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On a new formulation of the real-time propagator

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The development of theoretical tools for the study of dynamical phenomena of many-particle systems on the quantum level is a fundamental challenge since many decades. A lot of efforts have been invested on Feynman's path integral approach, however, no computationally tractable method for investigating realistic systems could be developed up to now. In this paper we propose an alternative representation of the real-time many-body evolution operator formulated within the framework of the auxiliary field formalism. Our goal is to derive a new auxiliary field functional integral representation, in which the large oscillations of the functional integrand are reduced, in order to render the auxiliary field approach more attractive for real-time computation. This objective is attained using a generalized version of the method of Gaussian equivalent representation of Efimov and Ganbold [Phys. Stat. Sol. 168 (1991) 165], which eliminates the low-order fluctuations of the auxiliary field from the interaction functional.

KEY WORDS: real-time propagator, auxiliary functional integral formalism, quantum dynamics

1. Introduction

The detailed understanding of dynamical phenomena represents an outstanding challenge in many areas of modern science and technology. In the last few years we could in particular witness a fast development of experimental techniques, which now allow us to investigate the dynamics of chemical reactions at the molecular scale and at very short time. On the theoretical level several methods have also been devised. Most of them are based on schemes [1–3] approximating the real-time propagator $\exp\{-i\widehat{H}(t_f - t_i)/\hbar\}$ formulated within Feynman's path integral approach [4]. Extensive efforts have also been devoted to calculate the exact real-time propagator using specific numerical integration techniques [5]. However, their success has so far been limited due to various numerical difficulties caused by strong oscillations of the complex integrand

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at longer propagation times. Though some progress has been made in circumventing this problem [6,7], there is as yet no satisfactory solution [8].

In this paper we propose an alternative approach to the real-time case by deriving the Gaussian equivalent representation (GER) of the many-body evolution operator within the framework of the auxiliary field functional integral formalism [9]. The goal is to devise a new auxiliary field representation, in which the main contributions to the functional integral (FI) are concentrated in a new Gaussian measure. In this way we aim to reduce the large oscillations of the functional integrand, which so far limit the usefulness of the auxiliary field approach for real-time computation. For the derivation we use the method of Gaussian equivalent representation of Efimov and Ganbold [10], which relies on the concept of normal-ordering developed in quantum field theory. It is a general prescription for finding an appropriate Gaussian measure of a FI in the strong coupling regime. The procedure efficiently removes the main divergences caused by the so-called tadpole Feynman diagrams by introducing the concept of normal product with respect to the new Gaussian measure in the interaction functional. This is of particular importance, since these diagrams are known to provide the main contributions to the FI under consideration. As a result we obtain a new exact FI representation of the evolution operator, in which the influence of the oscillatory interaction functional is significantly reduced in comparison to the quadratic term, and which consequently should be more suitable for analytical and numerical evaluation.

The GER technique has already been proven useful in classical statistical mechanical simulations of many-particle systems [11–14] and in several analytical calculations of quantum-mechanical applications [10]. In the small time-step regime it can be shown to shift the contour of integration through the mean field (MF) point of the FI providing the so-called mean field representation (MFR) [15]. In this range the GER technique has already been applied to the auxiliary field functional integral formulation of the imaginary-time evolution operator and has been found to be very efficient in numerical calculations of ground state properties of small and medium-sized molecules [16–18]. In particular, it has also been employed for the analytical computation of various quantities within the imaginary-time formulation of Feynman's path integral approach [10,19,20]. However, within this approach the GER technique cannot be trivially extended to the real time case. In this paper we show that this can be done within the auxiliary field functional integral formalism. Moreover, we generalize the GER technique for the treatment of interaction functionals which are nonlocal in the auxiliary field function.

The balance of the paper is the following. In section 2 we briefly review the basic derivation of the auxiliary field functional integral formulation of the many-body evolution operator in real time. Then, in section 3 we derive its Gaussian equivalent representation using the method of Efimov and Ganbold. Finally, we end the paper with conclusions and a brief outlook.

2. Basic field representation

Let us begin by considering the real-time propagator of a system of fermion particles [9]

$$\widehat{U}(t_\mathrm{f}-t_\mathrm{i}) = \exp\left\{-\frac{\mathrm{i}}{\hbar}(t_\mathrm{f}-t_\mathrm{i})\widehat{H}\right\} \tag{1}$$

with the Hamiltonian given by $\widehat{H} = \widehat{E}_\mathrm{k} + \widehat{E}_\mathrm{p} = (K\hat{\rho}) + \frac{1}{2}(\hat{\rho}V\hat{\rho})$, where $\hat{\rho}(\mathbf{x},\mathbf{y}) = \sum_{s=\uparrow\downarrow}\hat{\psi}_s^\dagger(\mathbf{x})\hat{\psi}_s(\mathbf{y})$ is the electron density operator expressed in the formalism of second quantization. The operator V is the positive Coulomb potential operator, $V(\mathbf{x},\mathbf{y};\mathbf{x}',\mathbf{y}') = e^2[\delta(\mathbf{x}-\mathbf{y})\delta(\mathbf{x}'-\mathbf{y}')]/|\mathbf{x}-\mathbf{x}'|$, describing the electron–electron repulsion and K a one-body term including the kinetic energy and the nuclear–electron attraction w, i.e., $K(\mathbf{x},\mathbf{y}) = \delta(\mathbf{x}-\mathbf{y})[-1/(2m_\mathrm{e})\boldsymbol{\nabla}_\mathbf{x}^2 + w(\mathbf{x})]$. A central step of the derivation is to introduce the auxiliary fields by employing the complex Hubbard–Stratonovich (HS) transformation [9],

$$\mathrm{e}^{-1/2\mathrm{i}c(r\Lambda r)} = C_\Lambda \int \mathcal{D}^N s\, \mathrm{e}^{-1/2(s\Lambda^{-1}s)}\, \mathrm{e}^{-\mathrm{i}\sqrt{\mathrm{i}}\sqrt{c}(sr)} \tag{2}$$

with $C_\Lambda = [\det(\Lambda)(2\pi)^N]^{-1/2}$ and c a positive constant. In this way one formally replaces the calculation of the full propagator with a simpler calculation of an ensemble average of single-particle propagators. For its application, one makes use of the Trotter separation,

$$\begin{aligned}\mathrm{e}^{-\mathrm{i}/\hbar(t_\mathrm{f}-t_\mathrm{i})\widehat{H}} &= \lim_{M\to\infty}\left(\mathrm{e}^{-\mathrm{i}/\hbar(t_\mathrm{f}-t_\mathrm{i})/M\widehat{E}_\mathrm{k}}\,\mathrm{e}^{-\mathrm{i}/\hbar(t_\mathrm{f}-t_\mathrm{i})/M\widehat{E}_\mathrm{p}}\right)^M \\ &\approx \mathrm{e}^{-\mathrm{i}/\hbar\widehat{E}_\mathrm{k}\Delta t}\,\mathrm{e}^{-\mathrm{i}/\hbar\widehat{E}_\mathrm{p}\Delta t}\cdots\mathrm{e}^{-\mathrm{i}/\hbar\widehat{E}_\mathrm{k}\Delta t}\,\mathrm{e}^{-\mathrm{i}/\hbar\widehat{E}_\mathrm{p}\Delta t},\end{aligned} \tag{3}$$

to break the real-time propagator into a large number M of short-time propagators with time-step $\Delta t = (t_\mathrm{f}-t_\mathrm{i})/M$. Since the operator $\widehat{E}_\mathrm{p}$ is in a quadratic form with respect to the density operator $\hat{\rho}$, we can apply the complex HS transformation to each $\exp\{-\mathrm{i}/\hbar\widehat{E}_\mathrm{p}\Delta t\}$, which provides the real-time propagator in its basic field representation

$$\begin{aligned}\widehat{U}(t_\mathrm{f}-t_\mathrm{i}) &= \mathrm{e}^{-\mathrm{i}/\hbar(t_\mathrm{f}-t_\mathrm{i})\widehat{H}} \\ &= C_V^M \int \mathcal{D}\sigma\, \mathrm{e}^{-1/2\sum_{m=1}^M(\sigma_{t_m}V\sigma_{t_m}) - \mathrm{i}\sum_{m=1}^M(K\hat{\rho})\Delta t/\hbar - \mathrm{i}\sqrt{\mathrm{i}}\sum_{m=1}^M(\sigma_{t_m}\hat{\rho})\sqrt{\Delta t/\hbar}},\end{aligned} \tag{4}$$

where $C_V = [\det(V)(2\pi)^N]^{-1/2}$ and $\mathcal{D}\sigma = \prod_{m=1}^M \mathcal{D}^N\sigma_{t_m}$ is the integration measure over all the field variables. The transition amplitude for some given initial state at time t_i and final state at time t_f is thus given by

$$\left\langle\Phi(t_\mathrm{f})\middle|\widehat{U}(t_\mathrm{f}-t_\mathrm{i})\middle|\Phi(t_\mathrm{i})\right\rangle = \int \mathcal{D}\mu_V[\sigma]\,\mathrm{e}^{W_V[\sigma]} \tag{5}$$

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

$$W_V[\sigma] = \ln \prod_{m=1}^{M} \langle \Phi(t_\mathrm{f}) | \mathrm{e}^{-\mathrm{i}(K\hat{\rho})\Delta t/\hbar - \mathrm{i}\sqrt{\mathrm{i}}(\sigma_{t_m}\hat{\rho})\sqrt{\Delta t/\hbar}} | \Phi(t_\mathrm{i}) \rangle. \tag{6}$$

3. Gaussian equivalent representation

The method of GER has been developed by Efimov and Ganbold [10] and bases on the assumption that in the strong coupling regime the FI remains of the Gaussian type, but with another Green function in the measure. The underlying concept originates from quantum field theory and makes use of the fact that the tadpole Feynman diagrams provide the main contributions to the FI under consideration. This implies that the FI over the Gaussian measure must be rewritten in a representation, where the interaction functional is given in normal-ordered form according to a new Gaussian measure and does not contain any linear and quadratic term in the field function. The technique can generally be applied to FI's of the following type:

$$I = \int \mathcal{D}\mu_{D_0}[\varphi] \exp\{g W_{D_0}[\varphi]\}, \tag{7}$$

where g is the coupling constant and

$$W_{D_0}[\varphi] = \int \mathcal{D}\nu[a]\, \mathrm{e}^{\mathrm{i}(a\varphi)} \tag{8}$$

represents the interaction functional with $\mathcal{D}\nu[a]$ as the functional measure and $(a\varphi) = \int \mathrm{d}x\, a(x)\varphi(x)$. The Gaussian measure, $\mathcal{D}\mu_{D_0}[\varphi] = C_{D_0}\mathcal{D}^N\varphi \exp\{-\frac{1}{2}(\varphi D_0^{-1}\varphi)\}$, obeys the normalization condition $\int \mathcal{D}\mu_{D_0}[\varphi]\cdot 1 = 1$. As a result we accomplish the transformation

$$\mathrm{e}^{-F} = \int \frac{\mathcal{D}^N\varphi}{\sqrt{\det D_0}}\, \mathrm{e}^{-1/2(\varphi D_0^{-1}\varphi) + W_{D_0}[\varphi]} \quad \longrightarrow \quad \mathrm{e}^{-F_0} \int \frac{\mathcal{D}^N\varphi}{\sqrt{\det D}}\, \mathrm{e}^{-1/2(\varphi D^{-1}\varphi) + W_D[\varphi]}, \tag{9}$$

where the zeroth-order approximation F_0 is the best variational Gaussian estimate of the initial FI, while the perturbation corrections over W_D give additional contributions to the zeroth-order approximation, i.e., $F = F_0 + F_1 + F_2 + \cdots$.

To derive the GER of the real-time propagator, let us now consider the matrix element of the evolution operator in a single time slice $t \to t + \Delta t$ [18]

$$M(t_\mathrm{f} - t_\mathrm{i}) \propto \int \mathcal{D}\mu_V[\sigma_t]\, \mathrm{e}^{W_V[\sigma_t]} = M_t, \tag{10}$$

where $\mathcal{D}\mu_V[\sigma_t] = C_V \mathcal{D}^N\sigma_t \exp\{-\frac{1}{2}(\sigma_t V^{-1}\sigma_t)\}$ and

$$W_V[\sigma_t] = \ln\langle \Phi_\mathrm{f}(t_\mathrm{f} - t) | \mathrm{e}^{-\mathrm{i}(K\hat{\rho})\Delta t/\hbar - \mathrm{i}\sqrt{\mathrm{i}}(\sigma_t\hat{\rho})\sqrt{\Delta t/\hbar}} | \Phi_i(t - \Delta t) \rangle. \tag{11}$$

Note that here $|\Phi_{\mathrm{i}}(t)\rangle$ and $\langle\Phi_{\mathrm{f}}(t)|$ represent time-dependent wave functions given through $|\Phi_{\mathrm{i}}(t)\rangle = U_\sigma(t-t_{\mathrm{i}})|\Phi(t_{\mathrm{i}})\rangle$ and $\langle\Phi_{\mathrm{f}}(t)| = \langle\Phi(t_{\mathrm{f}})|U_\sigma(t_{\mathrm{f}}-t)$ [21], where U_σ is a time-dependent one-body propagator defined by $U_\sigma(t_m) = \exp[-\mathrm{i}(K\hat{\rho})\Delta t/\hbar - \mathrm{i}\sqrt{\mathrm{i}}(\sigma_{t_m}\hat{\rho})\sqrt{\Delta t/\hbar}]U_\sigma(t_{m-1})$. We see that one recovers the integral representation (7), if one reformulates $W_V[\sigma_t]$ in terms of its functional Fourier transform

$$W_V[\sigma_t] = \frac{1}{(2\pi)^N}\int \mathcal{D}^N\omega_t\,\widetilde{W}_V[\omega_t]\,\mathrm{e}^{\mathrm{i}(\omega_t\sigma_t)} \tag{12}$$

with

$$(\omega_t\sigma_t) = \int \mathrm{d}\mathbf{x}\,\mathrm{d}\mathbf{y}\,\omega_t(\mathbf{x},\mathbf{y})\sigma_t(\mathbf{x},\mathbf{y}), \tag{13}$$

which leads to the functional measure $\mathcal{D}\nu[a] = \mathcal{D}^N\omega_t/(2\pi)^N\,\widetilde{W}_V[\omega_t] = \mathcal{D}\nu[\omega_t]$. In order to properly take into account the fermion MF contribution we perform a shift of the integration contour of integral (10) into the complex plane according to (see also appendix A)

$$\sigma_t(\mathbf{x},\mathbf{y}) \longrightarrow \sigma_t(\mathbf{x},\mathbf{y}) - \mathrm{i}\sqrt{\mathrm{i}}\,\alpha_t(\mathbf{x},\mathbf{y}) \tag{14}$$

and replace its Gaussian weight as follows:

$$V^{-1}(\mathbf{x},\mathbf{y};\mathbf{x}',\mathbf{y}') \longrightarrow D^{-1}\big(\mathbf{x},\mathbf{y};\mathbf{x}',\mathbf{y}'\big), \tag{15}$$

where $D(\mathbf{x},\mathbf{y};\mathbf{x}',\mathbf{y}')$ is an appropriate Green function of the differential operator D^{-1} satisfying the relation $\int \mathrm{d}\mathbf{y}\,\mathrm{d}\mathbf{y}'\,D^{-1}(\mathbf{x},\mathbf{x}';\mathbf{y},\mathbf{y}')D(\mathbf{y},\mathbf{y}';\mathbf{z},\mathbf{z}') = \delta(\mathbf{x}-\mathbf{z})\delta(\mathbf{x}'-\mathbf{z}')$. The FI (10) then reads

$$M_t = \sqrt{\frac{\det D}{\det V}}\exp\left\{\frac{\mathrm{i}}{2}\big(\alpha_t V^{-1}\alpha_t\big)\right\}\int \mathcal{D}\mu_D[\sigma_t]\,\mathrm{e}^{W'_D[\sigma_t,\alpha_t,D]}, \tag{16}$$

where $\mathcal{D}\mu_D[\sigma_t] = C_D\mathcal{D}^N\sigma_t\exp\{-\frac{1}{2}(\sigma_t D^{-1}\sigma_t)\}$ with $\int \mathcal{D}\mu_D[\sigma_t]\cdot 1 = 1$ and

$$W'_D[\sigma_t,\alpha_t,D] = \int \mathcal{D}\nu[\omega_t]\,\mathrm{e}^{\sqrt{\mathrm{i}}(\omega_t\alpha_t)}\,\mathrm{e}^{\mathrm{i}(\omega_t\sigma_t)} + \mathrm{i}\sqrt{\mathrm{i}}\big(\alpha_t V^{-1}\sigma_t\big) - \frac{1}{2}\big(\sigma_t\big[V^{-1}-D^{-1}\big]\sigma_t\big). \tag{17}$$

According to the strategy of the GER approach we must reformulate the interaction functional in (17) in normal-ordered form. For this, we introduce the concept of normal product according to the new Gaussian measure $\mathcal{D}\mu_D$ in the following way:

$$\mathrm{e}^{\mathrm{i}(\omega_t\sigma_t)} =: \mathrm{e}^{\mathrm{i}(\omega_t\sigma_t)} : \mathrm{e}^{-1/2(\omega_t D\omega_t)}, \tag{18}$$

so that $\int \mathcal{D}\mu_D[\sigma_t] : \mathrm{e}^{\mathrm{i}(\omega_t\sigma_t)} := 1$ and $\int \mathcal{D}\mu_D[\sigma_t] : \sigma_t(\mathbf{x}_1,\mathbf{y}_1)\cdots\sigma_t(\mathbf{x}_n,\mathbf{y}_n) := 0$. If we take into account that $\mathrm{e}^z = 1 + z + z^2/2 + e_2^z$ and insert this relation in (18), we obtain

$$\begin{aligned}\mathrm{e}^{\mathrm{i}(\omega_t\sigma_t)} &= \mathrm{e}^{-1/2(\omega_t D\omega_t)} + \mathrm{i}\,\mathrm{e}^{-1/2(\omega_t D\omega_t)}(\omega_t\sigma_t)\\ &\quad - \frac{1}{2} : (\omega_t\sigma_t)^2 : \mathrm{e}^{-1/2(\omega_t D\omega_t)} + : e_2^{\mathrm{i}(\omega_t\sigma_t)} : \mathrm{e}^{-1/2(\omega_t D\omega_t)}.\end{aligned} \tag{19}$$

Introducing (19) in expression (17) of $W'_D[\sigma_t, \alpha_t, D]$ and ordering the terms in powers of σ_t by using a consequence of the concept of normal product, i.e., $\sigma_t(\mathbf{x}, \mathbf{y})\sigma_t(\mathbf{x}', \mathbf{y}') =: \sigma_t(\mathbf{x}, \mathbf{y})\sigma_t(\mathbf{x}', \mathbf{y}') : +D(\mathbf{x}, \mathbf{y}; \mathbf{x}', \mathbf{y}')$, to reformulate the quadratic term in σ_t, we get

$$\begin{aligned} & W'_D[\sigma_t, \alpha_t, D] \\ &\quad = \left[\int \mathcal{D}\nu[\omega_t]\, \mathrm{e}^{\sqrt{\mathrm{i}}(\omega_t\alpha_t)}\, \mathrm{e}^{-1/2(\omega_t D\omega_t)} - \frac{1}{2}\big(\big[V^{-1} - D^{-1}\big]D\big)\right] \\ &\qquad + \left[\mathrm{i}\int \mathcal{D}\nu[\omega_t]\, \mathrm{e}^{\sqrt{\mathrm{i}}(\omega_t\alpha_t)}\, \mathrm{e}^{-1/2(\omega_t D\omega_t)}(\omega_t\sigma_t) + \mathrm{i}\sqrt{\mathrm{i}}\big(\alpha_t V^{-1}\sigma_t\big)\right] \\ &\qquad - \frac{1}{2} : \left[\int \mathcal{D}\nu[\omega_t]\, \mathrm{e}^{\sqrt{\mathrm{i}}(\omega_t\alpha_t)}\, \mathrm{e}^{-1/2(\omega_t D\omega_t)}(\omega_t\sigma_t)^2 + \big(\sigma_t\big[V^{-1} - D^{-1}\big]\sigma_t\big)\right] : \\ &\qquad + \int \mathcal{D}\nu[\omega_t]\, \mathrm{e}^{\sqrt{\mathrm{i}}(\omega_t\alpha_t)}\, \mathrm{e}^{-1/2(\omega_t D\omega_t)} : e_2^{\mathrm{i}(\omega_t\sigma_t)} : . \end{aligned} \tag{20}$$

To concentrate the main contributions to the FI in the new Gaussian measure $\mathcal{D}\mu_D$ we now demand that the linear and quadratic terms in $\sigma_t(\mathbf{x}, \mathbf{y})$ are removed from the interaction functional W'_D in (20). After rearrangement these two conditions give us , respectively, an equation for the shift $\alpha_t(\mathbf{x}, \mathbf{y})$ and the new Gaussian weight $D(\mathbf{x}, \mathbf{y}; \mathbf{x}', \mathbf{y}')$:

$$\alpha_t(\mathbf{x}, \mathbf{y}) = -\frac{1}{\sqrt{\mathrm{i}}}\int \mathrm{d}\mathbf{x}'\, \mathrm{d}\mathbf{y}'\, V\big(\mathbf{x}, \mathbf{y}; \mathbf{x}', \mathbf{y}'\big) W_1\big[\mathbf{x}', \mathbf{y}', \alpha_t\big] \tag{21}$$

$$\begin{aligned} & D\big(\mathbf{x}, \mathbf{y}; \mathbf{x}', \mathbf{y}'\big) \\ &\quad = V\big(\mathbf{x}, \mathbf{y}; \mathbf{x}', \mathbf{y}'\big) - \int \mathrm{d}\mathbf{x}''\, \mathrm{d}\mathbf{y}''\, \mathrm{d}\mathbf{x}'''\, \mathrm{d}\mathbf{y}'''\, V\big(\mathbf{x}, \mathbf{y}; \mathbf{x}'', \mathbf{y}''\big) \\ &\qquad\qquad \times W_2\big[\mathbf{x}'', \mathbf{y}'', \mathbf{x}''', \mathbf{y}''', \alpha_t\big] D\big(\mathbf{x}''', \mathbf{y}'''; \mathbf{x}', \mathbf{y}'\big) \end{aligned} \tag{22}$$

with:

$$W_1\big[\mathbf{x}', \mathbf{y}', \alpha_t\big] = \frac{1}{(2\pi)^N}\int \mathcal{D}^N\omega_t\, \omega_t\big(\mathbf{x}', \mathbf{y}'\big)\widetilde{W}_V[\omega_t]\, \mathrm{e}^{-1/2(\omega_t D[\alpha_t]\omega_t)}\, \mathrm{e}^{\sqrt{\mathrm{i}}(\omega_t\alpha_t)}, \tag{23}$$

$$\begin{aligned} & W_2\big[\mathbf{x}'', \mathbf{y}'', \mathbf{x}''', \mathbf{y}''', \alpha_t\big] \\ &\quad = \frac{1}{(2\pi)^N}\int \mathcal{D}^N\omega_t\, \omega_t\big(\mathbf{x}'', \mathbf{y}''\big)\omega_t\big(\mathbf{x}''', \mathbf{y}'''\big)\widetilde{W}_V[\omega_t]\, \mathrm{e}^{-1/2(\omega_t D[\alpha_t]\omega_t)}\, \mathrm{e}^{\sqrt{\mathrm{i}}(\omega_t\alpha_t)}. \end{aligned} \tag{24}$$

The functionals $W_1[\mathbf{x}', \mathbf{y}', \alpha_t]$ and $W_2[\mathbf{x}'', \mathbf{y}'', \mathbf{x}''', \mathbf{y}''', \alpha_t]$ can now further be recasted in terms of integral-representations depending on α_t. To this end, we first consider the functional expression (23), in which $\omega_t(\mathbf{x}', \mathbf{y}')\widetilde{W}_V[\omega_t]$ can easily be reformulated as (see also [15])

$$\omega_t\big(\mathbf{x}', \mathbf{y}'\big)\widetilde{W}_V[\omega_t] = \frac{1}{\mathrm{i}}\int \mathcal{D}^N\tilde{\alpha}_t\, \frac{\delta W[\tilde{\alpha}_t]}{\delta\tilde{\alpha}_t(\mathbf{x}', \mathbf{y}')}\exp\big[-\mathrm{i}\big(\omega_t\tilde{\alpha}_t\big)\big]. \tag{25}$$

Inserting this expression in (23) we get

$$W_1\big[\mathbf{x}', \mathbf{y}', \alpha_t\big] = \frac{1}{(2\pi)^N\mathrm{i}}\int \mathcal{D}^N\tilde{\alpha}_t\, \frac{\delta W_V[\tilde{\alpha}_t]}{\delta\tilde{\alpha}_t(\mathbf{x}', \mathbf{y}')}\int \mathcal{D}[\omega_t]\, \mathrm{e}^{-1/2(\omega_t D[\alpha_t]\omega_t) - (\omega_t[\mathrm{i}\tilde{\alpha}_t - \sqrt{\mathrm{i}}\alpha_t])}. \tag{26}$$

Then, performing the Gaussian integral over ω_t analytically by employing

$$\int_{-\infty}^{\infty} \mathcal{D}s^N \, \mathrm{e}^{-1/2(s\Lambda s)-(rs)} = \sqrt{\frac{(2\pi)^N}{\det(\Lambda)}} \, \mathrm{e}^{1/2(r\Lambda^{-1}r)},$$

we obtain

$$W_1\big[\mathbf{x}', \mathbf{y}', \alpha_t\big] = \frac{1}{\sqrt{(2\pi)^N \det(D)\mathrm{i}}} \int \mathcal{D}^N \tilde{\alpha}_t \frac{\delta W_V[\tilde{\alpha}_t]}{\delta\tilde{\alpha}_t(\mathbf{x}', \mathbf{y}')} \mathrm{e}^{-1/2([\tilde{\alpha}_t - \alpha_t/\sqrt{\mathrm{i}}]D^{-1}[\alpha_t][\tilde{\alpha}_t - \alpha_t/\sqrt{\mathrm{i}}])}. \quad (27)$$

Next, we consider the functional expression (24) of $W_2[\mathbf{x}'', \mathbf{y}'', \mathbf{x}''', \mathbf{y}''', \alpha_t]$, in which we can easily reexpress $\omega_t(\mathbf{x}'', \mathbf{y}'')\omega_t(\mathbf{x}''', \mathbf{y}''')\tilde{W}_V[\omega_t]$ using the relation [15]

$$\omega_t\big(\mathbf{x}'', \mathbf{y}''\big)\omega_t\big(\mathbf{x}''', \mathbf{y}'''\big)\tilde{W}_V[\omega_t] = -\int \mathcal{D}^N \tilde{\alpha}_t \frac{\delta W_V[\tilde{\alpha}_t]}{\delta\tilde{\alpha}_t(\mathbf{x}'', \mathbf{y}'')\delta\tilde{\alpha}_t(\mathbf{x}''', \mathbf{y}''')} \exp\big[-\mathrm{i}\big(\omega_t\tilde{\alpha}_t\big)\big]. \quad (28)$$

This leads then to

$$W_2\big[\mathbf{x}'', \mathbf{y}'', \mathbf{x}''', \mathbf{y}''', \alpha_t\big] = -\frac{1}{(2\pi)^N} \int \mathcal{D}^N \tilde{\alpha}_t \frac{\delta W_V[\tilde{\alpha}_t]}{\delta\tilde{\alpha}_t(\mathbf{x}'', \mathbf{y}'')\delta\tilde{\alpha}_t(\mathbf{x}''', \mathbf{y}''')} \times \int \mathcal{D}[\omega_t] \, \mathrm{e}^{-1/2(\omega_t D[\alpha_t]\omega_t)-(\omega_t[\mathrm{i}\tilde{\alpha}_t - \sqrt{\mathrm{i}}\alpha_t])}. \quad (29)$$

Performing again the Gaussian integral over ω_t analytically we finally get

$$W_2\big[\mathbf{x}'', \mathbf{y}'', \mathbf{x}''', \mathbf{y}''', \alpha_t\big] = -\frac{1}{\sqrt{(2\pi)^N \det(D)}} \int \mathcal{D}^N \tilde{\alpha}_t \frac{\delta W_V[\tilde{\alpha}_t]}{\delta\tilde{\alpha}_t(\mathbf{x}'', \mathbf{y}'')\delta\tilde{\alpha}_t(\mathbf{x}''', \mathbf{y}''')} \mathrm{e}^{-1/2[\tilde{\alpha}_t - \alpha_t/\sqrt{\mathrm{i}}]D^{-1}[\alpha_t][\tilde{\alpha}_t - \alpha_t/\sqrt{\mathrm{i}}]}. \quad (30)$$

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

$$M_t = \mathrm{e}^{-F_0} \int \mathcal{D}\mu_D[\sigma_t] \, \mathrm{e}^{W_D[\sigma_t]}, \quad (31)$$

where

$$W_D[\sigma_t] = \int \mathcal{D}\nu[\omega_t] \, \mathrm{e}^{\sqrt{\mathrm{i}}(\omega_t\alpha_t)} \, \mathrm{e}^{-1/2(\omega_t D\omega_t)} : e_2^{\mathrm{i}(\omega_t\sigma_t)} : \quad (32)$$

is the new interaction functional and

$$F_0 = -\frac{1}{2}\ln\det\left(\frac{D}{V}\right) - \frac{\mathrm{i}}{2}\big(\alpha_t V^{-1}\alpha_t\big) + \frac{1}{2}\big(\big[V^{-1} - D^{-1}\big]D\big) - \int \mathcal{D}\nu[\omega_t] \, \mathrm{e}^{\sqrt{\mathrm{i}}(\omega_t\alpha_t)} \, \mathrm{e}^{-1/2(\omega_t D\omega_t)} \quad (33)$$

is the zeroth-order approximation of M_t. To conclude, we point out that in the above representation the main contributions to the FI are isolated in the Gaussian measure, while the new interaction functional takes care for non-Gaussian contributions, which can be calculated either numerically by using MC algorithms or analytically by performing, e.g., a perturbation expansion of the new interaction functional $W_D[\sigma_t]$.

Finally, we wish to emphasize that by expanding the functional $W_V[\tilde{\alpha}_t]$ in (27) in a Taylor-series,

$$
\begin{aligned}
&W_V[\tilde{\alpha}_t] \\
&\quad = W_V\big[\tilde{\alpha}_t = 0\big] + \sum_{n=1}^{\infty} \frac{1}{n!} \int\int \cdots \int \left(\frac{\delta^{\{n\}} W_V[\tilde{\alpha}_t]}{\delta\tilde{\alpha}_t(\mathbf{x}_1, \mathbf{y}_1)\delta\tilde{\alpha}_t(\mathbf{x}_2, \mathbf{y}_2)\cdots\delta\tilde{\alpha}_t(\mathbf{x}_n, \mathbf{y}_n)} \right)_{\tilde{\alpha}_t=0} \\
&\qquad \times \tilde{\alpha}_t(\mathbf{x}_1, \mathbf{y}_1)\tilde{\alpha}_t(\mathbf{x}_2, \mathbf{y}_2)\cdots\tilde{\alpha}_t(\mathbf{x}_n, \mathbf{y}_n)\, \mathrm{d}\mathbf{x}_1\, \mathrm{d}\mathbf{x}_2 \cdots \mathrm{d}\mathbf{x}_n\, \mathrm{d}\mathbf{y}_1\, \mathrm{d}\mathbf{y}_2 \cdots \mathrm{d}\mathbf{y}_n, \qquad (34)
\end{aligned}
$$

we can easily derive the first-order approximation of $W_1[\mathbf{x}', \mathbf{y}', \alpha_t]$, which consequently provides the first-order approximation of the shifting function, $\alpha_t^{(1)}(\mathbf{x}, \mathbf{y}) = \sqrt{\Delta t/\hbar} \int \mathrm{d}\mathbf{x}'\, \mathrm{d}\mathbf{y}'\; V(\mathbf{x}, \mathbf{y}; \mathbf{x}', \mathbf{y}') \langle \Phi_\mathrm{f}(t_\mathrm{f} - t)|\hat{\rho}(\mathbf{x}', \mathbf{y}')|\Phi_\mathrm{i}(t)\rangle / \langle \Phi_\mathrm{f}(t_\mathrm{f} - t)|\Phi_\mathrm{i}(t)\rangle$. Since the nth-order functional derivative in (34) is proportional to $(\Delta t)^{n/2}$, we can readily convince ourselves that the approximation is valid in the limit of small time-steps. From this result we conclude that in this regime, the GER procedure shifts the integration path of the real-time propagator, i.e., FI (4), through the stationary point in the complex plane, which corresponds to the MF solution (for further details we refer to appendix A). Thus, we can safely predict that for systems with a relevant contribution from the MF the GER method will remove the overwhelming part of the oscillations of the functional integrand, which will considerably facilitate the calculation in such situations. The potential of this approach for handling physical problems in general can best be assessed by considering calculations based on the auxiliary field formulation of the imaginary-time evolution operator [16,17] or grand canonical partition function [12].

4. Summary and conclusions

In this paper we have shown that the method of Gaussian equivalent representation can also be applied to the real-time many-body evolution operator formulated within the framework of the auxiliary field functional integral formalism. For this, we developed and made use of a generalization of the method, which permits the treatment of interaction functionals nonlocal in the auxiliary field function. This allowed us to eliminate the low-order fluctuations from the interaction functional responsible for the large oscillations of the original functional integrand. As a result we have obtained a new auxiliary field representation, which should be more suitable for computation than the original one. By deriving a first-order approximation of the shifting function, we could already demonstrate that the new method will be useful for calculating systems, where the mean field configuration provides a relevant contribution to the functional integral. Currently, work is in progress, to investigate its efficiency in quantum-chemical applications and to develop accurate techniques for computing higher-order approximations of the shifting function [22].

We believe that the proposed approach will open new perspectives for the development of new computational and analytical tools, to investigate dynamical properties of quantum systems. The existence of claims that the problem is hard to solve [23] or even insoluble [8] is a strong indication of its severity. However, since the real world is a many-body quantum dynamical problem, there is no doubt that further research in this direction is worth the effort.

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Appendix A. Mean field approximation

In this section we derive the MF approximation of the FI representation of the matrix element of the evolution operator given in (10), i.e.,

$$M_t = C_V \int \mathcal{D}^N \sigma_t \, \mathrm{e}^{-S[\sigma_t]}, \tag{A.1}$$

where

$$S[\sigma_t] = \frac{1}{2}\big(\sigma_t V^{-1}\sigma_t\big) - \ln\Big\langle \Phi_\mathrm{f}(t_\mathrm{f}-t)\Big|\mathrm{e}^{-\mathrm{i}(K\hat{\rho})\Delta t/\hbar - \mathrm{i}\sqrt{\mathrm{i}}(\sigma_t\hat{\rho})\sqrt{\Delta t/\hbar}}\Big|\Phi_\mathrm{i}(t-\Delta t)\Big\rangle \tag{A.2}$$

represents the action of the FI. Applying the MF condition to the FI mentioned previously we get

$$\begin{aligned}
&\left(\frac{\delta S[\sigma_t]}{\delta\sigma_t(\mathbf{x},\mathbf{y})}\right)_{\sigma_t^\mathrm{MF}} \\
&\quad = \frac{1}{V^2}\int V^{-1}\big(\mathbf{x},\mathbf{y};\mathbf{x}',\mathbf{y}'\big)\sigma_t\big(\mathbf{x}',\mathbf{y}'\big)\,\mathrm{d}\mathbf{x}'\,\mathrm{d}\mathbf{y}' \\
&\qquad + \mathrm{i}\sqrt{\mathrm{i}}\sqrt{\frac{\Delta t}{\hbar}}\left(\frac{\langle\Phi_\mathrm{f}(t_\mathrm{f}-t)|\hat{\rho}(\mathbf{x},\mathbf{y})\,\mathrm{e}^{-\mathrm{i}(K\hat{\rho})\Delta t/\hbar-\mathrm{i}\sqrt{\mathrm{i}}(\sigma_t\hat{\rho})\sqrt{\Delta t/\hbar}}|\Phi_\mathrm{i}(t-\Delta t)\rangle}{\langle\Phi_\mathrm{f}(t_\mathrm{f}-t)|\mathrm{e}^{-\mathrm{i}(K\hat{\rho})\Delta t/\hbar-\mathrm{i}\sqrt{\mathrm{i}}(\sigma_t\hat{\rho})\sqrt{\Delta t/\hbar}}|\Phi_\mathrm{i}(t-\Delta t)\rangle}\right)_{\sigma_t^\mathrm{MF}} \\
&\quad = \frac{1}{V^2}\int V^{-1}\big(\mathbf{x},\mathbf{y};\mathbf{x}',\mathbf{y}'\big)\sigma_t^\mathrm{MF}\big(\mathbf{x}',\mathbf{y}'\big)\,\mathrm{d}\mathbf{x}'\,\mathrm{d}\mathbf{y}' \\
&\qquad + \mathrm{i}\sqrt{\mathrm{i}}\sqrt{\frac{\Delta t}{\hbar}}\frac{\langle\Phi_\mathrm{f}(t_\mathrm{f}-t)|\hat{\rho}(\mathbf{x},\mathbf{y})|\Phi_\mathrm{i}(t-\Delta t)\rangle}{\langle\Phi_\mathrm{f}(t_\mathrm{f}-t)|\Phi_\mathrm{i}(t-\Delta t)\rangle} = 0.
\end{aligned} \tag{A.3}$$

Solving this equation for $\sigma_t^{\mathrm{MF}}(\mathbf{x}, \mathbf{y})$, we finally obtain

$$\sigma_t^{\mathrm{MF}}(\mathbf{x}, \mathbf{y}) = -\mathrm{i}\sqrt{\mathrm{i}}\sqrt{\frac{\Delta t}{\hbar}} \int \mathrm{d}\mathbf{x}'\,\mathrm{d}\mathbf{y}'\,V\big(\mathbf{x}, \mathbf{y}; \mathbf{x}', \mathbf{y}'\big)\frac{\langle \Phi_{\mathrm{f}}(t_{\mathrm{f}} - t)|\hat{\rho}(\mathbf{x}', \mathbf{y}')|\Phi_{\mathrm{i}}(t)\rangle}{\langle \Phi_{\mathrm{f}}(t_{\mathrm{f}} - t)|\Phi_{\mathrm{i}}(t)\rangle}. \quad \text{(A.4)}$$

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