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Imaginary time correlations and the phaseless auxiliary field quantum Monte Carlo

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The phaseless Auxiliary Field Quantum Monte Carlo (AFQMC) method provides a well established approximation scheme for accurate calculations of ground state energies of many-fermions systems. Here we address the possibility of calculating imaginary time correlation functions with the phaseless AFQMC. We give a detailed description of the technique and test the quality of the results for static properties and imaginary time correlation functions against exact values for small systems. © 2014 AIP Publishing LLC. [http://dx.doi.org/10.1063/1.4861227]

I. INTRODUCTION

Over the last decades the study of many body quantum systems at zero temperature has been systematically supported by ab initio Quantum Monte Carlo (QMC) calculations. QMC are methods relying on a stochastic solution of the imaginary time Schrödinger equation of the system. As far as bosonic degrees of freedom are considered, QMC calculations allow static properties, energetics, and structure functions, to be computed exactly1–6 even for strongly correlated systems, for which analytic approaches yield only approximate results. Furthermore, the possibility of reconstructing dynamical properties of bosonic systems, like excitation spectra and response functions, from imaginary time correlation functions (ITCFs) has been explored with remarkable results.7–13 On the other hand, for fermionic degrees of freedom the situation is considerably complicated by the well-known sign problem:14, 15 the computational cost increases exponentially with the system size. The most widely employed scheme to reduce the problem to polynomial complexity is the Fixed-Node (FN) approximation:16, 17 FN restricts the stochastic sampling of the configurational space to regions where the sign of a reasonable approximation for the ground state wave function, the trial wave function, remains constant. Such approximation provides very accurate estimations of ground state properties.16–19 Nevertheless, FN may give inaccurate results for imaginary time correlation functions even when the nodal structure of the ground state wave function is exactly known: as an example, in Fig. 1 we show the comparison between exact and FN imaginary time correlation functions of the density fluctuations \( \langle \hat{\rho}_q(\tau) \hat{\rho}_q^\dagger \rangle \) for a 2D system of 5 noninteracting spinless fermions. Such mismatch arises from the imposition of the ground state nodal structure as a subset of the nodal structure of all excited states.

It is thus very interesting to investigate the accuracy of the imaginary time correlation functions calculated by QMC using nodal restrictions different from FN.

In recent years alternative QMC methods have been conceived, which simulate the imaginary time evolution with a suitable stochastic process taking place in the manifold of Slater determinants.18, 21–23, 25 In the present work we consider one of such QMC methods, the phaseless Auxiliary Field Quantum Monte Carlo (AFQMC)21, 23, 26 which is considered less sensitive than FN to the quality of the trial function.31

However, the phaseless approximation is less known than those characterizing configuration QMC methods, and its accuracy in the calculation of imaginary time correlation functions is unknown. We give a detailed description of AFQMC and present its application to the calculation of imaginary time correlation functions. To assess the accuracy of the phaseless AFQMC we compute ITCFs for a class of interacting fermionic models amenable to exact diagonalization of the hamiltonian.

The phaseless AFQMC and its extension to the calculation of imaginary time dynamics are described in Sec. II. The solvable fermionic systems are presented in Sec. III. Results of numeric calculations are presented in Sec. IV, and conclusions are drawn in Sec. V.

II. THE PHASELESS AFQMC

As mentioned in the Introduction, Quantum Monte Carlo are ab initio: this means that the starting point is the Hamiltonian operator of a physical system. We thus present the phaseless AFQMC relying on a very general hamiltonian operator:

\[
\hat{H} = \sum_{i,j=1}^{M} \beta_{ij} \hat{a}_i^\dagger \hat{a}_j + \sum_{i,j,k,l=1}^{M} \gamma_{ijkl} \hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_k \hat{a}_l. \tag{1}
\]

The creation and destruction operators appearing in (1) are related to an orthonormal complete set of orbitals \( \{|\psi_i\rangle\}_{i=1}^{M} \) in the single-particle Hilbert space, which we will denote \( \mathcal{H}_s \). \( M \) is the dimension of such Hilbert space; we will make the assumption that \( M < +\infty \). The above written Hamiltonian operator acts on the fermionic Fock space, \( \mathcal{F} \), built upon the one body space \( \mathcal{H}_s \). Throughout this paper, we will fix the number
of particles \(N\), which is a constant of motion for (1). Within the \(N\)-particles subspace of the Fock space \(\mathcal{F}\), the operator \(\hat{H}\) has the spectral resolution:

\[
\hat{H} = \sum_{\alpha} \epsilon_{\alpha} |\Phi_{\alpha}\rangle\langle\Phi_{\alpha}|,
\]

where \(\{\epsilon_{\alpha}\}_\alpha\) are the eigenvalues and \(\{|\Phi_{\alpha}\rangle\}_\alpha\) the eigenvectors. Naturally the above expression is \(N\)-dependent, but we will not include an explicit label \(N\) to simplify the notation. The sum over \(\alpha\) ranges from 0 to the dimension of the \(N\)-body fermionic space, equal to \(\binom{M}{N}\). While zero temperature equilibrium properties of an \(N\)-particle system are completely determined by the ground state of (1), \(|\Phi_0\rangle\), the study of dynamic properties requires knowledge of the spectrum \(\{\epsilon_{\alpha}\}_\alpha\).

Throughout the present work we shall make the technical assumption that \(\epsilon_0 < \epsilon_1 \leq \ldots\), i.e., the \(N\)-particle ground state is non-degenerate.

A wide class of QMC methods relies on the observation that the imaginary time propagator

\[
e^{-\tau \hat{H}}, \quad \tau \geq 0
\]

enables the ground state of an \(N\)-particle system to be recovered. In fact, as long as a trial state \(|\Psi_T\rangle\) has non-zero overlap with \(|\Phi_0\rangle\) the following relation holds:

\[
\lim_{\tau \to \infty} e^{-\tau (\hat{H} - \epsilon_0)} |\Psi_T\rangle = |\Phi_0\rangle \langle\Phi_0|\Psi_T\rangle,
\]

where the unknown quantity \(\epsilon_0\) is replaced with an adaptive estimate, according to a common procedure in Diffusion Monte Carlo (DMC) calculations.\(^{16}\) QMC methods rely on the observation that deterministic evolution driven by the family of operators (3) can be mapped onto suitable stochastic processes and solved by randomly sampling appropriate probability distributions.

Along with the typical approach in which (4) is associated with a diffusion process in the configurational space of the system,\(^{4,5,16}\) in a class of more recently developed QMC methods, the so-called determinantal\(^{18,19,21-23}\) methods, (4) is mapped onto a stochastic process in the abstract manifold, which we will denote \(\mathcal{D}(N)\), of \(N\)-particle Slater determinants.

In AFQMC\(^{20-24,26,28-30}\) the association between (4) and a stochastic process in \(\mathcal{D}(N)\) is made possible by a discretization:

\[
e^{-\tau (\hat{H} - \epsilon_0)} = (e^{-\delta \tau (\hat{H} - \epsilon_0)})^n,
\]

with \(\delta \tau = \frac{\tau}{n}\), and by a combined use of the Trotter-Suzuki decomposition of the propagator\(^{32,33}\) and of the Hubbard-Stratonovich transformation\(^{26,34,35}\) on the factors \(e^{-\delta \tau (\hat{H} - \epsilon_0)}\). The Hubbard-Stratonovich transformation is an operator identity guaranteeing that

\[
e^{-\delta \tau (\hat{H} - \epsilon_0)} = \int \text{d}g(\eta) \hat{G}(\eta) + \mathcal{O}(\delta \tau^2),
\]

with \(\text{d}g(\eta)\) standard 2\(M^2\)-dimensional normal probability measure, \(\hat{G}(\eta) = e^{\hat{A}(\eta)}\) and \(\hat{A}(\eta) = \sum_{i,j=1}^M \hat{A}_i \hat{A}_j\), a suitable one-particle operator, the structure of which is discussed in detail in Appendix A 2.

Equation (6) establishes a formal correspondence between an interacting fermion system and an ensemble of non-interacting fermion systems subject to fluctuating external potentials. The coupling with these external potentials is controlled by normally distributed parameters \(\eta\), called auxiliary fields, integration over which recovers the interaction.

To quantitatively realize that (6) provides a random walk representation of the imaginary time evolution, let us consider the stochastic process defined by the succession of wave functions:

\[
|\Psi_n\rangle = \hat{G}(\eta_{n-1}) \ldots \hat{G}(\eta_0) |\Psi_T\rangle,
\]

where the operators \(\hat{G}(\eta_{n})\) are functions of independent normally distributed random variables \(\eta_{n}\). It is known, and will be shown in details in Appendix A 1, that, if \(|\Psi_T\rangle \in \mathcal{D}(N)\), all the random variables \(|\Psi_n\rangle\) take values in \(\mathcal{D}(N)\). Furthermore, their average is given by

\[
\langle|\Psi_n\rangle|\Psi_{n-1}, \ldots, \eta_{0}\rangle = \langle\hat{G}(\eta_{n-1}) \ldots \hat{G}(\eta_0)|\Psi_T\rangle
\]

\[
= \int \text{d}g(\eta_{n-1}) \ldots \text{d}g(\eta_0) \hat{G}(\eta_{n-1}) \ldots \hat{G}(\eta_0) |\Psi_T\rangle
\]

\[
= e^{-n\delta \tau (\hat{H} - \epsilon_0)} |\Psi_T\rangle + \mathcal{O}(\delta \tau^2).
\]

Expression (8) clearly shows that the solution of the imaginary time Schrödinger equation (4) can be recovered as an average of a suitable stochastic process, the structure of which is suggested by (7). Combining (4) and (7) it is evident that numerical sampling of such stochastic process provides a stochastic linear combination of Slater determinants, representing an estimation of the ground state of (1). The most natural choice of the trial function \(|\Psi_T\rangle\), which will we use throughout the present work, is the Hartree-Fock ground state of the Hamiltonian, i.e., the lowest energy Slater determinant.

A. Control of the fermion sign problem: The phaseless AFQMC

Despite its formal simplicity, the straightforward numerical implementation leads in general to an exponential increase
in statistical errors with the imaginary time, due to the fact that complex random phases appear during the evolution (4).

S. Zhang invented a modification of the stochastic process through the introduction of an importance sampling transformation\textsuperscript{26} that guides the random walk, closely resembling the typical scheme adopted\textsuperscript{17} in configurational DMC simulations. The state $e^{-n\delta\tau(H-e_0)}|\Psi_T\rangle$ is rewritten in the following form, detailed in Appendix A3 and equivalent to (8):

$$e^{-n\delta\tau(H-e_0)}|\Psi_T\rangle \
\simeq \int dg(\eta_{-1})\ldots dg(\eta_0) \times \mathbb{M}[\eta_{-1},\xi_{-1},\ldots,\eta_0,\xi_0] \times \frac{\hat{G}(\eta_{-1}-\xi_{-1})\ldots\hat{G}(\eta_0-\xi_0)|\Psi_T\rangle}{|\Psi_T\rangle \hat{G}(\eta_{-1}-\xi_{-1})\ldots\hat{G}(\eta_0-\xi_0)} \tag{9}$$

where complex-valued shift parameters $\xi_{-1},\ldots,\xi_0$ and a weight function have been inserted. The latter satisfies the recursion relation:

$$\mathbb{M}[\eta_n,\xi_n;\eta_0,\xi_0] = \mathbb{M}[\eta_{-1},\xi_{-1},\ldots,\eta_0,\xi_0] \times \mathbb{I}[\eta_n,\xi_n;\hat{G}(\eta_{-1}-\xi_{-1})\ldots\hat{G}(\eta_0-\xi_0)|\Psi_T\rangle] \tag{10}$$

where the following importance function appears:

$$\mathbb{I}[\eta,\xi;|\Psi\rangle] = e^{-\frac{\delta\tau}{2} Im\langle\eta-\xi|\Psi\rangle} \tag{11}$$

appears. The shift parameters are chosen to minimize fluctuations in the importance function to first order in $\delta\tau$. The importance sampling expression (11) clearly shows the mechanism responsible for the appearance of the sign problem in the framework of AFQMC: when the overlap between one or more walkers and the trial state vanishes massive fluctuations in the importance function occur, determining drastic statistical errors in the AFQMC estimate (9) for the solution of (4). In the method conceived by S. Zhang, the exact complex-valued importance function appearing in (11) is replaced\textsuperscript{23} by the approximate form:

$$\mathbb{I}[\eta,\xi;|\Psi\rangle] \simeq e^{-\delta\tau(\epsilon_{loc}(\Psi)-\epsilon_0)} \times \max(0,\cos(\Delta\theta)) \tag{12}$$

where $\epsilon_{loc}(\Psi) = Re\left\{\frac{\langle\hat{G}(\eta-\xi)|\Psi\rangle}{|\Psi_T\rangle}\right\}$ is the local energy functional, and

$$\Delta\theta = \log\left(\frac{\langle\Psi_T|\hat{G}(\eta-\xi)|\Psi\rangle}{|\Psi_T\rangle}\right) \tag{13}$$

The derivation of such approximate form is detailed in Appendix A3. The first factor corresponds to the so-called real local energy approximation, which turns (11) into a real quantity, avoiding typical phase problems arising from complex weights. The second factor, together with the introduction of the shift parameters, has been argued in Refs. 23 and 26 to keep the overlap between the determinants involved in the random walk and the trial determinant far from zero. In fact, the angle $\Delta\theta$ corresponds to the flip in the phase of a determinant during a step of the random walk: the term max $(0, \cos(\Delta\theta))$ is meant to suppress determinants whose phase undergoes an abrupt change, under the assumption\textsuperscript{23,26} that such behavior indicates the vanishing of the overlap with the trial state.

Equation (9), together with the choice (12) for the evolution of the weights attached to the Slater determinants, gives rise to the so-called phaseless AFQMC method.

The underlying approximation is known to be good for the ground state, but ITCFs require sampling of excited states, related to the fluctuations around the asymptotic distribution of the random walk: this issue is largely unexplored, and the aim of the present work is to address its accuracy. There is no a priori motivation for concluding that the approximation (12) is better than the FN for the exploration of the manifold of excited states. One of the topics investigated in the present work is the verification of this important point for a model system by comparison with exact results.

We stress that the complex weights and the vanishing of the overlap with the trial state, responsible for the appearance of the sign problem in AFQMC, occur even for very small systems, such as two particles with opposite spins: for those systems, it is notoriously absent in configurational QMC.
methods, since the spatial part of the wave function is symmetric and positive.

**B. The algorithm**

The so-far introduced observations give rise to a polynomially complex algorithm for numerically sampling the solution (4), the efficiency of which relies on the observation that the walkers \( |\psi^{(w)}_k\rangle \) lie in \( \mathcal{D}(N) \) and can be therefore parametrized with an \( M \times N \) complex-valued matrix, as discussed in Appendix A1. The algorithm can be resumed in the following sequence of operations:

1. A collection \( |\psi^{(1)}_0\rangle \ldots |\psi^{(N_w)}_0\rangle \) of Slater determinants, henceforth referred to as walkers, is initialized to a trial state \( |\psi_T\rangle \).

2. For \( k = 0 \ldots n - 1 \) an adaptive estimate of the ground state energy is produced according to the formula:

\[
\epsilon_0 \simeq \frac{1}{\sum_{w=1}^{N_w} \eta^{(w)}_k} \sum_{w=1}^{N_w} \frac{\langle \psi_T | \hat{H} | \psi^{(w)}_k \rangle}{\langle \psi_T | \psi^{(w)}_k \rangle},
\]

(14)

normally distributed auxiliary field configurations \( \eta^{(1)}_k \ldots \eta^{(N_w)}_k \) are sampled, and walkers and weights are updated according to

\[
|\psi^{(w)}_{k+1}\rangle = \hat{G} (\eta^{(w)}_k - \xi^{(w)}_k) |\psi^{(w)}_k\rangle,
\]

\[
\eta^{(w)}_{k+1} = \eta^{(w)}_k \mathcal{J} [\xi^{(w)}_k, \xi^{(w)}_k; |\psi^{(w)}_k\rangle].
\]

(15)

3. An estimate for \( e^{-n\tau(H-e_0)} |\psi_T\rangle \) is given by

\[
e^{-n\tau(H-e_0)} |\psi_T\rangle \simeq \sum_{w=1}^{N_w} \mathcal{M}_n^{(w)} |\psi^{(w)}_n\rangle \langle \psi_T | \psi^{(w)}_n\rangle.
\]

(16)

The ground state average \( \langle \phi_0 | \hat{O} | \phi_0 \rangle \) of a many-body observable \( \hat{O} \) not commuting with \( \hat{H} \) is the \( m, n \rightarrow \infty \) limit of the following formula:

\[
\frac{\langle \psi_T | e^{-m\tau(H-e_0)} \hat{O} e^{-n\tau(H-e_0)} |\psi_T\rangle}{\langle \psi_T | e^{-n\tau(H-e_0)} |\psi_T\rangle},
\]

(17)

for which manipulations analogous to the importance sampling transformation, discussed in detail in Appendix A4, yield the following backpropagated estimate:

\[
\langle \phi^{(N)}_0 | \hat{O} | \phi^{(N)}_0 \rangle \simeq \frac{\sum_{w=1}^{N_w} \mathcal{M}_n^{(w)} \langle \psi^{(w)}_n | \hat{O} | \psi^{(w)}_n \rangle}{\sum_{w=1}^{N_w} \mathcal{M}_n^{(w)}},
\]

(18)

with

\[
|\psi^{(w)}_n\rangle = \hat{G} (\eta_{n-1} - \xi_{n-1}) \ldots \hat{G} (\eta_0 - \xi_0) |\psi^T\rangle,
\]

\[
|\psi^{(w)}_{BP,m}\rangle = \hat{G}^\dagger (\eta_n - \xi_n) \ldots \hat{G}^\dagger (\eta_{n+m-1} - \xi_{n+m-1}) |\psi^T\rangle.
\]

(19)

Notice that the backpropagation technique is necessary to obtain ground state averages from the random walk. In the absence of backpropagation, only mixed estimates of the form \( \langle \psi_T | \hat{O} | \psi_0 \rangle / \langle \psi_T | \psi_0 \rangle \) can be obtained, which coincide with ground state
TABLE I. Exact (column 6) and calculated (column 5) ground state energy per particle in Hartree units, and overlap between exact and reconstructed ground state (column 7) for various systems (parameters are listed in columns 1 to 4).

| $N_\uparrow$ | $N_\downarrow$ | $r_s$ | $M$ | $\epsilon_0/N$ (AFQMC) | $\epsilon_0/N$ (exact) | $\langle \Phi_0 | \Psi_1 \rangle$ |
|----------|------------|------|-----|-----------------|-------------------|----------------|}
| 1        | 1          | 1    | 5   | $-0.82255(5)$   | $-0.82259$        | $0.99999(5)$ |
| 1        | 1          | 1    | 13  | $-0.8315(1)$    | $-0.8313$        | $0.9999(1)$  |
| 1        | 1          | 1    | 21  | $-0.83338(6)$   | $-0.83307$       | $0.9989(7)$  |
| 1        | 1          | 1    | 49  | $-0.83476(7)$   | $-0.83441$       | $0.9882(4)$  |
| 1        | 2          | 5    |     | $-0.4282(1)$    | $-0.4282$        | $0.9629(3)$  |
| 1        | 2          | 13   |     | $-0.4351(1)$    | $-0.4330$        | $0.9650(2)$  |
| 1        | 2          | 21   |     | $-0.4359(3)$    | $-0.4339$        | $0.9586(2)$  |
| 1        | 2          | 49   |     | $-0.4362(3)$    | $-0.4345$        | $0.9594(5)$  |
| 1        | 3          | 21   |     | $-0.3020(3)$    | $-0.2972$        | $0.9253(8)$  |
| 1        | 4          | 21   |     | $-0.2320(4)$    | $-0.2272$        | $0.904(1)$   |
| 5        | 0          | 1    | 9   | $0.11327(2)$    | $0.11247$        | $0.99185(1)$ |
| 5        | 0          | 2    | 9   | $-0.19485(1)$   | $-0.19751$       | $0.9863(4)$  |
| 5        | 0          | 2    | 13  | $-0.19878(2)$   | $-0.20311$       | $0.9683(3)$  |

expectations (17) only if $\hat{O}$ commutes with the Hamiltonian $\hat{H}$.

C. Imaginary time correlation functions

In a well-established approach \cite{7–12,19} to the reconstruction of dynamic properties of many body systems, the dynamic structure factor of the single-particle operators $\hat{A}, \hat{B}$:

$$ S_{\hat{A}, \hat{B}}(\omega) = \int_{\mathbb{R}} dt \frac{e^{i\omega t}}{2\pi} \langle \Phi_0 | \hat{A}(t) \hat{B} | \Phi_0 \rangle $$

is recovered from their imaginary time correlation function:

$$ F_{\hat{A}, \hat{B}}(\tau) = \langle \Phi_0 | \hat{A}(\tau) \hat{B} | \Phi_0 \rangle = \frac{\langle \Phi_0 | \hat{A} e^{-\tau(\hat{H} - \epsilon_0)} \hat{B} | \Phi_0 \rangle}{N} $$

though a numeric inverse Laplace transform. Being constructed with the imaginary time evolution operator, the ITCF (21) is a natural quantity to be evaluated in QMC calculations. Its evaluation in determinantal QMC methods, however, is not as simple as in configurational QMC: straightforward extension of the backpropagation technique to the evaluation of (21) is in fact prevented because the single-particle

FIG. 4. Imaginary time correlation function of the momentum shift operator relative to $M = 5, 21, 49$ at $r_s = 1$ for $N_\uparrow = 1, N_\downarrow = 1$. In the right lower box, comparison between AFQMC and exact Path Integral QMC calculations is given. When not visible, error bars are smaller than the symbol size.

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operator $\hat{B}$ does not preserve $\mathcal{D}(N)$. To overcome this difficulty, we generalize the clever approach conceived by Feldbacher and Assaad\textsuperscript{24} for the calculation of dynamical Green functions: we introduce the Hubbard-Stratonovich representation (6) of the imaginary time propagator in (21) and move the operators $\hat{G}(\tau)$ to the right of $\hat{B} = \sum_{ij} \mathcal{B}_{ij} \hat{a}_i^\dagger \hat{a}_j$ commuting them with the operators $\hat{a}_i^\dagger$, $\hat{a}_j$. As discussed in detail in Appendix A5, this procedure determines the appearance of two random matrices in the estimator for (21):

$$F_{\hat{A}, \hat{B}}(r\delta \tau) = \frac{1}{N} \sum_{kl} \mathcal{B}_{kl} \int d\mathcal{g}(\eta_{n-1}) \ldots d\mathcal{g}(\eta_{n-r})$$

$$\times \langle \Phi_0 | \hat{A} \hat{G}(\eta_{n-1}) \ldots \hat{G}(\eta_{n-r}) \hat{a}_k^\dagger \hat{a}_l | \Phi_0 \rangle$$

$$= \frac{1}{N} \sum_{ijkl} \mathcal{B}_{ijkl} \int d\mathcal{g}(\eta_{n-1}) \ldots d\mathcal{g}(\eta_{n-r})$$

$$\times \langle \Phi_0 | \hat{A} \hat{a}_k^\dagger \hat{a}_j \hat{G}(\eta_{n-1}) \ldots \hat{G}(\eta_{n-r}) | \Phi_0 \rangle$$

$$\times \mathcal{D}(\eta_{n-1}, \ldots, \eta_{n-r})_j \mathcal{D}^{-1}(\eta_{n-1}, \ldots, \eta_{n-r})_k,$$

where $\mathcal{D}(\eta_{n-1}, \ldots, \eta_{n-r}) = e^{A(\eta_{n-1})} \ldots e^{A(\eta_{n-r})}$.

Further application of the importance sampling transformation and of the backpropagation technique yields, as explained in Appendix A5:

$$F_{\hat{A}, \hat{B}}(r\delta \tau) \simeq \frac{1}{N} \sum_{w_{1}, \ldots, w_{N_{w}}} \frac{1}{\mathcal{M}_{w_{N_{w}}} - (22)} \sum_{w_{1}} \sum_{ijkl} \mathcal{B}_{ijkl} \mathcal{M}_{w_{N_{w}}}$$

$$\times \frac{\langle \psi^{(w)}_{B,P,m} | \hat{A} \hat{a}_k^\dagger \hat{a}_j | \psi^{(w)}_{n} \rangle}{\langle \psi^{(w)}_{B,P,m} | \psi^{(w)}_{n} \rangle}$$

$$\times \mathcal{D}(\eta_{n-1}^{(w)} - \xi_{n-1}^{(w)}, \ldots, \eta_{n-r}^{(w)} - \xi_{n-r}^{(w)})_j$$

$$\times \mathcal{D}^{-1}(\eta_{n-1}^{(w)} - \xi_{n-1}^{(w)}, \ldots, \eta_{n-r}^{(w)} - \xi_{n-r}^{(w)})_k. \quad (23)$$

where the single-particle Hilbert space $\mathcal{H}$ is spanned by the plane wave orbitals $|n, \sigma\rangle$ with $n \in \mathbb{Z}^2$, $|n|^2 \leq n_{\text{max}}$ for some integer $n_{\text{max}}$ and $\sigma = \pm 1$. The parameter $r_s \in (0, \infty)$ controls the relevance of the interaction part and $N$ stands for the number of particles, and the constant $\xi = -3.900265$ arises from an Ewald summation procedure.\textsuperscript{37} For small number of particles $N$ and low kinetic energy cutoff $n_{\text{max}}$ the above Hamiltonian defines a simple model which can be solved exactly.\textsuperscript{36, 39}

Knowledge of eigenvalues $\{\epsilon_\alpha\}_\alpha$ and eigenvectors $\{\Phi_\alpha\}_\alpha$ of $\hat{H}$ allows exact calculation of the imaginary time propagator:

$$e^{-\tau(\hat{H} - \epsilon_\alpha)} = \sum_\alpha e^{-\tau(\epsilon_\alpha - \epsilon_\alpha)} |\Phi_\alpha\rangle \langle \Phi_\alpha|, \quad (25)$$

III. A CLASS OF SOLVABLE SYSTEMS

We test the accuracy of the AFQMC results on a class of simple systems for which exact numeric expression for the spectral decomposition (2) of the Hamiltonian operator $\hat{H}$ can be given. Let us consider the Hamiltonian of the 2D electron gas:

$$\hat{H} = \frac{\xi \sqrt{N}}{\sqrt{4\pi r_s}} + \sum_{m,\sigma} \frac{2\pi}{N} \frac{|n_m|^2}{r_s} \hat{a}_m^\dagger \hat{a}_m,\sigma$$

$$+ \sum_{m,\sigma} \sum_{n,\sigma} \frac{1}{\sqrt{4N\pi r_s}} \delta_{n_m, n_m - n} \hat{a}_m^\dagger \hat{a}_{n_m} \hat{a}_{n_m}^\dagger \hat{a}_{n_m},\sigma, \quad (24)$$

FIG. 5. Imaginary time correlation function of the momentum shift operator relative to $r_s = 2, 3, 4$ (top to bottom) for $N_1 = 1$, $N_2 = 1$ at $M = 21$. When not visible, error bars are smaller than the symbol size.
of the projector $|\Phi_0\rangle\langle\Phi_0|$ onto the minimum energy eigenspace, of backpropagated ground state averages:

$$\frac{\langle\Psi_{\tau}|e^{-\tau(e_{\alpha}-\epsilon_0)}\hat{O}|\Phi_0\rangle}{\langle\Psi_{\tau}|e^{-\tau(e_{\alpha}-\epsilon_0)}|\Phi_0\rangle} = \sum_\alpha \frac{\langle\Psi_{\tau}|\Phi_\alpha\rangle e^{-\tau(e_{\alpha}-\epsilon_0)} \langle\Phi_\alpha|\hat{O}|\Phi_0\rangle}{\langle\Psi_{\tau}|\Phi_0\rangle}$$

and of backpropagated imaginary time correlation functions (21):

$$F_{\hat{A},\hat{B}}(\tau) = \frac{1}{N} \frac{\langle\Psi_{\tau}|e^{-\tau\hat{H}}\hat{A}e^{-\tau\hat{H}}\hat{B}|\Phi_0\rangle}{\langle\Psi_{\tau}|e^{-\tau\hat{H}}|\Phi_0\rangle} = \frac{1}{N} \sum_{\alpha,\beta} \frac{\langle\Psi_{\tau}|\Phi_\alpha\rangle e^{-\tau(e_{\alpha}-\epsilon_0)} \langle\Phi_\alpha|\hat{A}\hat{B}|\Phi_\beta\rangle \langle\Phi_\beta|\hat{B}|\Phi_0\rangle}{\langle\Psi_{\tau}|\Phi_0\rangle}$$

and the comparison of such quantities with AFQMC results.

IV. RESULTS

We focus on the ITCF $F_n(\tau) = \frac{1}{N} \langle\Psi_0|\hat{\rho}_n(\tau)\hat{\rho}^\dagger_n|\Psi_0\rangle$ of the density fluctuation operator:

$$\hat{\rho}_n = \sum_{j,\sigma} \delta_{n,j} \hat{a}^\dagger_{j,\sigma} \hat{a}_{j,\sigma}$$

and of its adjoint $\hat{\rho}^\dagger_n = \hat{\rho}^{-\dagger}$.

The phaseless AFQMC method represents the ground state as a stochastic linear combination of Slater determinants (16) from which accurate estimates of the ground state energy can be obtained.\cite{22,26} However, much more information can be obtained from the simulation. Here we present results for the components of the ground state on the chosen basis of the Hilbert space and for the imaginary time correlation functions.

Each of the simulations presented below is characterized by two sets of parameters: $(N_1, N_1^f, r_s, M)$ define the system under study, whereas $(\delta\tau, m, N_w)$ control the details of the simulation. In particular, $N_1$ ($N_1^f$) is the number of spin-up (spin-down) fermions, $r_s$ controls the strength of the

![Graphs showing imaginary time correlation functions](Image)

FIG. 6. Imaginary time correlation function of the momentum shift operator relative to $M = 9$, 97 at $r_s = 1$ (upper panel) and to $M = 13$, 97 at $r_s = 2$ (lower panel) for $N_1 = 5$, $N_1^f = 0$. In the right box of each panel comparison between AFQMC and FN calculations (green crosses) is given. When not visible, error bars are smaller than the symbol size.
interaction, $M$ fixes the order of the matrices with which the algorithm deals, while $m$ corresponds to the number of backpropagation steps.

Apart from the basis set size $M$, which we keep small to allow comparison with exact diagonalization, and we extrapolate to the joint limit $\delta \tau \to 0$, $N_m \to \infty$, and $m \to \infty$ to eliminate sources of systematic errors.

As an example, we show in Fig. 2 the extrapolations for a calculation with $(N_1, N_4, r_s, M) = (1, 1, 1, 49)$. Discrepancies with respect to the exact results are therefore due to the only uncontrolled approximations of the method, namely the real local energy and the phase approximations (12).

### A. Assessment of the accuracy

In Fig. 3 we show results relative to the simulation of systems with $r_s = 1$, $M = 13$, for some values of $N_1$ and $N_4$. The left panels of Fig. 3 show the components of the stochastic solution on the Hilbert space basis functions. The little statistical fluctuations around the $x$ axis show that the random walk visits a large number of states, while the significant components of the AFQMC solution match those of the exact ground state with good accuracy. The ITCF $F_A$ of the density fluctuation operator (28) for $n = (1, 0)$ is reported in the right column of Fig. 3. The wave vector $\mathbf{n}$ has been chosen in the lowest energy shell since it gives rise to nonvanishing ITCFs even for small $M$. The agreement with exact values is remarkable, in particular if compared with the discrepancy observed for the FN result, Fig. 1: this constitutes the central result of the present work.

For all these systems we computed also the ground state energy per particle, and the overlap between exact and reconstructed ground state: the results are listed in Table I, the bias of the energy resulting of the order of $10^{-3} \Delta E_{distr}$, which is smaller than the FN bias using a Slater-Jastrow trial function with plane-wave nodes.41

### B. Computational issues

Although our primary interest is the assessment of the accuracy of AFQMC in calculating the ITCFs addressed in Sec. IV A, we explored the behavior of the method for larger values of $r_s$ and $M$.

As $r_s$ increases, the interaction becomes more and more important, and the overlap of the exact wave function with the trial function becomes smaller. Also the increase in $M$, which is required for the study of realistic models, makes the stochastic exploration of the Hilbert space more difficult: in particular, the calculation of ITCFs is further complicated by the need of multiplying many exponentials of large matrices, see (23), which induces instabilities at large imaginary time. This problem is already known in the literature.24,42

In Fig. 4 results appear relative to systems with $N_1 = 1$, $N_4 = 1$, showing that AFQMC estimations of static and dynamic properties remain in satisfactory agreement with exact values even if $M$ is raised to 49. For $M = 49$ we are also in good agreement with exact Path Integral QMC calculations, providing the exact result in the limit $M \to +\infty$, which cannot be explored via exact diagonalization.

The algorithm is able to reproduce exact values even at $r_s = 2, 3, 4$ and $M = 21$, as shown in Fig. 5. Since it is known that the degree of correlation in the uniform electron gas is significantly higher in 2D than in 3D for given $r_s$, the range of densities covered well represents the typical realistic density values in 3D (up to $r_s \sim 5$).

We complete the study with calculations relative to systems with $N_1, N_4 = (5, 0)$. Results are shown in Fig. 6. For $M = 9$ the quality of AFQMC calculations is still satisfactory, even if we observe a small overestimate of $F_A$ for $\tau \sim 1$. For $M = 97$ we compared our results with FN calculations. We observe good agreement between the estimates of the static property $F_n(0)$ yield by both algorithms. As far as finite $\tau$ ITCFs are concerned, we found that the discrepancy between the two results qualitatively resembles the discrepancy between exact solution and FN in the case of noninteracting particles in Fig. 1: an encouraging result.

To quantify the quality of the presented results, the reader may refer to Table II, where we report an average reduced chi-squared.

### V. CONCLUSIONS

In the present work we gave a detailed description of the phaseless AFQMC algorithm, we proposed a scheme for its application to the calculation of dynamical properties of zero temperature fermion systems and we tested the methodology against exact diagonalization for interacting few fermion systems. Such tests revealed that it is actually possible to compute imaginary time correlation functions with satisfactory accuracy, at least for systems with moderate number of particles and interaction strength. This is a very interesting result since it is known that there exist situations when the well established and widely employed FN approximation scheme provides inaccurate results for ITCFs. The present work indicates that the AFQMC algorithm can become an accurate tool to calculate dynamical properties of few body systems. We hope that the accuracy of our results will encourage the development of technical tools necessary to study larger systems.

### TABLE II. Values of $\chi^2 = \frac{1}{N} \sum_{\tau=1}^{N-1} \frac{|\chi_{\text{AFQMC}}(\tau) - \chi_{\text{FN}}(\tau)|^2}{\sigma^2}$ for the various systems presented. $N_\tau$ is the number of imaginary time instants.

<table>
<thead>
<tr>
<th>$N_1$</th>
<th>$N_4$</th>
<th>$r_s$</th>
<th>$M$</th>
<th>$\chi^2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1</td>
<td>1</td>
<td>5</td>
<td>1.02</td>
</tr>
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<td>13</td>
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<tr>
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<td>1</td>
<td>4</td>
<td>21</td>
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</tr>
<tr>
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<td>1</td>
<td>9</td>
<td>0.69</td>
</tr>
<tr>
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<td>1</td>
<td>13</td>
<td>2.87</td>
</tr>
<tr>
<td>5</td>
<td>0</td>
<td>2</td>
<td>9</td>
<td>1.09</td>
</tr>
</tbody>
</table>
such as the numeric stabilization\(^{40,42}\) of the products of matrix exponentials involved both in the backpropagation\(^{27}\) and in the calculation of imaginary time correlation functions. In perspective, an accurate calculation of ITCFs is a prerequisite for the analytic continuation\(^{7}\) leading to real-time dynamics of quantum systems.

**ACKNOWLEDGMENTS**

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**APPENDIX A: ALGORITHMIC DETAILS**

The aim of this appendix is completing the description of the extended AFQMC outlined in Sec. II.

1. Properties of Slater determinants

For a generic Slater determinant \( |\Psi \rangle \) there exist single-particle orbitals \( |\psi_i \rangle \ldots |\psi_N \rangle \in \mathcal{H} \) for which \( |\Psi \rangle = |\psi_1 \rangle \ldots |\psi_N \rangle \). As a consequence the state

\[
|\Psi \rangle = \sum_{i_1 \ldots i_N} \langle \psi_{i_1} | \ldots | \psi_{i_N} \rangle |\psi_{i_1} \rangle \ldots |\psi_{i_N} \rangle = \sum_{i_1 \ldots i_N} \Psi_{i_1 \ldots i_N} \hat{a}_{i_1} \ldots \hat{a}_{i_N} |0 \rangle
\]

is completely and uniquely described by the \( M \times N \) matrix \( \Psi_{ij} = \langle \psi_i | \psi_j \rangle \).

In the light of such parametrization it can be proved\(^{43}\) that for a generic \( N \)-particle Slater determinant \( |\Psi \rangle \) and a generic one-body operator \( \hat{O} = \sum_{i,j} \hat{O}_{ij} \hat{a}_i \hat{a}_j \) the state \( e^{\hat{O}} |\Psi \rangle \) is still a Slater determinant, described by the matrix \( e^{\hat{O}}|\Psi \rangle \), so that the manifold \( \mathcal{D}(N) \) of Slater determinants is closed under the action of exponentials of single-particle operators.

Equation (A1) also enables the concrete calculation overlaps and matrix elements of one-body and two-body operators. In particular, if \( |\Psi \rangle, |\Phi \rangle \) are generic non-orthogonal \( N \)-particle Slater determinants the following properties\(^{26,43,44}\) hold:

\[
\langle \Phi | \Psi \rangle = \frac{\det[\Phi^\dagger \Psi]}{N!},
\]

\[
\frac{\langle \Phi | \hat{a}_i \hat{a}_j | \Psi \rangle}{\langle \Phi | \Psi \rangle} = \Psi_{ij} \left[ \Phi \right]_{ij},
\]

\[
\frac{\langle \Phi | \hat{a}_i \hat{a}_j \hat{a}_k | \Psi \rangle}{\langle \Phi | \Psi \rangle} = \Psi_{ij} \Gamma_{jk} - \Psi_{ik} \Gamma_{jj}.
\]

2. The Hubbard-Stratonovich transformation

It is well known that the coefficients \( \gamma_{ijk} \) describing the interaction part of (1) satisfy the relation \( \gamma_{ijk} = \gamma_{jki} \) and can be consequently cast in a hermitian matrix \( \Gamma_{(K)(J)} \) = \( \gamma_{ijk} \) of order \( M^2 \). Due to the spectral theorem \( \Gamma_{(K)(J)} \) = \( \sum_{\xi=1}^{M^2} U_{\xi(J)} U_{\xi(I)} \) for some real-valued coefficients \( \Gamma_{\xi} \) and some unitary matrix \( U \) of order \( M^2 \). As a consequence, (1) can be put in the form

\[
\hat{H} = \hat{H}_0 - \frac{1}{2} \sum_{\xi=1}^{M^2} \Gamma_{\xi} \left[ \frac{\hat{O}_\xi - \hat{O}_\xi \dagger}{2} + \frac{\hat{O}_\xi - i \hat{O}_\xi \dagger}{2} \right],
\]

(A3)

with

\[
\hat{H}_0 = \sum_{ij} \beta_{ij} + \sum_{ij} \sum_{j} \gamma_{ijj} \hat{a}_i \hat{a}_j, \quad \hat{O}_\xi = \sum_{ij} U_{\xi(j)} \hat{a}_j \hat{a}_i U_{\xi(I)}^\dagger.
\]

(A4)

Notice that the interaction part of (A4) has been replaced with a sum of squares of single-particle hermitian operators. Inserting such expression in \( e^{-\delta \tau (\hat{H}_0 - \epsilon_0)} \) and applying a Trotter-Suzuki decomposition:

\[
e^{-\delta \tau (\hat{H}_0 - \epsilon_0)} = e^{\delta \tau (\hat{H}_0 - \epsilon_0)} \prod_{\xi=1}^{M^2} e^{\delta \tau \Gamma_{(k)} \sum_{j} \hat{a}_j \hat{a}_j} e^{\delta \tau \sum_{j} \hat{a}_j \hat{a}_j}.
\]

(A5)

To each of the factors appearing in (A5) the Hubbard-Stratonovich Transformation applies, yielding (6) with

\[
\hat{A}(\eta) = \delta \tau \left( \hat{H}_0 - \epsilon_0 \right) - \sqrt{\delta \tau} \eta \cdot \hat{n}.
\]

(A6)

which can be compactly written as

\[
\hat{A}(\eta) = \frac{\delta \tau}{2} \left( \hat{H}_0 - \epsilon_0 \right) - \sqrt{\delta \tau} i \hat{B} \cdot \eta.
\]

(A7)

3. The importance sampling transformation

We now explain in detail the derivation of Eq. (9). First we introduce in the expression (8) \( n \) arbitrary and possibly complex-valued shift parameters \( \xi_0 \ldots \xi_{n-1} \) obtaining

\[
e^{-\delta \tau (\hat{H}_0 - \epsilon_0)} |\Psi_T \rangle \propto \int \ldots \int d(\eta_0 - \xi_0) \ldots d(\eta_n - \xi_n) |\Psi_T \rangle.
\]

(A8)

Then we recall that

\[
d(\eta - \xi) = d(\eta) e^{-\frac{\eta^2}{2} - \eta \xi}
\]

(A9)
and obtain (9) inserting the identity
\[ \hat{G}(\eta_{n-1} - \xi_{n-1}) \ldots \hat{G}(\eta_0 - \xi_0) |\Psi_T \rangle \]
\[ = \hat{G}(\eta_{n-1} - \xi_{n-1}) \ldots \hat{G}(\eta_0 - \xi_0) |\Psi_T \rangle \frac{\langle \Psi_T | \hat{G}(\eta_{n-1} - \xi_{n-1}) \ldots \hat{G}(\eta_0 - \xi_0) |\Psi_T \rangle}{\langle \Psi_T | \hat{G}(\eta_{n-1} - \xi_{n-1}) \ldots \hat{G}(\eta_0 - \xi_0) |\Psi_T \rangle} \]
\[ \times \prod_{k=0}^{n-1} \frac{\langle \Psi_T | \hat{G}(\eta_k - \xi_k) \ldots \hat{G}(\eta_0 - \xi_0) |\Psi_T \rangle}{\langle \Psi_T | \hat{G}(\eta_k - \xi_k) \ldots \hat{G}(\eta_0 - \xi_0) |\Psi_T \rangle} \]
\[ \times \langle \Psi_T | \hat{G}(\eta - \xi) |\Psi_T \rangle \]
\[ G^\prime(\eta - \xi) = I + i \sqrt{\delta \tau} (\eta - \xi) \cdot \hat{B} + \mathcal{O}(\delta \tau). \] (A11)

Introducing this approximation in (11) leads to

\[ \log[\mathcal{Z}[\eta, \xi; |\Psi \rangle]] = -\frac{\langle \Psi_T | |\hat{B} \rangle |\Psi_T \rangle}{2} + \eta \cdot \xi - i \sqrt{\delta \tau} \frac{\langle \Psi_T | \hat{B} |\Psi_T \rangle}{\langle \Psi_T | |\Psi_T \rangle} \cdot (\eta - \xi), \] (A12)

where the operation \( \langle \Psi_T | \hat{B} |\Psi_T \rangle \) shall be henceforth abbreviated with \( \langle \hat{B} \rangle \). Imposing \( \eta \cdot \xi = 0 \) fixes the value of the shift parameters to \( \xi_{opt} = -i \sqrt{\delta \tau} \langle \hat{B} \rangle \). \( \quad \) (A13)

Insertion of (A13) into (11) yields the stabilized expression for the importance function. A straightforward expansion of this quantity in powers of \( \sqrt{\delta \tau} \) leads to

\[ \mathcal{Z}[\eta, \xi_{opt}; |\Psi \rangle] = 1 - \delta \tau \langle \hat{H} \rangle - \epsilon_0 \]
\[ - \frac{\delta \tau}{2} \left[ \langle \eta \cdot (\hat{B} - \langle \hat{B} \rangle) \rangle \right]^2 - \langle (\hat{B} - \langle \hat{B} \rangle) \rangle^2 \]
\[ + \mathcal{O}(\delta \tau \tau^{3/2}). \] (A14)

The real local energy approximations (12) are suggested by the observation that the term in square brackets in (A14) has zero average over auxiliary field configurations, and it consists in neglecting all terms of order \( \delta \tau \) in (A14) except for the real part of \( \langle \hat{H} \rangle \). The imaginary part of \( \langle \hat{H} \rangle \) is neglected because it vanishes for \( |\Psi \rangle \) equal to the ground state. Empirical evidence shows that it is a reasonable approximation, but to our knowledge it is not supported by mathematical arguments.

### 4. The backpropagation technique

We now discuss the emergence of the backpropagated estimator (18). We express all imaginary time propagators appearing in (A7) with (A8) and obtain the following representations for the numerator and the denominator:

\[ \langle \Psi_T | e^{-m+n/\tau \hat{H} - \epsilon_0} |\Psi_T \rangle \]
\[ = \int dg(\eta_{m+n-1}) \ldots dg(\eta_0) |\Psi_T \rangle \prod_{i=0}^{m+n-1} \hat{G}(\eta_i) |\Psi_T \rangle, \] (A15)

\[ \langle \Psi_T | e^{-m/\tau \hat{H} - \epsilon_0} \hat{O} e^{-n/\tau \hat{H} - \epsilon_0} |\Psi_T \rangle \]
\[ = \int dg(\eta_{m+n-1}) \ldots dg(\eta_0) |\Psi_T \rangle \prod_{i=n}^{m+n-1} \hat{G}(\eta_i) \hat{O} \prod_{i=0}^{m+n-1} \hat{G}(\eta_i) |\Psi_T \rangle, \] (A16)

where the symbol \( \prod_{i=n}^{m+n} \hat{G}(\eta_i) \) stands for the product \( \hat{G}(\eta_{m+n-1}) \ldots \hat{G}(\eta_n) \). Further application of the importance sampling transformation and of identity (A10) yields

\[ \langle \Psi_T | e^{-(m+n)/\tau \hat{H} - \epsilon_0} |\Psi_T \rangle \]
\[ = \int dg(\eta_{m+n-1}) \ldots dg(\eta_0) \mathcal{Z}^{2n|\Psi_T |} \prod_{i=n}^{m+n-1} \hat{G}(\eta_i) \hat{O} \prod_{i=0}^{m+n-1} \hat{G}(\eta_i) |\Psi_T \rangle, \] (A17)

the estimator for which is obviously (18). Notice that the same weights appearing in (15) are involved in (18).

### 5. The phaseless AFQMC estimator for ITCFs

We now explain in detail the derivation of Eqs. (22) and (23). The last passage of (22) is a manipulation of the operator product \( \hat{G}(\eta_{n-1}) \ldots \hat{G}(\eta_{n-2}) \hat{A}_i \hat{A}_j \). First, we observe that if \( \hat{A} = \sum_{i,j} \hat{A}_{ij} \hat{A}_j^\dagger \) is a one-body operator:

\[ e^{\hat{A}} \hat{B} e^{-\hat{A}} = \sum_j e^{\hat{A}_j^\dagger} \hat{B} j e^{\hat{A}_j^\dagger}, \] (A18)

As an immediate consequence:

\[ e^{\hat{A}} \hat{A}_i^\dagger e^{-\hat{A}} = \sum_{ij} e^{\hat{A}_i^\dagger} \hat{A}_j e^{-\hat{A}_j^\dagger} e^{\hat{A}_i^\dagger} \] (A19)

showing that the exponential of a one-body operator can be moved to the right of a product \( \hat{A}_i \hat{A}_j \) at the cost of introducing the matrix \( e^{\hat{A}} \) and its inverse. Iterated application of formula (A18) to the operator product \( \hat{G}(\eta_{n-1}) \ldots \hat{G}(\eta_{n-2}) \hat{A}_i \hat{A}_j \) yields

\[ \hat{G}(\eta_{n-1}) \ldots \hat{G}(\eta_{n-2}) \hat{A}_i \hat{A}_j \]
\[ = \sum_{ij} e^{\hat{A}_i^\dagger} \hat{A}_j e^{-\hat{A}_j^\dagger} \hat{G}(\eta_{n-1}) \ldots \hat{G}(\eta_{n-2}) \hat{A}_i \hat{A}_j \hat{G}(\eta_{n-1}) \ldots \hat{G}(\eta_{n-2}) \] (A20)
and justifies the last passage of Eq. (22). To obtain (23) we observe, as in the backpropagation technique, that

$$F_{\tilde{A}, \tilde{B}}(r, \delta r) \simeq \frac{1}{N} \langle \Psi_T | e^{-\bar{m} + n - \bar{r} - \delta r} \tilde{A} e^{-\bar{r} \delta r} | \Psi_T \rangle \cdot \langle \Psi_T | e^{-\bar{m} + n - \bar{r} - \delta r} \tilde{B} e^{-\bar{r} \delta r} | \Psi_T \rangle;$$

(A20)

notice that, unlike in (17), at the denominator of the previous equation only \( m + n - r \) integrations over auxiliary fields configurations are involved. Expressing all imaginary time propagators appearing in (A20) with (A8), recalling (22), and applying the importance sampling transformation to both numerator and denominator of the previous equation lead to

$$\langle \Psi_T | e^{-(m + n - r) \bar{r} \delta r} | \Psi_T \rangle = \int d\bar{q} d\bar{p} \rho_{\bar{q}}(\bar{q}) \rho_{\bar{p}}(\bar{p}) \langle \Psi_T | e^{-\bar{m} + n - \bar{r} - \delta r} \tilde{A} e^{-\bar{r} \delta r} \tilde{B} e^{-\bar{r} \delta r} | \Psi_T \rangle \langle \tilde{A} e^{-\bar{r} \delta r} \tilde{B} e^{-\bar{r} \delta r} | \Psi_T \rangle$$

(A21)

$$= \sum_{ijkl} \langle \Psi_T | e^{-\bar{m} + n - \bar{r} - \delta r} \tilde{A} e^{-\bar{r} \delta r} \tilde{B} e^{-\bar{r} \delta r} | \Psi_T \rangle \langle \tilde{A} e^{-\bar{r} \delta r} \tilde{B} e^{-\bar{r} \delta r} | \Psi_T \rangle.$$  

(A22)

Further application of the importance sampling transformation and of identity (A10) yields

$$\langle \Psi_T | e^{-(m + n - r) \bar{r} \delta r} | \Psi_T \rangle = \int d\bar{q} d\bar{p} \rho_{\bar{q}}(\bar{q}) \rho_{\bar{p}}(\bar{p}) \langle \Psi_T | e^{-\bar{m} + n - \bar{r} - \delta r} \tilde{A} e^{-\bar{r} \delta r} \tilde{B} e^{-\bar{r} \delta r} | \Psi_T \rangle \langle \tilde{A} e^{-\bar{r} \delta r} \tilde{B} e^{-\bar{r} \delta r} | \Psi_T \rangle$$

(A23)

expanding the propagators involved in (A23) we find

$$\langle \Psi_T | e^{-(m + n - r) \bar{r} \delta r} | \Psi_T \rangle = \sum_{ijkl} \langle \Psi_T | e^{-\bar{m} + n - \bar{r} - \delta r} \tilde{A} e^{-\bar{r} \delta r} \tilde{B} e^{-\bar{r} \delta r} | \Psi_T \rangle \langle \tilde{A} e^{-\bar{r} \delta r} \tilde{B} e^{-\bar{r} \delta r} | \Psi_T \rangle.$$  

(A24)

an estimator for which is precisely (23). Notice that the numerator of (A24) of the estimator (A20) involves an integration over \( n + m \) auxiliary fields configurations, whereas the denominator of (A23) involves an integration over \( n + m - r \) auxiliary fields configurations. Due to this circumstance, the weights \( \omega_k^{(n)} \), appearing in the numerator of (23) coincide with those appearing in (18), whereas at the denominator other weights \( \omega_k^{(n)} \) appear, which are constructed with a slightly modified recursion relation:

$$\omega_k^{(n)} = \begin{cases} \omega_k^{(n)} & \text{if } n - r \leq k \leq n - 1 \\ \omega_k^{(n)} \mathbb{I}[\hat{\eta}_k^{(w)} | \hat{\eta}_k^{(w)}] & \text{otherwise}. \end{cases}$$  

(A25)

**APPENDIX B: ITCF S FOR THE IDEAL FERMI GAS**

In the case of a noninteracting system, the ITCF \( F_q(\tau) \) takes the form

$$F_q(\tau) = \frac{1}{N} \langle \Psi_0 | \hat{\rho}_q(\tau) \hat{\rho}_{-q} | \Psi_0 \rangle = \frac{1}{N} \sum_{p, p', \sigma, \sigma'} \langle \Psi_0 | \hat{a}_{p', \sigma}^{\dagger} \hat{a}_{p, \sigma}(\tau) \hat{a}_{p', \sigma}^{\dagger} \hat{a}_{p, \sigma}(\tau) | \Psi_0 \rangle.$$  

(B1)

For a spin polarized system, using Heisenberg representation and Wick’s theorem, formula (B1) can be reduced to

$$F_q(\tau) = \frac{1}{N} \sum_p e^{-\tau\xi - \tau\tau - \tau} \Theta(k_F - p - q) \Theta(|p| - k_F).$$  

(B2)

Numeric evaluation of (B2) yields \( F_q(\tau) \). For \( N_T = 5, N_g = 0, r_s = 1, \) and \( q = \frac{2\pi}{\tau} (1, 0) \) the nonvanishing contributions to (B2) come from \( p = \frac{2\pi}{\tau} (1, 0), \frac{2\pi}{\tau} (0, 1), \frac{2\pi}{\tau} (0, -1) \). Consequently,

$$F_q(\tau) = \frac{e^{-\frac{2\pi}{\tau}}}{5} + \frac{2 e^{-\frac{2\pi}{\tau}}}{5}.$$  

(B3)