result! These results prove that even in the continuum limit, one can not ommit the terms of order $\epsilon^2\Delta^2$ in the propagation of n and Ω in order to obtain the exact result.

VI. CONCLUSIONS

The above derivations demonstrate that there is a close relation between AFQMC and the Gaussian Monte Carlo method of Ref.[1]. However, care has to be taken when translating the expressions of Ref.[1] into finite time steps: terms that are of quadratic order in the time step have to be included. The averaging over the auxiliary fields will transform some of these terms to first order because the variance of the auxiliary fields scales as $1/\epsilon$. If one applies the correct finite time-step expressions, one arrives at the same decomposition as the one used in shifted-contour auxiliary-field method, and hence one should find the same sign properties. Otherwise the Gaussian Monte Carlo method is only an approximate method, that might be improved upon using symmetry projections [19].

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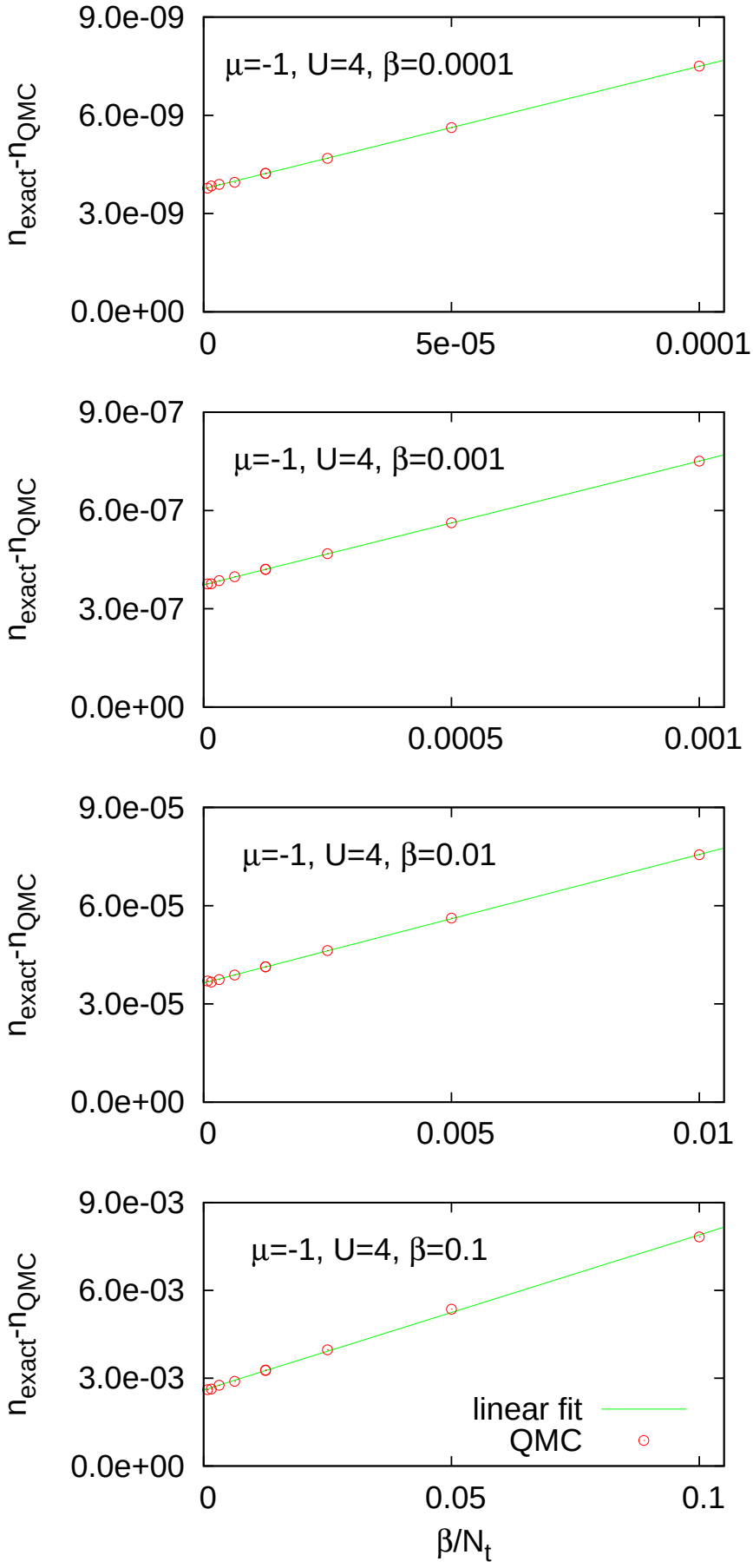

FIG. 1: Deviation from the exact result for the average density for the one-site Hubbard model with chemical potential $\mu = -1$ and interaction strength $U = 4$, evaluated using Eqs.(25,26) with $N_t = 1, 2, 4, \ldots 128$ time steps, for small values of β. Results obtained using 200 000 Monte Carlo samples per data point. The statistical errors are smaller than the symbols.

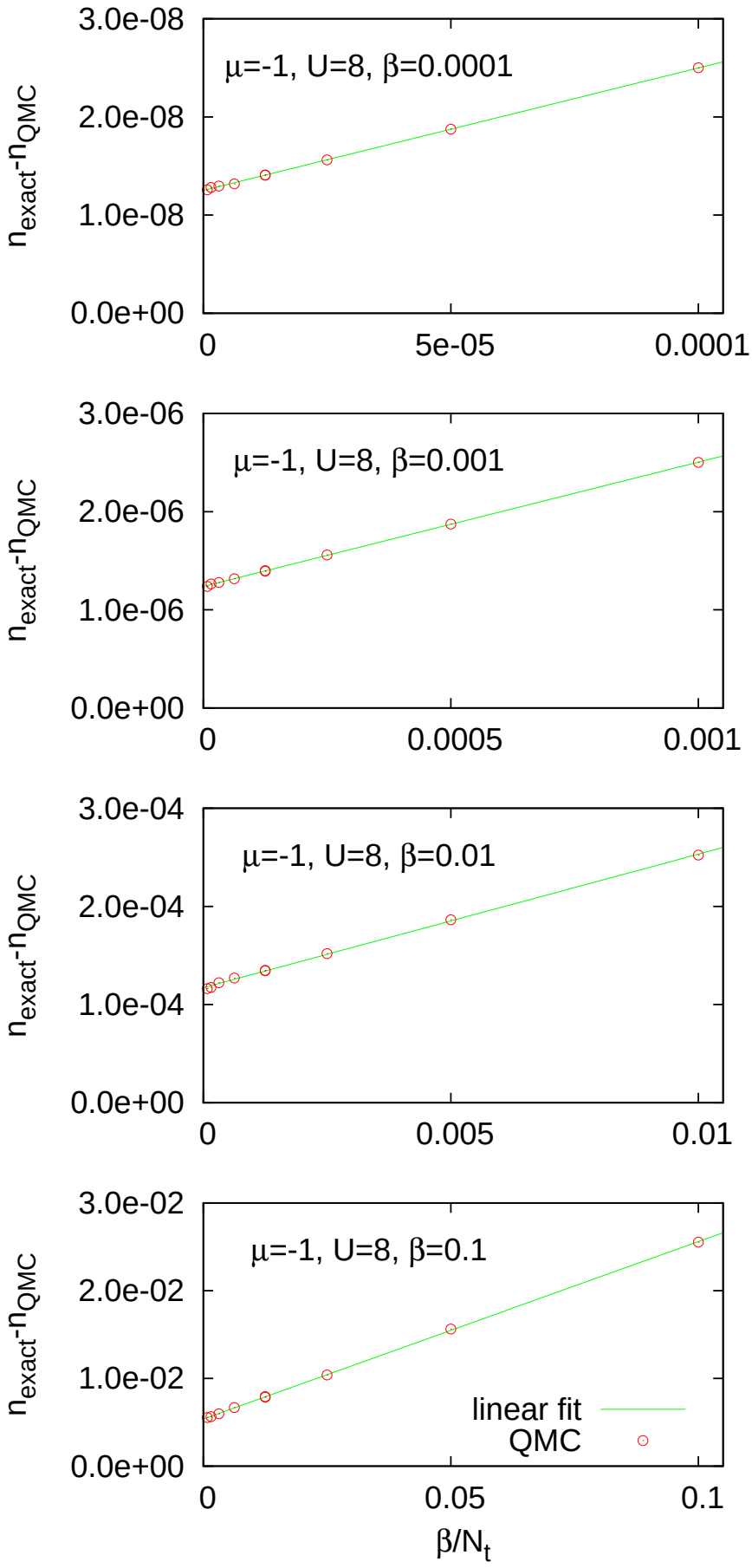

FIG. 2: Deviation from the exact result for the average density for the one-site Hubbard model with chemical potential $\mu = -1$, interaction strength $U = 8$, evaluated using Eqs.(25,26) with $N_t = 1, 2, 4, \ldots 128$ time steps, for small values of β. Results obtained using 200 000 Monte Carlo samples per data point. The statistical errors are smaller than the symbols.