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Auxiliary Field Functional Integral Representation of the Many-Body Evolution Operator

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Finding an appropriate functional integral representation of the many-body evolution operator is a crucial task for performing efficient calculations of fermionic systems within the auxiliary field approach. In this paper we derive a new field representation of the imaginary-time evolution operator using the method of Gaussian equivalent representation of Efimov and Ganbold (1991, *Physica Status Solidi* **168**, 165). The goal is to obtain a functional integral representation, in which the main divergences caused by the tadpole Feynman diagrams are efficiently eliminated. These diagrams provide the main contributions to the ground state of the system under consideration, and therefore it is important to take them into account adequately, especially at lower temperatures. In addition, we show that the well-known mean field representation of the imaginary-time evolution operator is only the limiting case of the Gaussian equivalent representation in the small time-step regime.

KEY WORDS: imaginary-time many-body evolution operator; Fermion systems; auxiliary field formalism; functional integral representation.

1. INTRODUCTION

In the past decade we noticed a rapid growth of interest in methods relying on the auxiliary field functional integral approach due to their increased aptitude in treating relevant problems of physics and chemistry. In this framework the original imaginary-time many-body propagator is decomposed into a superposition of one-body propagators, which formally describe a system of noninteracting particles moving in a time-dependent auxiliary field. The resulting auxiliary field representation can then be employed to derive expectation values, which can be calculated either in an analytical or numerical way.

Actually, the numerical techniques are most promising. They have recently found first applications in quantum chemical calculations of atoms and small molecules (Baer, 2000a,b, 2001; Baer and Neuhauser, 2000; Rom *et al.*, 1997,

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1998), as well as in statistical computations of classical many-particle systems (Baeurle, 2000, 2002; Baeurle *et al.*, 2002). The goal of the so-called auxiliary field quantum Monte Carlo (AFQMC) method (Charutz and Neuhauser, 1994; Rom *et al.*, 1997, 1998; Silvestrelli *et al.*, 1993), for instance, is to compute various chemical properties of molecules, such as the ground-state energy or low-lying excited-state energies, with high accuracy at affordable computational cost. Another worthy goal, particularly useful for larger systems of fermions, is also the calculation of thermodynamic properties. It appears that in all these objectives, the imaginary-time propagator $e^{-\beta H}$ plays a key role. At small temperatures it can be utilized to project out the low energy manyfold of molecules, while at higher temperatures it can be employed to compute the thermodynamic expectation values. The basic technique (Silvestrelli *et al.*, 1993; Sugiyama and Koonin, 1986), however, suffers from a convergence problem, called the numerical sign problem, which causes a bad statistical convergence of the observable averages. To circumvent these convergence difficulties, several strategies have been conceived. The most efficient one is the shifted-contour auxiliary field quantum Monte Carlo (SC-AFQMC) method of Rom *et al*. (1997, 1998). It takes advantage of Cauchy's integral theorem to accomplish an exact transformation of the auxiliary field functional integral representation of the imaginary-time evolution operator. Recently, also a classical auxiliary field Monte Carlo (AFMC) method (Baeurle, 2000; Baeurle *et al.*, 2002) has been developed, in which similar convergence problems could be significantly reduced (Baeurle, 2002). This technique provides a framework for performing classical statistical simulations of many-particle systems within a continuum formalism, which can be particularly useful for multiscale modeling. Moreover, in the grand-canonical case it represents an alternative to standard grand-canonical Monte Carlo methods.

The auxiliary field functional integral representation also constitutes a starting point for various approximating schemes. For instance, one can derive the self-consistent mean field (MF) approximation at finite temperature (Levit, 1980) by applying the method of stationary phase. Moreover, by additionally considering time-dependent fluctuations of the auxiliary field around the MF solution in the Gaussian approximation, one can obtain the random phase approximation (Kerman *et al.*, 1983; Kerman and Levit, 1981). Besides, it is also worth mentioning that within the auxiliary field formulation one can also apply approximation schemes that are nonperturbative. One of the simplest is the static path approximation in which the integral over a time-dependent auxiliary field is reduced to one of a time-independent field (Lauritzen and Negele, 1991). Recently, new methods have also been developed to go beyond these approximations by taking into account small amplitude time-dependent fluctuations around the static value of the auxiliary field (Attias and Alhassid, 1997).

A crucial aspect of all the methods mentioned previously is to deal with an appropriate functional integral (FI) representation of the evolution operator, which

is decisive for the efficiency of the calculation and/or validity of the approximation (Baeurle, 2000, 2002). The goal of this paper is to derive an alternative exact representation of the auxiliary field functional integral of the evolution operator, which remains useful beyond the small time-step regime. For this, we employ the method of Gaussian equivalent representation (GER) of Efimov and Ganbold (1991, 1995), which has recently proven to be very effective for improving the statistical convergence of the AFMC method (Baeurle, 2002). The procedure efficiently eliminates the main divergences caused by the so-called tadpole Feynman diagrams by introducing the normal-ordered product of operators in the interaction functional. From quantum field theory we know that these diagrams provide the main contributions to the ground state of the system under consideration. As a result we accomplish the transformation

$$e^{-F} = \int \frac{\mathcal{D}\sigma}{\sqrt{\det V}} e^{-\frac{1}{2}(\sigma V^{-1}\sigma)+W_V[\sigma]} \rightarrow e^{-F_0} = \int \frac{\mathcal{D}\sigma}{\sqrt{\det D}} e^{-\frac{1}{2}(\sigma D^{-1}\sigma)+W_D[\sigma]}, \tag{1}$$

where the zero-order approximation F_0 is the best variational Gaussian estimate of the initial integral. The calculation of the perturbation corrections over W_D give us the additional contributions to the zero-order approximation

$$F = F_0 + F_1 + F_2 + \cdots. \tag{2}$$

Within this approach the Gaussian leading term takes care of all the quadratic fluctuations around the ground state and the remaining higher orders for non-Gaussian contributions, which can be calculated in an analytical or numerical way. In other words, the GER methodology gives a guidance for how to find the most optimal Gaussian functional measure for our FI and provides a regular prescription for the calculation of higher-order corrections to the lowest-order approximation.

Our paper is structured as follows. In Section 2 we review the derivation of the basic field representation of the imaginary-time evolution operator followed, in Section 3, by the derivation of the mean field representation (MFR) proposed by Rom *et al.* Then, in Section 4 we make use of the method of GER, to derive the GER of the evolution operator. In Section 5 we show by analytical approximation that the MFR of the evolution operator is only a first-order approximation of the GER. Finally, we end the paper with a discussion of the main achievements and the conclusions.

2. BASIC FIELD REPRESENTATION

To start, let us consider the imaginary-time propagator of a system of fermion particles

$$U(\beta) = \exp\{-\beta H\}, \tag{3}$$

with the Hamiltonian given by $H = E_k + E_p = (K\rho) + \frac{1}{2}(\rho V \rho)$, where $\rho(x, y) = \sum_{s=\uparrow\downarrow} = \psi_s^{\dagger}(x)\psi_s(y)$ is the electron density operator expressed in the

formalism of second quantization. The operator V is the positive Coulomb potential operator describing the electron–electron repulsion and K a one-body term, including the kinetic energy and the nuclear–electron attraction (Baer *et al.*, 1998; Rom *et al.*, 1997).

A central step of the derivation is to apply the complex Hubbard–Stratonovich (HS) transformation (Baer *et al.*, 1998)

$$e^{-\frac{1}{2}(r\Lambda r)} = C_\Lambda \int \mathcal{D}^N s e^{-\frac{1}{2}(s\Lambda s)} e^{-i(s\Lambda r)} \tag{4}$$

with $C_\Lambda = [\det(\Lambda)(2\pi)^{-N}]^{1/2}$, which replaces the calculation of the full propagator with a simpler calculation of an ensemble average of single-particle propagators; that is, the HS transformation formally substitutes the electron–electron repulsion with an electron-field interaction. For its application one makes use of the Trotter separation to break the imaginary-time propagator into a large number M of short-time propagators with time-step $\Delta\tau = \beta/M$

$$e^{-\beta H} = \lim_{M\to\infty} \left(e^{-\frac{\beta}{M}E_k} e^{-\frac{\beta}{M}E_p}\right)^M \approx e^{-E_k\Delta\tau} e^{-E_p\Delta\tau} \cdots e^{-E_k\Delta\tau} e^{-E_p\Delta\tau}.$$

Since the operator E_p is in a quadratic form with respect to the density operator ρ, we can apply the complex HS transformation (4) to each $\exp\{-E_p\Delta\tau\}$ according to

$$e^{-\frac{1}{2}(\rho V\rho)\Delta\tau} = C_V \int \mathcal{D}\sigma_{\tau_m} e^{-\frac{1}{2}(\sigma_{\tau_m} V\sigma_{\tau_m})\Delta\tau} e^{-i(\sigma_{\tau_m} V\rho)\Delta\tau}, \tag{5}$$

which provides the imaginary-time propagator in its basic field representation

$$U(\beta) = e^{-\beta H} = C_V^M \int \mathcal{D}\sigma\, e^{-\frac{1}{2}\sum_{m=1}^M(\sigma_{\tau m}V_{\sigma_{\tau m}})\Delta\tau - \sum_{m=1}^M((K+i\sigma_{\tau m})\rho)\Delta\tau}, \tag{6}$$

where $C_V = [\det(V)(\Delta\tau/2\pi))^N]^{1/2}$ and $\mathcal{D}\sigma = \prod_{m=1}^M \mathcal{D}^N\sigma_{\tau m}$ is the integration measure over all the field variables. For the sake of simplicity we here just consider ground state properties, for which one can define a pseudopartition function

$$Z(\beta, N_e) = \langle\Phi(0)|U(\beta)|\Phi(0)\rangle = \int \mathcal{D}\mu_V[\sigma]\, e^{\bar{W}_V[\sigma]}, \tag{7}$$

with the Gaussian measure $\mathcal{D}\mu_V[\sigma] = C_V^M\mathcal{D}\sigma \exp\{-\frac{1}{2}\sum_{m=1}^M(\sigma_{\tau m}V_{\sigma_{\tau m}})\Delta\tau\}$ and the interaction functional

$$\bar{W}_V[\sigma] = \ln\prod_{m=1}^M \langle\Phi(0)|e^{-(K_\rho)\Delta\tau + i(\sigma\tau_m V_\rho)\Delta\tau}|\Phi(0)\rangle, \tag{8}$$

where the initial N_e-electron wave function $|\Phi(0)\rangle$ is typically chosen as a conventional Slater-determinant. Substituting Z into the respective standard

thermodynamic relation, we finally get the desired ground state expectation value of the observable $\mathcal{O}$ with the formula

$$\langle \mathcal{O} \rangle = \lim_{\beta \to \infty} \frac{\int \mathcal{D}\mu_V[\sigma] \mathcal{O}(\sigma)\, e^{\bar{W}_V[\sigma]}}{\int \mathcal{D}\mu_V[\sigma]\, e^{\bar{W}_V[\sigma]}}. \tag{9}$$

For further details concerning the basic derivation, we refer to Rom *et al.* (1997) and Baer *et al.* (1998).

The above multidimensional integral over the field variables should now be evaluated in an analytical or numerical way. However, since the resulting integrand is complex, this is generally an unfeasible task at lower temperatures or/and large system-sizes. For instance, a straightforward use of standard MC methods is faced with the well-known sign problem due to strong oscillations of the original distribution resulting in large statistical fluctuations (Silvestrelli *et al.*, 1993; Sugiyama and Koonin, 1986).

3. MEAN FIELD REPRESENTATION

It has recently been recognized by Rom *et al.* (1997) that an alternative exact representation of the imaginary-time evolution operator is more useful in numerical application. Their strategy bases on Cauchy's integral theorem, which guarantees that the FI (7) is invariant with respect to a deformation of its integration path. It consists in shifting the contour away from the real axis to cross the domain of integration in vicinity to the imaginary stationary point corresponding to the MF solution. In cases where the largest contribution to the FI comes from the region near to this critical point a significant reduction of the fluctuations can be achieved. Rom *et al.* (1997, 1998) and Baer *et al.* (1998) found out that an overwhelming part of the sign problem is removed by taking proper account of the fermion MF contribution, which is achieved, for example, when an approximate density calculated on the Hartree–Fock level of theory is employed.

Baer *et al.* (1998) have subsequently provided a rigorous theoretical basis to this methodology. They have recognized that one properly shifts the integration contour through the imaginary stationary point, only if one makes use of the exact one-electron density. As a result one obtains the so-called MFR of the FI. For practical purposes it is however sufficient to use an approximated density of the quality mentioned previously.

To derive the MFR of Baer *et al.*, let us now consider the matrix element of the evolution operator in a single time slice $\tau \to \tau + \Delta\tau$ (Baer *et al.*, 1998),

$$Z(\beta, N_e) \propto \int \mathcal{D}\mu_V[\sigma_\tau],\ e^{\bar{W}_V[\sigma_\tau]} = Z_\tau, \tag{10}$$

where $\mathcal{D}\mu_V[\sigma_\tau] = C_V \mathcal{D}\sigma_\tau \ \exp\{-\frac{1}{2}(\sigma_\tau V \sigma_\tau)\Delta\tau\}$ and

$$\bar{W}_V[\sigma_\tau] = \ln\langle\Phi(\beta-\tau)|\, e^{-(K\rho)\Delta\tau - i(\sigma_\tau V\rho)\Delta\tau}|\Phi(\tau-\Delta\tau)\rangle. \tag{11}$$

Each short-time propagator is independently stabilized by adding a constant shift to each field σ_τ, i.e.

$$\sigma_\tau(x, y) \to \sigma_\tau(x, y) - i\alpha_\tau(x, y), \tag{12}$$

where $\alpha_\tau(x, y)$ is an arbitrary function called the shifting function. We then get

$$Z_\tau = e^{\frac{1}{2}(\alpha_\tau V \alpha_\tau)\Delta\tau} \int \mathcal{D}\mu_V[\sigma_\tau]\, e^{\bar{W}'_V[\sigma_\tau]}, \tag{13}$$

with

$$\begin{aligned}\bar{W}'_V[\sigma_\tau] = {} & \ln\langle\Phi(\beta-\tau)|e^{(K\rho)\Delta\tau - i(\sigma_\tau V\rho)\Delta\tau - (\alpha_\tau V_\rho)\Delta\tau}|\Phi(\tau-\Delta\tau)\rangle \\ & + i(\sigma_\tau V\alpha_\tau)\end{aligned} \tag{14}$$

To derive the MF solution, one has to choose the shift α_τ in such way that $\bar{W}'_V[\sigma_\tau]$ is insensitive to first-order changes in the auxiliary field σ_τ, i.e.

$$\frac{\bar{W}'_V[\sigma_\tau]}{\delta\sigma_\tau} = i(V\alpha_\tau) - i\left(V\frac{\langle\Phi(\beta-\tau)|\rho(x, y)|\Phi(\tau)\rangle}{\langle\Phi(\beta-\tau)|\Phi(\tau)\rangle}\right) = 0. \tag{15}$$

The stationary condition thus provides the following solution:

$$\alpha_\tau(x, y) = \frac{\langle\Phi(\beta-\tau)|\rho(x, y)|\Phi(\tau)\rangle}{\langle\Phi(\beta-\tau)|\Phi(\tau)\rangle}. \tag{16}$$

We note that the resulting shift α_τ is a matrix element of the exact one-electron density matrix normalized by the matrix element of the evolution operator. Under the assumption that $\beta, \tau, \beta-\tau \to \infty$, the above expression leads to

$$\alpha_\tau(x, y) = \frac{\langle\Phi_{\rm gs}|\rho(x, y)|\Phi_{\rm gs}\rangle}{\langle\Phi_{\rm gs}|\langle\Phi_{\rm gs}\rangle} = \langle\rho(x, y)\rangle_{\rm gs}, \tag{17}$$

where $\Phi_{\rm gs}$ represents the exact ground state wave function and $\langle\rho(x, y)\rangle_{\rm gs}$ the exact ground state one-electron density. Moreover, it is also worth emphasizing that $\alpha_\tau(x, y) \to \langle\rho(x, y)\rangle_{\rm gs}$ for $\beta \to \infty$ and therefore becomes independent of the time τ. Finally, substituting the shifting function in FI (13), we obtain the MFR of Z_τ.

4. GAUSSIAN EQUIVALENT REPRESENTATION

To derive the GER of the evolution operator, let us again consider the matrix element in single time slice defined in Eq. (10). For the derivation we make use of the method of GER of Efimov and Ganbold (1991, 1995), which provides an optimized representation of the FI in the strong coupling regime with the advantageous property that the influence of the oscillatory interaction functional is small

compared to the quadratic term. It is supposed that in this regime the FI remains of the Gaussian-type, but with another Green function in the measure. The technique is generally applicable to FIs of the following type:

$$I = \int \mathcal{D}\mu_{D_0}[\varphi]\, \exp\{g W_{D_0}[\varphi]\}, \tag{18}$$

where g is the coupling constant and

$$W_{D_0}[\varphi] = \int d\nu_a\, e^{i(a\varphi)} \tag{19}$$

is the interaction functional with $d\nu_a$ as the functional measure and $(a\varphi) = \int dy\, a(y)\varphi(y)$. The Gaussian measure $\mathcal{D}\mu_{D_0}[\varphi] = C_{D_0}\mathcal{D}\varphi\, \exp\{-\frac{1}{2}(\varphi D_0^{-1}\varphi)\}$ is normalized in such a way that $\int \mathcal{D}\mu_{D_0}[\varphi]\cdot 1 = 1$. We can easily reformulate the FI (10) in the form of (18) by performing the substitution $\sigma_\tau = (\Delta t)^{-1/2}(V^{-1}\sigma'_\tau)$ and immediately dropping the prime. We then get

$$Z_\tau = \int \mathcal{D}\mu_V[\sigma_\tau] e^{\bar{W}_V[\sigma_\tau]}, \tag{20}$$

where $\mathcal{D}\mu_V[\sigma_\tau] = C'_V\, \exp\{-\frac{1}{2}(\sigma_\tau V^{-1}\sigma_\tau)\}$ with $C'_V = [\det(V)(2\pi)^N]^{-1/2}$ and

$$\bar{W}_V[\sigma_\tau] = \ln\langle\Phi(\beta-\tau)|\, e^{-(K\rho)\Delta\tau - i(\sigma_\tau\rho)\sqrt{\Delta\tau}}|\Phi(\tau-\Delta\tau)\rangle. \tag{21}$$

We subsequently expand the functional $\bar{W}_V$ in a Taylor series (Parr and Yang, 1998)

$$\begin{aligned}\bar{W}_V[\sigma_\tau] &= \bar{W}_V[\sigma_\tau = 0] \\ &\quad + \sum_{n=1}^{\infty}\frac{1}{n!}\int\int\cdots\int\left(\frac{\delta^{\{n\}}\bar{W}_V[\sigma_\tau]}{\delta\sigma_\tau(x_1,y_1)\delta\sigma_\tau(x_2,y_2)\cdots\delta\sigma_\tau(x_n,y_n)}\right)_{\sigma_\tau=0} \\ &\quad \times \sigma_\tau(x_1,y_1)\sigma_\tau(x_2,y_2)\cdots\sigma_\tau(x_n,y_n)\, dx_1\, dx_2\cdots dx_n\, dy_1\, dy_2\cdots dy_n,\end{aligned} \tag{22}$$

and then define the interaction functional as

$$W_V[\sigma_\tau] = \bar{W}_V[\sigma_\tau] - \bar{W}_V[\sigma_\tau = 0] = \int dx_1\, dy_1\, J[\sigma_\tau(x_1,y_1)] \tag{23}$$

with

$$\begin{aligned}J[\sigma_\tau(x_1,y_1)] &= \sum_{n=1}^{\infty}\frac{1}{n!}\int\cdots\int\left(\frac{\delta^{\{n\}}\bar{W}_V[\sigma_\tau]}{\delta\sigma_\tau(x_1,y_1)\delta\sigma_\tau(x_2,y_2)\cdots\delta\sigma_\tau(x_n,y_n)}\right)_{\sigma_\tau=0} \\ &\quad \times \sigma_\tau(x_1,y_1)\sigma_\tau(x_2,y_2)\cdots\sigma_\tau(x_n,y_n)\, dx_2\cdots dx_n\, dy_2\cdots dy_n.\end{aligned} \tag{24}$$

Solving Eq. (23) for $\bar{W}_V[\sigma_\tau]$ and inserting it in Eq. (10), we get

$$Z_\tau = e^{\bar{W}_V[\sigma_\tau=0]} \int \mathcal{D}\mu_V[\sigma_\tau]\, e^{W_V[\sigma_\tau]}, \tag{25}$$

where

$$\bar{W}_V[\sigma_\tau = 0] = \ln\langle \Phi(\beta - \tau)|\, e^{-(K\rho)\Delta\tau} |\Phi(\tau - \Delta\tau)\rangle. \tag{26}$$

We see that one recovers the integral representation (18), if one rewrites $W_V[\sigma_\tau]$ in form of expression (19). This is achieved by reformulating $J[\sigma_\tau(x_1, y_1)]$ in terms of its Fourier transform

$$J[\sigma_\tau(x_1, y_1)] = \int \frac{dk}{2\pi}\, \tilde{J}(k)\, e^{i(k\sigma_\tau)} \tag{27}$$

with

$$(k\sigma_\tau) = \int dx_1'\, dy_1'\, k\delta(x_1 - x_1'; y_1 - y_1')\sigma_\tau(x_1', y_1'), \tag{28}$$

where the functional measure $dx_1\, dy_1\, dk/(2\pi)\, \tilde{J}(k) = d\nu_a = d\nu_k$. Next, we perform a parallel shift of the integration contour of FI (25) along the real axis

$$\sigma_\tau(x, y) \to \sigma_\tau(x, y) - i\alpha_\tau(x, y) \tag{29}$$

and replace its Gaussian weight according to

$$V^{-1}(x, y; x', y') \to D^{-1}(x, y; x', y'), \tag{30}$$

where $D(x, y; x', y')$ is an appropriate Green function of the differential operator D^{-1} satisfying the relation

$$\int dy\, dy'\, D^{-1}(x, x'; y, y')D(y, y'; z, z') = \delta(x - z)\delta(x' - z'). \tag{31}$$

The FI (25) then takes the form

$$Z_\tau = \sqrt{\frac{\det D}{\det V}}\, \exp\left\{\frac{1}{2}(\alpha_\tau V^{-1}\alpha_\tau)\right\}\, e^{\bar{W}_V[\sigma_\tau=0]} \int \mathcal{D}\mu_D[\sigma_\tau]\, e^{W_D'[\sigma_\tau,\alpha_\tau,D]}, \tag{32}$$

where

$$W_D'[\sigma_\tau, \alpha_\tau, D] = W_V[\sigma_\tau - i\alpha_\tau] + i(\alpha_\tau V^{-1}\sigma_\tau) - \frac{1}{2}(\sigma_\tau[V^{-1} - D^{-1}]\sigma_\tau) \tag{33}$$

and $\mathcal{D}\mu_D[\sigma_\tau] = C_D\mathcal{D}\sigma_\tau\, \exp\{\frac{1}{2}(\sigma_\tau D^{-1})\}$ obeying the normalization condition $\int \mathcal{D}\mu_D[\sigma_\tau] \cdot 1 = 1$.

From quantum field theory we know that the tadpole Feynman diagrams provide the main quantum contributions to the ground state of the system under consideration (Efimov and Ganbold, 1995). Since with growing β its influence becomes more significant, it is important to take them into account in an adequate

way. In quantum theory the main divergences caused by these diagrams are efficiently eliminated from consideration if the normal-ordered product of operators is introduced in the interaction Hamiltonian. According to this strategy, the interaction functional in (32), W'_D, must be reformulated in normal-ordered form. For this, we make use of the concept of the normal product according to the given Gaussian measure $\mathcal{D}\mu_D$, in the following way:

$$\begin{aligned} e^{i(k\sigma_\tau)} &=: e^{i(k\sigma_\tau)} : e^{-\frac{1}{2}k^2 \int dx'_1\, dy'_1\, dx''_1\, dy''_1\, \sigma(x_1-x'_1;y_1-y'_1)D(x'_1,y'_1;x''_1,y''_1)\sigma(x_1-x''_1;y_1-y''_1)} \\ &=: e^{i(k\sigma_\tau)} : e^{-\frac{1}{2}k^2 D(x_1,y_1;x_1,y_1)}. \end{aligned} \tag{34}$$

so that:

$$\int \mathcal{D}\mu_D[\sigma_\tau] : e^{i(k\sigma_\tau)} := 1, \qquad \int \mathcal{D}\mu_D[\sigma_\tau] : \sigma_\tau(x_1, y_1)\cdots\sigma_\tau(x_n, y_n) := 0. \tag{35}$$

If we take into account that $e^z = 1 + z + z^2/2 + e_2^z$ and insert this relation in Eq. (34), we obtain

$$\begin{aligned} e^{i(k\sigma_\tau)} &=: 1 + i(k\sigma_\tau) - \frac{1}{2}(k\sigma_\tau)^2 + e_2^{i(k\sigma_\tau)} : e^{-\frac{1}{2}k^2 D(x_1,y_1;x_1,y_1)} \\ &= e^{-\frac{1}{2}k^2 D(x_1,y_1;x_1,y_1)} + i\, e^{-\frac{1}{2}k^2 D(x_1,y_1;x_1,y_1)}(k\sigma_\tau) \\ &\quad - \frac{1}{2} : (k\sigma_\tau)^2 : e^{-\frac{1}{2}k^2 D(x_1,y_1;x_1,y_1)} + : e_2^{i(k\sigma_\tau)} : e^{-\frac{1}{2}k^2 D(x_1,y_1;x_1,y_1)}. \end{aligned} \tag{36}$$

Introducing Eq. (36) in the functional

$$W'_D[\sigma_\tau, \alpha_\tau, D] = \int d\nu_k\, e^{(k\alpha_\tau)}\, e^{i(k\alpha_\tau)} + i(\alpha_\tau V^{-1}\sigma_\tau) - \frac{1}{2}(\sigma_\tau[V^{-1} - D^{-1}]\sigma_\tau), \tag{37}$$

we obtain

$$\begin{aligned} W'_D[\sigma_\tau, \alpha_\tau, D] = \int d\nu_k\, e^{(k\alpha_\tau)} \Big[& e^{-\frac{1}{2}k^2 D(x_1,y_1;x_1,y_1)} \\ & + i\, e^{-\frac{1}{2}k^2 D(x_1,y_1;x_1,y_1)}(k\sigma_\tau) - \frac{1}{2} : (k\sigma_\tau)^2 : e^{-\frac{1}{2}k^2 D(x_1,y_1;x_1,y_1)} \\ & + : e_2^{i(k\sigma_\tau)} : e^{-\frac{1}{2}k^2 D(x_1,y_1;x_1,y_1)} \Big] + i(\alpha_\tau V^{-1}\sigma_\tau) \\ & - \frac{1}{2}(\sigma_\tau[V^{-1} - D^{-1}]\sigma_\tau). \end{aligned} \tag{38}$$

Afterwards, ordering the terms of the functional in powers of σ_τ, this results in

$$W'_D[\sigma_\tau, \alpha_\tau, D] = \int d\nu_k\, e^{(k\alpha_\tau)}\, e^{-\frac{1}{2}k^2 D(x_1,y_1;x_1,y_1)}$$

$$+\left[i\int d\nu_k\, e^{(k\alpha_\tau)}\, e^{-\frac{1}{2}k^2 D(x_1,y_1;x_1,y_1)}(k\sigma_\tau)+i(\alpha_\tau V^{-1}\sigma_\tau)\right]$$

$$-\frac{1}{2}\left[:\int d\nu_k\, e^{(k\alpha_\tau)}\, e^{-\frac{1}{2}k^2 D(x_1,y_1;x_1,y_1)}(k\sigma_\tau)^2:\right.$$

$$\left.+(\sigma_\tau[V^{-1}-D^{-1}]\sigma_\tau)\right]+\int d\nu_k\, e^{(k\alpha_\tau)}\, e^{-\frac{1}{2}k^2 D(x_1,y_1;x_1,y_1)}$$

$$\times\ :e_2^{i(k\sigma_\tau)}:. \tag{39}$$

The concept of the normal product implies that

$$\sigma_\tau(x,y)\sigma_\tau(x',y')=:\sigma_\tau(x,y)\sigma_\tau(x',y'):+D(x,y;x',y'), \tag{40}$$

which permits to reformulate the quadratic term in σ_τ

$$W'_D[\sigma_\tau,\alpha_\tau,D]=\left[\int d\nu_k\, e^{(k\alpha_\tau)}\, e^{-\frac{1}{2}k^2 D(x_1,y_1;x_1,y_1)}-\frac{1}{2}([V^{-1}-D^{-1}]D)\right]$$

$$+\left[i\int d\nu_k\, e^{(k\alpha_\tau)}\, e^{-\frac{1}{2}k^2 D(x_1,y_1;x_1,y_1)}(k\sigma_\tau)+i(\alpha_\tau V^{-1}\sigma_\tau)\right]$$

$$-\frac{1}{2}:\left[\int d\nu_k\, e^{(k\alpha_\tau)}\, e^{-\frac{1}{2}k^2 D(x_1,y_1;x_1,y_1)}(k\sigma_\tau)^2\right.$$

$$\left.+\ (\sigma_\tau[V^{-1}-D^{-1}]\sigma_\tau)\right]:+\int d\nu_k\, e^{(k\alpha_\tau)}\, e^{-\frac{1}{2}k^2 D(x_1,y_1;x_1,y_1)}$$

$$\times\ :e_2^{i(k\sigma_\tau)}:. \tag{41}$$

Now, we demand that the linear and quadratic terms in the integration variable $\sigma_\tau(x,y)$ should be absent in the interaction functional W'_D in (41). These two conditions provide us with the GER equations:

$$i\int d\nu_k\, e^{(k\alpha_\tau)}\, e^{-\frac{1}{2}k^2 D(x_1,y_1;x_1,y_1)}(k\sigma_\tau)+i(\alpha_\tau V^{-1}\sigma_\tau)=0, \tag{42}$$

$$\int d\nu_k\, e^{(k\alpha_\tau)}\, e^{-\frac{1}{2}k^2 D(x_1,y_1;x_1,y_1)}(k\sigma_\tau)^2+(\sigma_\tau[V^{-1}-D^{-1}]\sigma_\tau)=0,$$

which after rearrangement give vs, respectively, an equation for the shift $\alpha_\tau(x,y)$ and the new Gaussian weight $D(x,y;x',y')$:

$$\alpha_\tau(x,y)=-\int dx'\,dy'\,V(x',y';x,y)J_1[\alpha_\tau(x',y')], \tag{43}$$

$$D(x,y;x',y')=V(x,y;x',y')-\int dx''\,dy''\,V(x'',y'';x',y')$$

$$\times J_2[\alpha_\tau(x'',y'')]D(x,y;x'',y''), \tag{44}$$

where

$$J_1[\alpha_\tau(x,y)] = \int \frac{dk}{2\pi} k\tilde{J}(k)\, e^{-\frac{1}{2}k^2 D(x,y;x,y)}\, e^{(k\alpha_\tau)}, \tag{45}$$

$$J_2[\alpha_\tau(x,y)] = \int \frac{dk}{2\pi} k^2\tilde{J}(k)\, e^{-\frac{1}{2}k^2 D(x,y;x,y)}\, e^{(k\alpha_\tau)}, \tag{46}$$

As a result we obtain a new exact field representation of the imaginary-time evolution operator, i.e. the so-called GER

$$Z_\tau = e^{-F_0} \int d\mu_D[\sigma_\tau]\, e^{W_D[\sigma_\tau]}, \tag{47}$$

where

$$W_D[\sigma_\tau] = \int d\nu_k\, e^{(k\alpha_\tau)}\, e^{-\frac{1}{2}k^2 D(x_1,y_1;x_1,y_1)} : e_2^{i(k\sigma_\tau)} : \tag{48}$$

is the new interaction functional and

$$F_0 = -\frac{1}{2}\ln\det\left(\frac{D}{V}\right) - \frac{1}{2}(\alpha_\tau V^{-1}\alpha_\tau) + \frac{1}{2}([V^{-1} - D^{-1}]D) - \int d\nu_k\, e^{(k\alpha_\tau)} e^{-\frac{1}{2}k^2 D(x_1,y_1;x_1,y_1)} \tag{49}$$

the zero-order approximation of Z_τ. Since the exponential within the double dots in Eq. (48) now only contains terms of higher order than two, we can expect that the new FI formulation is more suitable for numerical and analytical calculation than the original one.

5. FIRST-ORDER APPROXIMATION OF THE SHIFTING FUNCTION

To derive the first-order approximation of the shifting function, we consider the functional expression (45),

$$J_1[\alpha_\tau(x,y)] = \int \frac{dk}{2\pi} k\tilde{J}(k)\, e^{-\frac{1}{2}k^2 D(x,y;x,y)}\, e^{(k\alpha_\tau)}, \tag{50}$$

in which $k\tilde{J}(k)$ can be written as (for further details, see Appendix A)

$$k\tilde{J}(k) = \frac{1}{i}\int d\tilde{\alpha}_\tau \int dx'\, dy'\, \frac{\delta J[\tilde{\alpha}_\tau(x,y)]}{\delta\tilde{\alpha}_\tau(x',y')}\, \exp[-i(k\tilde{\alpha}_\tau)], \tag{51}$$

with

$$J[\tilde{\alpha}_\tau(x,y)] = \sum_{n=1}^{\infty}\frac{1}{n!}\int\cdots\int\left(\frac{\delta^{\{n\}}\bar{W}_V[\sigma_\tau]}{\delta\sigma_\tau(x,y)\delta\sigma_\tau(x_2,y_2)\cdots\delta\sigma_\tau(x_n,y_n)}\right)_{\sigma_\tau=0} \times\tilde{\alpha}_\tau(x,y)\tilde{\alpha}_\tau(x_2,y_2)\cdots\tilde{\alpha}_\tau(x_n,y_n)dx_2\cdots dx_n\, dy_2\cdots dy_n. \tag{52}$$

It can easily be shown that the nth-order functional derivative is proportional to $(\Delta t)^{n/2}$. Therefore, truncating the functional $J[\tilde{\alpha}_\tau(x, y)]$ at low order is a reasonable approximation of the GER shifting function for small Δt. Here we truncate the functional at first order and obtain

$$J[\tilde{\alpha}_\tau(x, y)] \approx \left(\frac{\delta^1 \bar{W}_V[\sigma_\tau]}{\delta\sigma_\tau(x, y)}\right)_{\sigma_\tau=0} \tilde{\alpha}_\tau(x, y), \tag{53}$$

where

$$\bar{W}_V[\sigma_\tau] = \ln\langle\Phi(\beta - \tau)|\, e^{-(K\rho)\Delta t - i(\sigma_\tau\rho)\sqrt{\Delta t}}|\Phi(\tau - \Delta t)\rangle, \tag{54}$$

which provides the first-order derivative

$$\begin{aligned}\left(\frac{\delta^1 \bar{W}_V[\sigma_\tau]}{\delta\sigma_\tau(x, y)}\right)_{\sigma_\tau=0} &= -i\sqrt{\Delta t}\frac{\langle\Phi(\beta - \tau)|\rho(x, y)\, e^{-(K\rho)\Delta t - i(\sigma_\tau\rho)\sqrt{\Delta t}}|\Phi(\tau - \Delta t)\rangle}{\langle\Phi(\beta - \tau)|\, e^{-(K\rho)\Delta t - i(\sigma_\tau\rho)\sqrt{\Delta t}}|\Phi(\tau - \Delta t)\rangle} \\ &= -i\sqrt{\Delta t}\frac{\langle\Phi(\beta - \tau)|\rho(x, y)|\Phi(\tau)\rangle}{\langle\Phi(\beta - \tau)|\Phi(\tau)\rangle}.\end{aligned} \tag{55}$$

Introducing expression (53) into expression (51), we approximately get for $k\tilde{J}(k)$

$$k\tilde{J}(k) \approx \frac{1}{i}\left(\frac{\delta^1 \bar{W}_V[\sigma_\tau]}{\delta\sigma_\tau(x, y)}\right)_{\sigma_\tau=0} \int d\tilde{\alpha}_\tau\, \exp[-i(k\tilde{\alpha}_\tau)]. \tag{56}$$

Then, inserting the above expression into the functional $J_1[\alpha_\tau(x, y)]$, we obtain its first-order approximant

$$J_1^{(1)}(x, y) = \frac{1}{i}\left(\frac{\delta^1 \bar{W}_V[\sigma_\tau]}{\delta\sigma_\tau(x, y)}\right)_{\sigma_\tau=0} \int d\tilde{\alpha}_\tau \int \frac{dk}{2\pi}\, e^{-\frac{1}{2}k^2 D^{(1)}(x,y;x,y)k^2 + [(\alpha_\tau) - i(\tilde{\alpha}_\tau)]k}. \tag{57}$$

where $D^{(1)}(x, y; x, y) = V(x, y; x, y) > 0$ (see also Appendix B).

For the explicit evaluation of integral (57) we use the following Gaussian integral relation (Gröbner and Hofreiter, 1966)

$$\int_{-\infty}^{\infty} \exp[-(ax^2 + 2bx + c)]\, dx = \sqrt{\frac{\pi}{a}}\, \exp\left[\frac{b^2 - ac}{a}\right] \tag{58}$$

with $a > 0$, which leads to

$$\begin{aligned}J_1^{(1)}(x, y) = \frac{1}{i}\left(\frac{\delta^1 \bar{W}_V[\sigma_\tau]}{\delta\sigma_\tau(x, y)}\right)_{\sigma_\tau=0} \frac{1}{2\pi} \int d\tilde{\alpha}_\tau \sqrt{\frac{2\pi}{V(x, y; x, y)}} \\ \times \exp\left[\frac{[(\alpha_\tau - i(\tilde{\alpha}_\tau)]^2}{2V(x, y; x, y)}\right]\end{aligned}$$

$$= \frac{1}{i}\left(\frac{\delta^1 \bar{W}_V[\sigma_\tau]}{\delta\sigma_\tau(x,y)}\right)_{\sigma_\tau=0}\sqrt{\frac{1}{2\pi V(x,y;x,y)}}$$
$$\times \int d\tilde{\alpha}_\tau \exp\left[\frac{(\alpha_\tau)^2 - 2i(\alpha_\tau)(\tilde{\alpha}_\tau) - (\tilde{\alpha}_\tau)^2}{2V(x,y;x,y)}\right]. \quad (59)$$

Performing the remaining Gaussian integral with the integral relation (58), we finally get for the first-order approximant of $J_1(x,y)$

$$J_1^{(1)}(x,y) = \frac{1}{i}\left(\frac{\delta^1 \bar{W}_V[\sigma_\tau]}{\delta\sigma_\tau(x,y)}\right)_{\sigma_\tau=0} = -\sqrt{\Delta t}\frac{\langle\Phi(\beta-\tau)|\rho(x,y)|\Phi(\tau)\rangle}{\langle\Phi(\beta-\tau)|\Phi(\tau)\rangle}. \quad (60)$$

The first-order approximant of the GER shifting function is thus given by

$$\alpha_\tau^{(1)}(x,y) = \sqrt{\Delta t}\int dx'\,dy'\,V(x',y';x,y)\frac{\langle\Phi(\beta-\tau)|\rho(x',y')|\Phi(\tau)\rangle}{\langle\Phi(\beta-\tau)|\Phi(\tau)\rangle}, \quad (61)$$

or alternatively by

$$\alpha_\tau'^{(1)}(x,y) = \frac{\langle\Phi(\beta-\tau)|\rho(x,y)|\Phi(\tau)\rangle}{\langle\Phi(\beta-\tau)\mid\Phi(\tau)\rangle}, \quad (62)$$

under the assumption of the substitution $\alpha'_\tau = (V^{-1}\alpha_\tau)/\sqrt{\Delta t}$.

6. DISCUSSION AND CONCLUSIONS

By analyzing expression (62), we see that it is identical to the shifting function used by Baer *et al.*, i.e., expression (16). Therefore, we can conclude that their result is only a first-order approximation of the GER methodology, which becomes a valuable approximation of the exact GER shifting function for small Δt. It also demonstrates that the GER methodology is the underlying theory containing the MFR approach as a limiting case.

In conclusion, the above derivation provides a strong indication that the GER is a more useful representation for analytical and numerical calculation than previously proposed representations. Currently, work is in progress employing the methodology in conjuction with the AFQMC method in quantum chemical applications (Baeurle *et al.*, in preparation).

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APPENDIX A

To derive an explicit expression for $k\,\tilde{J}(k)$, let us consider the Fourier representation of $J[\alpha_\tau(x, y)]$,

$$J[\alpha_\tau(x, y)] = \int \frac{dk}{2\pi}\,\tilde{J}(k)\,e^{i(k\alpha_\tau)}. \tag{A1}$$

By taking the functional derivative with respect to α_τ and integrating over the variables x' and y', we get

$$\begin{aligned}\int dx'\,dy'\frac{\delta J[\alpha_\tau(x, y)]}{\delta\alpha_\tau(x', y')} &= i\int \frac{dk}{2\pi}k\tilde{J}(k)\int dx'\,dy'\delta(x - x'; y - y')\,e^{i(k\alpha_\tau)}\\ &= i\int \frac{dk}{2\pi}k\tilde{J}(k)\,e^{i(k\alpha_\tau)}.\end{aligned} \tag{A2}$$

Then, multiplying the equation with $\exp[-i(k\alpha_\tau)]$ and integrating over α_τ, this results in

$$\begin{aligned}\int d\alpha_\tau\int dx'\,dy'\frac{\delta J[\alpha_\tau(x, y)]}{\delta\alpha_\tau(x', y')}\,\exp[-i(k\alpha_\tau)] &= i\int d\alpha_\tau\int \frac{dk'}{2\pi}k'\,\tilde{J}(k')\,e^{i([k'-k]\alpha_\tau)}\\ &= ik\tilde{J}(k).\end{aligned}$$

where we have taken into account that the integral on the right-hand side is the Fourier representation of the δ-function.

Next, we wish to derive an explicit expression for $k^2\tilde{J}(k)$. To this end, we take the second-order functional derivative with respect to α_τ and integrate over the variables x', y' and x'', y''. Then, we obtain

$$\begin{aligned}&\int dx'\,dy'\,dx''\,dy''\frac{\delta J[\alpha_\tau(x, y)]}{\delta\alpha_\tau(x', y')\delta\alpha_\tau(x'', y'')}\\ &\quad= -\int \frac{dk}{2\pi}k^2\,\tilde{J}(k)\int dx'\,dy'\,dx''dy''\delta(x - x'; y - y')\\ &\quad\times\delta(x - x''; y - y'')\,e^{i(k\alpha_\tau)} = -\int \frac{dk}{2\pi}k^2\,\tilde{J}(k)\,e^{i(k\alpha_\tau)}.\end{aligned} \tag{A3}$$

We subsequently multiply the equation with $\exp[-i(k\alpha_\tau)]$ and integrate over α_τ, which finally gives

$$\begin{aligned}&\int d\alpha_\tau\int dx'\,dy'\,dx''\,dy''\frac{\delta J[\alpha_\tau(x, y)]}{\delta\alpha_\tau(x', y')\delta\alpha_\tau(x'', y'')}\,\exp[-i(k\alpha_\tau)]\\ &\quad= -\int d\alpha_\tau\int \frac{dk'}{2\pi}k'^2\,\tilde{J}(k')\,e^{i([k'-k]\alpha_\tau)} = -k^2\,\tilde{J}(k).\end{aligned} \tag{A4}$$

APPENDIX B

To perform the integration, we must ensure that the first-order approximant $D^{(1)}$ of the new Gaussian weight D is positive. For this, let us consider the functional (46)

$$J_2[\alpha_\tau(x, y)] = \int \frac{dk}{2\pi} k^2 \tilde{J}(k)\, e^{-\frac{1}{2}k^2 D(x,y;x,y)}\, e^{(k\alpha_\tau)}, \tag{B1}$$

where $k^2 \tilde{J}(k)$ can be explicitely expressed as (see Appendix A)

$$k^2 \tilde{J}(k) = -\int d\tilde{\alpha}_\tau \int dx'\, dy'\, dx''\, dy'' \frac{\delta J[\tilde{\alpha}_\tau(x, y)]}{\delta\tilde{\alpha}_\tau(x', y')\delta\tilde{\alpha}_\tau(x'', y'')} \exp[-i(k\tilde{\alpha}_\tau)]. \tag{B2}$$

By introducing the first-order approximant of $J[\tilde{\alpha}_\tau(x, y)]$, i.e. expression (53), into expression (B2), it can easily be demonstrated that $J_2^{(1)}(x, y) \approx 0$, because

$$\int \frac{\delta J[\tilde{\alpha}_\tau(x, y)]}{\delta\tilde{\alpha}_\tau(x', y')\delta\tilde{\alpha}_\tau(x'', y'')} dx'\, dy'\, dx''\, dy'' \approx 0, \tag{B3}$$

and therefore

$$D^{(1)}(x, y; x', y') = V(x, y; x', y'). \tag{B4}$$

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