Gauge-*P* representation and *N*-boson problem with binary interactions

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Recently, the gauge-*P* representation has been introduced to eliminate boundary term problems arising in some cases with the positive-*P* representation. We show that the gauge-*P* representation does not solve the problem in the case of a many-body system with binary interactions, unless the number of atoms is definite. In this case we find a set of stochastic equations for the gauge-*P* representation that reduces the statistical errors with respect to the equations suggested in a previous work. We also analyze the possibility to reduce the statistical errors with appropriate decompositions of the diffusion matrix. Finally, we study the relation between the gauge-*P* and alternative representations.

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I. INTRODUCTION

In this paper we will consider the dynamics of a multidimensional system described by the creation and annihilation Bose operators $\hat{\phi}_i^\dagger$, $\hat{\phi}_i$, respectively, and with the following associated Hamiltonian, normalized to $\hbar$,

$$\hat{\mathcal{H}}=\sum_{i,j} H_{ij}^0 \hat{\phi}_i^\dagger \hat{\phi}_j+\frac{1}{2}\sum_{i,j} V_{ij}\hat{\phi}_i^\dagger \hat{\phi}_j^\dagger \hat{\phi}_i \hat{\phi}_j . \tag{1}$$

With a suitable choice of H_{ij}^0, this is the discretized version of the Hamiltonian of a gas with binary interactions and it is used to describe the dynamics of dilute Bose-Einstein condensates. In the continuum limit we have the correspondence $\hat{\phi}_i \rightarrow \hat{\phi}(\vec{x})$. When the field fluctuations are sufficiently small it is possible to describe the system with the mean-field Gross-Pitaevskii equation of a collective wave-function [1]. However, in this approximation genuine quantum effects are lost. An exact quantum solution is a formidable task for large systems. In quantum mechanics, a system with *N* coordinates is described by a function of *N* variables, thus the quantum state is an element of a functional space with infinite dimensions. Suppose to discretize the variables with a lattice of *M* elements for each dimension, the quantum state is described by M^N elements. On increasing *N*, the dynamical problem becomes rapidly numerically intractable. In these cases Monte Carlo techniques can be useful, since the state is obtained with different suitably weighted statistical realizations of the evolution of *N* classical variables. A statistical method is obtained by the Feynmann's path integral formulation and is used to calculate the thermodynamical properties. However, the path integral is not suitable to evaluate the dynamics, because of well-known phase problems. Alternatively, the stochastic approach can be extended for quasiprobability distributions in the phase space. A Monte Carlo technique has been dealt with in Ref. [2] using the positive-*P* representation. In this representation the density operator is written as a superposition of the operators

$$\hat{\Lambda}(\vec{\alpha},\vec{\beta})\equiv \exp(-\vec{\beta}^*\cdot\vec{\alpha})||\vec{\alpha}\rangle\langle\vec{\beta}||, \tag{2}$$

i.e.,

$$\hat{\rho}=\int \mathcal{D}\alpha\mathcal{D}\beta\hat{\Lambda}(\vec{\alpha},\vec{\beta})P(\vec{\alpha},\vec{\beta}), \tag{3}$$

where $\vec{\alpha}\equiv(\alpha_1,\alpha_2,\ldots)$, $\vec{\beta}\equiv(\beta_1,\beta_2,\ldots)$ are multidimensional complex vectors and $||\vec{\alpha}\rangle$ is a Bargmann state, defined by

$$||\vec{\alpha}\rangle\equiv\sum_{i,n}(\alpha_i\hat{\phi}_i^\dagger)^n/n!|0\rangle. \tag{4}$$

It can be proved that the positive-*P* function $P(\vec{\alpha},\vec{\beta})$ can be chosen positive for any density matrix [3,4]. It is well-known that among the infinite evolution equations of the *P* function there exists a Fokker-Planck equation with a positive definite diffusion matrix [3,4]. Thus, the evolution of *P* can be evaluated using stochastic equations for $\vec{\alpha}$ and $\vec{\beta}$ [5]. However, in some cases, as for Hamiltonian (1), these equations have unstable solutions that diverge at a finite time.

The gauge-*P* representation introduced in Ref. [6] allows us to eliminate the instabilities of the stochastic equations, but it is not able to solve another problem. Smith and Gardiner [7] have demonstrated that the dynamics may not be properly described by the stochastic equations, even though the solutions do not diverge. This occurs because, in the derivation of the equations, nonzero boundary terms arising from an integration by parts are neglected. Such an anomaly occurs also for the system described by Hamiltonian (1) unless a definite number of atoms is considered. In this last case, we introduce a set of stochastic equations that reduces the statistical errors with respect to the equations suggested in Ref. [6]. We also analyze the possibility to reduce the statistical errors with appropriate decompositions of the diffusion matrix. Finally, we find that the stochastic equations in Refs. [8,9] can be recovered from the gauge-*P* representation. In Sec. II we show, with the gauge choice in Ref. [6], that the boundary terms cannot be neglected even by using the gauge-*P* representation. In Sec. III we consider a system with a fixed number of atoms and show that problems with the boundary terms do not occur. Then, we find the optimized stochastic equations. In Sec. IV we analyze the possibility to reduce the statistical errors with appropriate decom-

positions of the diffusion matrix. In Sec. V we study the relation between the gauge-P and alternative representations.

II. GAUGE-P REPRESENTATION AND BOUNDARY TERMS

The equation of motion of $\hat{\rho}$ is $\partial_t\hat{\rho}=-i\hat{\mathcal{H}}\hat{\rho}+i\hat{\rho}\hat{\mathcal{H}}$, which by using Eq. (3) becomes,

$$\int \mathcal{D}\alpha\mathcal{D}\beta\hat{\Lambda}(\vec{\alpha},\vec{\beta})\partial_t P(\vec{\alpha},\vec{\beta}) = \int \mathcal{D}\alpha\mathcal{D}\beta[-i\hat{\mathcal{H}},\hat{\Lambda}(\vec{\alpha},\vec{\beta})]P(\vec{\alpha},\vec{\beta}). \tag{5}$$

It is easily proved that

$$\begin{aligned}\hat{\phi}_i\hat{\Lambda}(\vec{\alpha},\vec{\beta})&=\alpha_i\hat{\Lambda}(\vec{\alpha},\vec{\beta}),\\ \hat{\Lambda}(\vec{\alpha},\vec{\beta})\hat{\phi}_i^\dagger&=\beta_i^*\hat{\Lambda}(\vec{\alpha},\vec{\beta}),\\ \hat{\phi}_i^\dagger\hat{\Lambda}(\vec{\alpha},\vec{\beta})&=(\beta_i^*+\partial_{\alpha_i})\hat{\Lambda}(\vec{\alpha},\vec{\beta}),\\ \hat{\Lambda}(\vec{\alpha},\vec{\beta})\hat{\phi}_i&=(\alpha_i+\partial_{\beta_i^*})\hat{\Lambda}(\vec{\alpha},\vec{\beta}).\end{aligned} \tag{6}$$

Furthermore, because of the analyticity of $\hat{\Lambda}$, we have

$$\partial_{\alpha_i^*}\hat{\Lambda}(\vec{\alpha},\vec{\beta})=\partial_{\beta_i}\hat{\Lambda}(\vec{\alpha},\vec{\beta})=0. \tag{7}$$

Thus, we find that

$$[-i\hat{\mathcal{H}},\hat{\Lambda}]=\sum_{ij}\left\{-iH_{ij}\alpha_j\partial_{\alpha_i}-iV_{ij}\alpha_j\beta_j^*\alpha_i\partial_{\alpha_i} -\frac{i}{2}V_{ij}\alpha_i\alpha_j\partial_{\alpha_i}\partial_{\alpha_j}+\alpha\leftrightarrow\beta+\text{c.c.}\right\}\hat{\Lambda}. \tag{8}$$

At this point, we integrate by parts and obtain

$$\int \mathcal{D}\alpha\mathcal{D}\beta\hat{\Lambda}O_{F.P.}P=0, \tag{9}$$

where

$$O_{F.P.}=\left[\partial_t+\left(iH_{ij}\partial_{\alpha_i}\alpha_j+iV_{ij}\partial_{\alpha_i}\alpha_j\beta_j^*\alpha_i -\frac{i}{2}V_{ij}\partial_{\alpha_i}\partial_{\alpha_j}\alpha_i\alpha_j+\alpha\leftrightarrow\beta+\text{c.c.}\right)\right] \tag{10}$$

This equation is fulfilled if

$$O_{F.P.}P=0. \tag{11}$$

Note that it is not a necessary condition, since $\hat{\Lambda}(\alpha,\beta)$ is an overcomplete set. The Fokker-Planck equation (11) does not have a positive-definite diffusion matrix and, consequently, it does not have an associated stochastic equation. We can use Eqs. (7) to add terms into Eq. (8) which lead to a positive-definite diffusion matrix. A simple choice is the following

$$\left\{\sum_{ij}U_{ij}\alpha_i\alpha_j^*\partial_{\alpha_i}\partial_{\alpha_j^*}+\alpha\leftrightarrow\beta\right\}\hat{\Lambda}, \tag{12}$$

where $U\equiv ZZ^\dagger$ and the matrix Z is, by definition, the square root of $-iV$, i.e., $ZZ\equiv-iV$. Thus, we obtain a Fokker-Planck equation with the following associated stochastic equations

$$\dot{\alpha}_i=-i\sum_j H_{ij}\alpha_j-i\alpha_i\sum_j V_{ij}\alpha_j\beta_j^*+\alpha_i\sum_j Z_{ij}\xi_j^{(1)}, \tag{13}$$

$$\dot{\beta}_i=-i\sum_j H_{ij}\beta_j-i\beta_i\sum_j V_{ij}\beta_j\alpha_j^*+\beta_i\sum_j Z_{ij}\xi_j^{(2)}, \tag{14}$$

where $\xi_i^{(k)}(t)$ are real stochastic functions with $\overline{\xi_i^{(k)}(t)\xi_j^{(l)}(t')}=\delta_{kl}\delta_{ij}\delta(t-t')$. A different choice of the additional terms leads to alternative equations (see Sec. IV). If we neglect the stochastic term and put $\vec{\alpha}=\vec{\beta}$, the equations become the mean-field nonlinear equation which is generally used to study the Bose-Einstein condensates. The two equations have independent noises, thus it is not possible that $\vec{\alpha}=\vec{\beta}$ at every time. This implies that the nonlinear coefficient $-i\Sigma_j V_{ij}\alpha_j\beta_j^*$ of Eqs. (13) and (14) have in general a real part, which is the reason of the well-known instability of these stochastic equations. In the gauge-P representation it is possible to eliminate the destabilizing drift term by adding a diffusion term [6]. In this representation a new complex variable Ω is introduced and the density operator is expanded in the overcomplete basis

$$\hat{\Lambda}_g(\Omega,\vec{\alpha},\vec{\beta})\equiv\Omega\exp(-\vec{\beta}^*\cdot\vec{\alpha})||\vec{\alpha}\rangle\langle\vec{\beta}||=\Omega\hat{\Lambda}(\vec{\alpha},\vec{\beta}). \tag{15}$$

Equation (3) becomes

$$\hat{\rho}=\int \mathcal{D}\alpha\mathcal{D}\beta d\Omega\hat{\Lambda}_g(\Omega,\vec{\alpha},\vec{\beta})P_g(\Omega,\vec{\alpha},\vec{\beta}). \tag{16}$$

Infinite choices of $P_g(\Omega,\vec{\alpha},\vec{\beta})$ are possible for each density operator. One of them is the following

$$P_g(\Omega,\vec{\alpha},\vec{\beta})=\delta(\Omega-1)P(\vec{\alpha},\vec{\beta}), \tag{17}$$

where $P(\vec{\alpha},\vec{\beta})$ is the positive-P representation.

Suppose that in the positive-P representation the stochastic equations are

$$\begin{aligned}\dot{\alpha}_i&=A_i^a+\sum_k B_{ik}^a\xi_k^{(1)}\\ \dot{\beta}_i&=A_i^b+\sum_k B_{ik}^b\xi_k^{(2)},\end{aligned} \tag{18}$$

it is possible to obtain the following equations for $\vec{\alpha}$, $\vec{\beta}$, and Ω in the gauge-P representation [6]

$$\dot{\alpha}_i = \left[A_i^a - \sum_k g_{a,k} B_{ik}^a \right] + \sum_k B_{ik}^a \xi_k^{(1)},$$

$$\dot{\beta}_i = \left[A_i^b - \sum_k g_{b,k} B_{ik}^b \right] + \sum_k B_{ik}^b \xi_k^{(2)},$$

$$\dot{\Omega} = \Omega \sum_k [g_{a,k} \xi_k^{(1)} + g_{b,k}^* \xi_k^{(2)}]. \tag{19}$$

In Ref. [6] the proof is obtained using a real notation. For pedagogical reasons we demonstrate again Eqs. (19), using a complex notation. Since $(\Omega \partial_\Omega - 1)\hat{\Lambda}_g = 0$ and $\partial_{\Omega *} \hat{\Lambda}_g = 0$, by integration by parts it is easy to show that the following terms can be added to the Fokker-Planck equation without modifying the dynamics of the density operator $\hat{\rho}$,

$$\left(\frac{\partial}{\partial \Omega} \Omega - 1 \right) F_1(\Omega, \vec{\alpha}, \vec{\beta}, \partial_\Omega, \partial_{\vec{\alpha}}, \partial_{\vec{\beta}}) P_g(\Omega, \vec{\alpha}, \vec{\beta}),$$

$$\frac{\partial}{\partial \Omega *} F_2(\Omega, \vec{\alpha}, \vec{\beta}, \partial_\Omega, \partial_{\vec{\alpha}}, \partial_{\vec{\beta}}) P_g(\Omega, \vec{\alpha}, \vec{\beta}), \tag{20}$$

where $F_{1,2}$ are generic functions of Ω, α_i, β_i, and their derivatives. It is obvious that Eqs. (18) are valid also in the gauge-P representation, with

$$\dot{\Omega} = 0 \tag{21}$$

for Ω. The Fokker-Planck equation associated with Eqs. (18) and (21) is

$$\frac{\partial P_g}{\partial t} = \left[-\sum_i \frac{\partial}{\partial \gamma_i} D_i + \frac{1}{2} \sum_{ij} \frac{\partial^2}{\partial \gamma_i \partial \gamma_j^*} C_{ij} \gamma_i \gamma_j^* \right] P_g,$$

where

$$\vec{\gamma} = \begin{pmatrix} \vec{\alpha} \\ \vec{\alpha}^* \\ \vec{\beta} \\ \vec{\beta}^* \\ \Omega \\ \Omega^* \end{pmatrix}, \quad \vec{D} = \begin{pmatrix} \vec{A}^a \\ \vec{A}^{a*} \\ \vec{A}^b \\ \vec{A}^{b*} \\ 0 \\ 0 \end{pmatrix}, \quad C = MM^\dagger, \tag{22}$$

and

$$M = \begin{pmatrix} B^a & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ B^{a*} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & B^b & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & B^{b*} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & 0 & 0 \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & 0 & 0 \end{pmatrix}. \tag{23}$$

$\vec{\alpha}$, $\vec{\beta}$, Ω, and their conjugate values are considered as independent variables. Bold zeros are zero submatrices, whose dimensions are consistent with the dimension of the six elements in the column vector $\vec{\gamma}$.

The presence of the redundant variable Ω allows us to obtain a larger set of stochastic equations by means of Eqs. (20). Let us replace M with the following matrix

$$M' = \begin{pmatrix} B^a & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ B^{a*} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & B^b & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & B^{b*} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \vec{g}_a^T & \mathbf{0} & \vec{g}_b^\dagger & \mathbf{0} & 0 & 0 \\ \vec{g}_a^\dagger & \mathbf{0} & \vec{g}_b^T & \mathbf{0} & 0 & 0 \end{pmatrix}, \tag{24}$$

where $\vec{g}_a$ and $\vec{g}_b$ are the column vectors whose elements are $g_{a,i}$ and $g_{b,i}$, respectively. With this modification second-order terms in ∂_{γ_i} are added. Terms with the left-hand factors $\partial_\Omega^2 \Omega^2 = (\partial_\Omega \Omega - 1)\partial_\Omega \Omega$ and $\partial_{\Omega *}$ do not modify the dynamics of the density operator because of Eqs. (20). Thus the only terms that have to be counterbalanced are the following

$$\sum_{ki} \partial_\Omega \Omega (\partial_{\alpha_i} g_{a,k} B_{ik}^a \alpha_i + \partial_{\beta_i} g_{b,k} B_{ik}^b \beta_i + \text{c.c.}) P_g. \tag{25}$$

They can be compensated by adding the following drift terms [see the first of Eqs. (20)]

$$-\sum_{ki} (\partial_{\alpha_i} g_{a,k} B_{ik}^a \alpha_i + \partial_{\beta_i} g_{b,k} B_{ik}^b \beta_i + \text{c.c.}) P_g. \tag{26}$$

So, we obtain the Fokker-Planck equation associated with the stochastic Eqs. (19).

In our case $B_{ij}^a = \alpha_i Z_{ij}$ and $B_{ij}^b = \beta_i Z_{ij}$, thus the second drift term of Eqs. (13) and (14) can be removed with $g_{a,i} = \Sigma_j Z_{ij} \alpha_j \beta_j^*$ and $g_{b,i} = \Sigma_j Z_{ij} \beta_j \alpha_j^*$. We have the following stochastic equations

$$\dot{\alpha}_i = -i \sum_j H_{ij} \alpha_j + \alpha_i \sum_j Z_{ij} \xi_j^{(1)},$$

$$\dot{\beta}_i = -i \sum_j H_{ij} \beta_j + \beta_i \sum_j Z_{ij} \xi_j^{(2)},$$

$$\dot{\Omega} = \Omega \sum_{ij} \alpha_i \beta_i^* [Z_{ij} \xi_j^{(1)} + Z_{ij}^* \xi_j^{(2)}]. \tag{27}$$

They have solutions that do not diverge at a finite time.

It is important to remark an interesting result by Smith and Gardiner [7]. They studied a single mode which is damped by both linear and nonlinear couplings to a zero-temperature reservoir and found that the stochastic equations associated with the standard positive-P distribution lead to large, but finite, excursions. They demonstrated that the dynamics is not properly described by the stochastic equations, even though the solutions do not diverge. The issue of this

anomaly, reported also in [10,11], is the validity of neglecting the boundary terms arising from integration by parts. Let us define the modulus of an operator $\hat{C}$ as follows, $|\hat{C}| \equiv [\mathrm{Tr}(\hat{C}\hat{C}^{\dagger})]^{1/2}$. It is easily proved that $\Omega \exp(-\vec{\beta}^{*}\cdot\vec{\alpha})$ is a constant of motion of Eqs. (27). Indeed, it is sufficient to show that $\delta \ln[\Omega \exp(-\vec{\beta}^{*}\cdot\vec{\alpha})] = \delta[\ln\Omega - \vec{\beta}^{*}\cdot\vec{\alpha}]$ is zero up to the first order in δt. Now suppose that at the initial time the density operator is $|\alpha_0\rangle\langle\alpha_0|$ we can choose at this time the distribution $P_g(\Omega,\vec{\alpha},\vec{\beta}) = \delta[\Omega - \exp(|\vec{\alpha}_0|^2)]\delta(\vec{\alpha}-\vec{\alpha}_0)\delta(\vec{\beta}-\vec{\alpha}_0)$, thus we have $\Omega \exp(-\vec{\beta}^{*}\cdot\vec{\alpha}) = 1$ at every time, where P_g is different from zero. Then, since the modulus of $\hat{\Lambda}_g(\Omega,\boldsymbol{\alpha},\boldsymbol{\beta})$ is $exp(|\alpha|^2/2 + |\beta|^2/2)$, the distribution P_g has to decay rather quickly by increasing $|\alpha|$ and $|\beta|$ in order that the argument of the integral in Eq. (16) has a suitable behavior at the boundary. This is not the case in our system. At sufficiently small times we can neglect the deterministic terms. We diagonalize Z with a unitary transformation of α_i, β_i, and $\xi_i^{(1,2)}$, thus the equations of motion become

$$\dot{\alpha}_i^t \simeq \alpha_i^t \overline{Z_i}\,\overline{\xi_i^{(1)}}, \tag{28}$$

$$\dot{\beta}_i^t \simeq \beta_i^t \overline{Z_i}\,\overline{\xi_i^{(2)}}, \tag{29}$$

where α_i^t, β_i^t and $\overline{\xi_i^{(1,2)}}$ are the transformed variables and noises, respectively, and $\overline{Z_i}$ are the complex eigenvalues of Z. If the initial state is a Dirac's delta centered in (α_i^0, β_i^0), the probability distribution P of $|\alpha_i^t|$ and $|\beta_i^t|$ at the time δt is

$$P(|\alpha_i^t|,|\beta_i^t|,\delta t) \propto \exp\left[-\frac{(\ln|\alpha_i^t| - \ln|\alpha_i^0|)^2}{2\,\delta t Z_R} + (\alpha_i,\alpha_i^0) \leftrightarrow (\beta_i,\beta_i^0) \right]. \tag{30}$$

The modulus of $\hat{\Lambda}_g(\vec{\alpha}^t,\vec{\beta}^t)$ is $\exp[(|\vec{\alpha}^t|^2 + |\vec{\beta}^t|^2)/2]$ that multiplied by P of Eq. (30), diverges for $|\vec{\alpha}^t|, |\vec{\beta}^t| \to \infty$, i.e., the boundary terms are not negligible. Since for an initial coherent state $\Omega \exp(-\vec{\beta}^{*}\cdot\vec{\alpha}) = 1$, the gauge-$P$ representation becomes a Bargmann state representation, where $\hat{\Lambda}_g$ of Eq. (15) is replaced by $\hat{\Lambda}^B \equiv ||\alpha\rangle\langle\beta||$. In this case, it has been shown that the statistical method not only gives erroneous results, but leads also to an infinite statistical uncertainty at every time [8].

In the following section we consider the case of a fixed number of atoms and show that the boundary terms are always negligible in contrast with the preceding case. We introduce a set of stochastic equations that reduce the statistical error with respect to the equations suggested in Ref. [6].

III. *N* PARTICLE SYSTEM

Let $\hat{Q}_N$ be the projector onto the Hilbert subspace S_N associated with a fixed number of atoms. We consider only the states in this subspace. The corresponding density operator can be written in the following way:

$$\hat{\rho} = \hat{Q}_N \hat{\rho} \hat{Q}_N = K \int d\Omega \mathcal{D}\alpha \mathcal{D}\beta \hat{\Lambda}_g^N(\Omega,\vec{\alpha},\vec{\beta}) P_g^N(\Omega,\vec{\alpha},\vec{\beta}),$$

where

$$\hat{\Lambda}_g^N \equiv \Omega \exp(-\vec{\alpha}\cdot\vec{\beta}^{*}) |N{:}\vec{\alpha}\rangle\langle N{:}\vec{\beta}| \propto \hat{Q}_N \hat{\Lambda}_g \hat{Q}_N \tag{31}$$

with $|N{:}\vec{\alpha}\rangle \equiv (\vec{\alpha}\cdot\hat{\vec{\phi}}^{\dagger})^N/\sqrt{N!}|0\rangle$ and $\hat{\vec{\phi}} \equiv (\hat{\phi}_1, \hat{\phi}_2, \ldots)$. K is a normalization constant.

In the representation of Ref. [9] the density operator is written as a superposition of the operators $\hat{\Lambda}_C \equiv |N{:}\alpha\rangle\langle N{:}\beta|$. So, this representation differs from the gauge-P representation, in the subspace S_N, by a factor $\Omega \exp(-\vec{\alpha}\cdot\vec{\beta})$ (see Sec. V).

Let us show that the boundary terms are negligible. The modulus of $\hat{\Lambda}_g^N$ is

$$|\Omega \exp(-\vec{\alpha}\cdot\vec{\beta}^{*})||\vec{\alpha}|^N |\vec{\beta}|^N. \tag{32}$$

Since $|\Omega \exp(-\vec{\alpha}\cdot\vec{\beta}^{*})|$ is a constant of motion of the stochastic Eqs. (27) (see preceding section), the modulus of $\hat{\Lambda}_g^N$ is $\overline{K}|\vec{\alpha}|^N|\vec{\beta}|^N$, $\overline{K}$ being a multiplicative constant. Once multiplied by P of Eq. (30), this modulus does not diverge for $\vec{\alpha},\vec{\beta} \to \infty$. It is reasonable to suppose that this occurs also at a finite time. Thus, the stochastic equations are exact. However, the statistical error with a fixed number of realizations can grow very rapidly in time for high N since fluctuations of $|\alpha|$ and $|\beta|$ are amplified by the exponent N in Eq. (32).

We have seen that in the gauge-P representation we can add diffusion terms in the Fokker-Planck equation if we add also suitable drift terms. We now use this property to reduce the statistical fluctuations. We impose that the variation of the modulus of $\hat{\Lambda}_g^N$ is zero at the order of the square root of the time integration step δt. This condition is fulfilled if we choose the following equation for Ω

$$\dot{\Omega} = \Omega \sum_{ij} \{\alpha_i \beta_i^{*}[Z_{ij}\xi_j^{(1)} + Z_{ij}^{*}\xi_j^{(2)}] - N[|\alpha_i|^2/|\alpha|^2 Z_{ij}\xi_j^{(1)} + |\beta_i|^2/|\beta|^2 Z_{ij}^{*}\xi_j^{(2)}]\}. \tag{33}$$

From Eqs. (19), we find that the corresponding equations for α_i and β_i are

$$\dot{\alpha}_i = \sum_j \left[-iH_{ij}\alpha_j - iN\alpha_i V_{ij} \frac{|\alpha_j|^2}{|\alpha|^2} + \alpha_i Z_{ij}\xi_j^{(1)} \right],$$

$$\dot{\beta}_i = \sum_j \left[-iH_{ij}\beta_j - iN\beta_i V_{ij} \frac{|\beta_j|^2}{|\beta|^2} + \beta_i Z_{ij}\xi_j^{(2)} \right]. \tag{34}$$

They have stable solutions, as Eqs. (27). Even though $|\hat{\Lambda}_g^N|$ is constant at the order $(\delta t)^{1/2}$, it is not the case at the order δt. Now, let us evaluate the variation of the modulus of $\hat{\Lambda}_g^N$ at this order. It corresponds to the evaluatation of variation of $\ln|\hat{\Lambda}_g^N|$ multiplied by $|\hat{\Lambda}_g^N|$ since $|\hat{\Lambda}_g^N|$ is constant at the order $(\delta t)^{1/2}$. We have

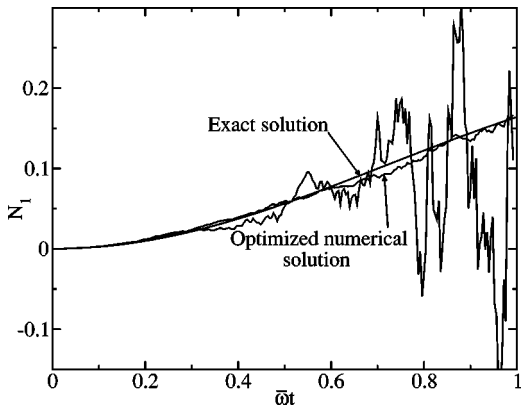

FIG. 1. Mean fraction of atoms in level 1 in the two-mode model for $\omega=\bar{\omega}=1$ and $N=2$. The optimized numerical solution is evaluated by means of Eqs. (33) and (34). The line with larger fluctuations is obtained from Eqs. (19) [6]. We have used 200 realizations.

$$\delta \ln|\hat{\Lambda}_g^N| = \frac{N}{2}\left(U_{00} - \sum_{ij} U_{ij} \frac{|\alpha_i|^2|\alpha_j|^2}{|\alpha|^4} \right) \delta t + \frac{N}{2}\left(U_{00} - \sum_{ij} U_{ij} \frac{|\beta_i|^2|\beta_j|^2}{|\beta|^4} \right) \delta t \leqslant N U_{00} \delta t. \tag{35}$$

This equation is obtained by supposing that $U_{00}=U_{ii}$, for every i. This result is identical to the one that we can obtain by the stochastic formulation in Refs. [8,9]. In Sec. V we show the relation between that approach and Eqs. (33) and (34). Note that the aspectation value of $\hat{\Lambda}_g^N$ has to be equal to one, thus if its modulus increases exponentially with the coefficient NU_{00}, then interference cancellation among the statistical realizations has to occur. This implies also a statistical fluctuation of the aspectation value over a finite number of realizations. The statistical error increases exponentially in the time. It is indeed the negative aspect of a Monte Carlo method, whereby the equations have a reduced number of variables, but a number of realizations growing exponentially by increasing t and N is necessary to reduce the statistical error. Thus, the exponential complexity of a quantum system is not circumvented by using a statistical method. However, such a method can be very useful when $NU_{00}\Delta t$ is not too large, Δt being the time integration.

We test the stochastic Eqs. (33) and (34) by considering a two-mode problem with $V_{ij}=2\omega\delta_{ij}$, $H_{12}=H_{22}=0$, and $H_{12}=H_{21}=\bar{\omega}/2$. In Fig. 1, we report the mean fraction N_1 of atoms in the level 1 for $\omega=\bar{\omega}=1$ and $N=2$. At the initial time $\Omega=1$ and $\alpha_1=\beta_1=0$ (every atom is in level 2). Note that the solution of Eqs. (33) and (34) has considerably smaller statistical errors than the one of Eqs. (19). We have chosen a small number of atoms to have a rapid convergence with Eqs.(19).

In Fig. 2 we plot, with the error bars, the same quantity as in Fig. 1, but with the parameters $N=17$, $\bar{\omega}=1$, and $\omega=0.1$, which have been used in Ref. [9]. The number of realizations is 2×10^5. In this case we have considered only the optimized Eqs. (33) and (34), since with Eqs. (19) the statistical errors are too large. Equations (33) and (34) yield statistical errors compatible with the ones in Ref. [9] (see Fig. 1(d) in Ref. [9]), as suggested by Eq. (35).

During the dynamical evolution almost all the atoms remain in level 2, so the variation $\delta\ln|\hat{\Lambda}_g^N|$ in Eq. (35) is $\ll NU_{00}\delta t$. This is not the case if we choose a different initial state. In Fig. 3, we consider the same case as in Fig. 2, but at the initial time the variables are $\Omega=1$, $\alpha_1=\beta_1=\sqrt{0.2N}$, and $\alpha_2=\beta_2=-\sqrt{0.8N}$. The statistical errors are larger. This occurs also with the approach in Ref. [9].

Note that the stochastic term in Eq. (33) is of the order of $\Omega N\sqrt{V}\xi$, in contrast with the ones of α_i and β_i that are of the order $\alpha\sqrt{V}\xi$ and $\beta\sqrt{V}\xi$, respectively. Thus, in general, the equation for Ω requires a smaller integration step. To circumvent this inconvenience, we can replace Ω in Eq. (15) with Ω^N so that the stochastic term becomes of the order $\Omega\sqrt{V}\xi$. However, a more suitable replacement is performed with $\exp(\Omega)$. With this choice the $\dot{\Omega}$ in Eq. (33) is replaced by $\Omega\dot{\Omega}$. However, since the stochastic equations are written in the Ito formalism, the substitution in these equations has to be accomplished with the addition of a drift term in the

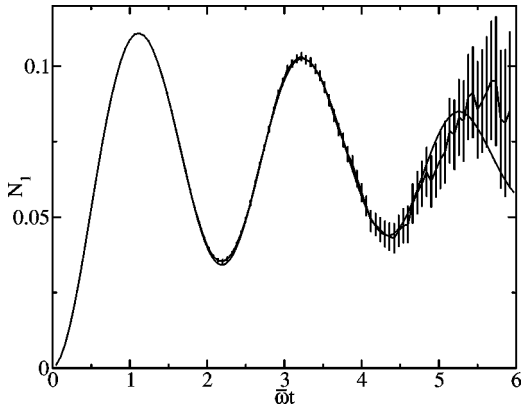

FIG. 2. Mean fraction of atoms in level 1 in the two-mode model for $\omega=0.1$, $\bar{\omega}=1$, $N=2$, and 2×10^5 realizations. At the initial time $\alpha_1=\beta_1=0$ and $\Omega=1$.

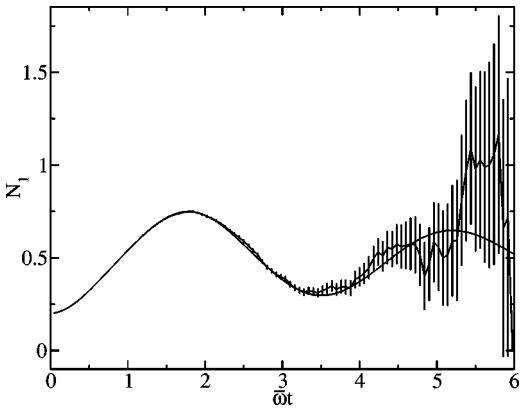

FIG. 3. The same as in Fig. 2, but with $\Omega=1$, $\alpha_1=\beta_1=\sqrt{0.2N}$, and $\alpha_2=\beta_2=-\sqrt{0.8N}$ at the initial time.

equation for Ω [5], which then becomes

$$\dot{\Omega}=\sum_{ij}\left\{\alpha_i\beta_i^*[Z_{ij}\xi_j^{(1)}+Z_{ij}^*\xi_j^{(2)}]\right.$$
$$-N[|\alpha_i|^2/|\alpha|^2 Z_{ij}\xi_j^{(1)}+|\beta_i|^2/|\beta|^2 Z_{ij}^*\xi_j^{(2)}]$$
$$\times\frac{i}{2}N^2\frac{|\alpha_i|^2|\alpha_j|^2}{|\alpha|^4}V_{ij}-\frac{i}{2}N^2\frac{|\beta_i|^2|\beta_j|^2}{|\beta|^4}V_{ij}$$
$$\left.+iN\frac{|\alpha_i|^2}{|\alpha|^2}\alpha_j\beta_j^*V_{ij}-iN\frac{|\beta_i|^2}{|\beta|^2}\alpha_j\beta_j^*V_{ij}\right\}. \quad (36)$$

IV. ALTERNATIVE DECOMPOSITIONS OF THE DIFFUSION MATRIX

In Ref. [12] it has been shown that the stochastic error can be reduced by choosing a different decomposition of the diffusion matrix. We investigate if a different decomposition can reduce the exponential growth of $|\hat{\Lambda}_g^N|$. Let us indicate with $\vec{z}$ the set of complex variables α_i and β_i^*. The diffusion term with only derivative in z can be written in the following way:

$$\frac{1}{2}\sum_{i,j}\frac{\partial^2}{\partial z_i\partial z_j}(BB^{\dagger *})_{i,j}P_g^N$$
$$=\frac{1}{2}\sum_{i,j}\frac{\partial^2}{\partial z_i\partial z_j}(BOO^{\dagger *}B^{\dagger *})_{i,j}P_g^N, \quad (37)$$

where B is the matrix in a particular decomposition and O is a complex matrix such that $OO^{\dagger *}=1$. As previously done, we use a matrix with 2×2 blocks for B, with the blocks of the first column equal to Z and Z^*. Also BO is a valid decomposition matrix. Note that the terms with one derivative in z^* and one in z are not in general invariant with respect to the transformation $B\rightarrow BO$, however these terms do not influence the evolution of the density operator because of Eqs. (7). Also terms with one derivative in Ω and one in z are not invariant unless a suitable transformation of $\vec{g}_a$, $\vec{g}_b$ is performed. The transformation of $\vec{g}_a$, $\vec{g}_b$, and B is equivalent to replacing the real noises $\xi_i^{(1,2)}$ with the following complex noises:

$$\eta_i^{(1)}=\sum_j[\Xi_{ij}^{(1,1)}\xi_j^{(1)}+\Xi_{ij}^{(1,2)}\xi_j^{(2)}],$$

$$\eta_i^{(2)}=\left\{\sum_j[\Xi_{ij}^{(2,1)}\xi_j^{(1)}+\Xi_{ij}^{(2,2)}\xi_j^{(2)}]\right\}^*, \quad (38)$$

where the complex coefficients $\Xi_{ij}^{(a,b)}$ fulfill the conditions

$$\sum_k[\Xi_{ik}^{(a,1)}\Xi_{jk}^{(b,1)}+\Xi_{ik}^{(a,2)}\Xi_{jk}^{(b,2)}]=\delta_{ij}\delta_{ab}. \quad (39)$$

We now show that the exponential growth of $\hat{\Lambda}_g^N$ is minimal with the standard decomposition. Replacing $\xi_i^{(1,2)}$ with the complex noises $\eta_i^{(1,2)}$, we have

$$\frac{d}{dt}\ln|\hat{\Lambda}_g^N|=\frac{N}{2}\sum_{ijr}[A_{ij}(R_{ir}R_{jr}^*+S_{ir}S_{jr}^*)$$
$$+B_{ij}(\overline{R}_{ir}\overline{R}_{jr}^*+\overline{S}_{ir}\overline{S}_{jr}^*)], \quad (40)$$

where $A_{ij}=|\alpha_i|^2/|\alpha|^2\delta_{ij}-|\alpha_i|^2|\alpha_j|^2/|\alpha|^4$, $B_{ij}=|\beta_i|^2/|\beta|^2\delta_{ij}-|\beta_i|^2|\beta_j|^2/|\beta|^4$, $R_{ir}\equiv\Sigma_k Z_{ik}\Xi_{kr}^{(1,1)}$, $S_{ir}\equiv\Sigma_k Z_{ik}\Xi_{kr}^{(1,2)}$, $\overline{R}_{ir}\equiv\Sigma_k Z_{ik}\Xi_{kr}^{(2,2)}$, and $\overline{S}_{ir}\equiv\Sigma_k Z_{ik}\Xi_{kr}^{(2,1)}$. Let O_A and O_B be orthogonal matrices that diagonalize A_{ij} and B_{ij}, i.e., $(O_A^\dagger AO_A)_{ij}=\delta_{ij}a_i$ and $(O_B^\dagger BO_B)_{ij}=\delta_{ij}b_i$, a_i and b_i being the eigenvalues of A and B, respectively. Using these transformations in Eq. (40) we have

$$\frac{d}{dt}\ln|\hat{\Lambda}_g^N|=\frac{N}{2}\sum_{ir}[a_i(O_A^tR)_{ir}(O_A^tR^*)_{ir}$$
$$+a_i(O_A^tS)_{ir}(O_A^tS^*)_{ir}$$
$$+b_i(O_B^t\overline{R})_{ir}(O_B^t\overline{R}^*)_{ir}b_i(O_B^t\overline{S})_{ir}(O_B^t\overline{S}^*)_{ir}]. \quad (41)$$

Note that $O_{A,B}$ can be chosen with real coefficients, since A and B are real matrices. The eigenvalues of A and B are positive, since $\Sigma_{ij}v_iv_jA_{ij}$ and $\Sigma_{ij}v_iv_jB_{ij}$ are positive for every v_i. This implies the following inequality:

$$\frac{d}{dt}\ln|\hat{\Lambda}_g^N|\geq\frac{N}{2}\left|\sum_{ir}[a_i(O_A^tR)_{ir}(O_A^tR)_{ir}+a_i(O_A^tS)_{ir}(O_A^tS)_{ir}\right.$$
$$\left.+b_i(O_B^t\overline{R})_{ir}(O_B^t\overline{R})_{ir}b_i(O_B^t\overline{S})_{ir}(O_B^t\overline{S})_{ir}]\right|$$
$$=\frac{N}{2}\left|\sum_{ir}[a_i(O_A^tZ)_{ir}(O_A^tZ^*)_{ir}\right.$$
$$\left.+b_i(O_B^tZ)_{ir}(O_B^tZ^*)_{ir}]\right|$$
$$=\frac{N}{2}\sum_{ij}[A_{ij}U_{ij}+B_{ij}U_{ij}]$$
$$=\frac{N}{2}\left(U_{00}-\sum_{ij}U_{ij}\frac{|\alpha_i|^2|\alpha_j|^2}{|\alpha|^4}\right)+\alpha\leftrightarrow\beta\equiv\Gamma_m. \quad (42)$$

In this chain of derivations we have used Eqs. (39) and the fact that Z can be decomposed into a real matrix and a complex factor. The inequality (42) implies that the minimal value of $d/dt\ln|\hat{\Lambda}_g^N|$ is obtained with the standard decomposition, for which Eq. (35) is fulfilled.

It is important to understand that the minimization of $d/dt\ln|\hat{\Lambda}_g^N|$ is a single-step optimization. It is the simplest attempt to reduce the statistical errors. However, this does

not warrant a minimization of the fluctuations at a finite evolution time, since Γ_m is a function of α_i and β_i, whose evolutions depend on the decomposition choice. Furthermore, we can obtain a single-step optimization for a specific observable that does not coincide with the minimization of $d/dt \ln|\hat{\Lambda}_g^N|$. These observations are in accordance with the results in Ref. [12], where an error reduction is obtained with respect to the standard decomposition for a specific problem that is solvable analytically.

Note that in a Bose-Einstein condensate the quantity $\Sigma_{ij} U_{ij}|\alpha_i|^2|\alpha_j|^2/|\alpha|^4$ is in general negligible with respect to U_{00}. In the s-wave approximation, the interparticle potential $V(\vec{r}-\vec{r}')$ is replaced with an effective interaction

$$V(\vec{r}-\vec{r}') = g\,\delta(\vec{r}'-\vec{r}), \tag{43}$$

where the coupling constant is related to the scattering length a through $g=4\pi\hbar^2 a/m$. When the stochastic equations are solved using a spatial lattice, the Dirac's delta in Eq. (43) is replaced by a Kronecker delta, that is,

$$U_{ij} = |V_{ij}| = \frac{|g|}{r_0^3}\,\delta_{ij}, \tag{44}$$

r_0 being the lattice step. We have

$$\sum_{ij} U_{ij}\frac{|\alpha_i|^2|\alpha_j|^2}{|\alpha|^4} = \sum_i \frac{|g|}{r_0^3}\frac{|\alpha_i|^4}{|\alpha|^4} \sim \frac{|g|}{r_0^3}\frac{v}{r_0^3} \ll \frac{|g|}{r_0^3} = U_{00},$$

where v is the volume of the condensate. Thus, Γ_m is nearly independent on α_i and β_i and the single-step optimization minimizes the growth of $|\hat{\Lambda}_g^N|$ also at a finite time.

V. RELATION OF THE GAUGE-P REPRESENTATION WITH OTHER REPRESENTATIONS

In the previous sections we have considered the gauge-P representation. It is possible to introduce a more general distribution that includes the positive-P, the gauge-P and the Bargmann representations. In the N-particle case, the last two become the represention used in Sec. III and Ref. [9].

First let us generalize the positive-P representation in the following way:

$$\hat{\rho} = \int \mathcal{D}\alpha\mathcal{D}\beta\,\hat{\Lambda}_f(\vec{\alpha},\vec{\beta})P_f(\vec{\alpha},\vec{\beta}), \tag{45}$$

where

$$\hat{\Lambda}_f(\vec{\alpha},\vec{\beta}) \equiv \exp[f(\vec{\beta}^*\cdot\vec{\alpha})]|\,|\vec{\alpha}\rangle\langle\vec{\beta}\,|| \tag{46}$$

and f is generic function. To obtain a Fokker-Planck equation with a positive-definite diffusion matrix, it is necessary that $\hat{\Lambda}_f$ is analytic, i.e.,

$$\partial_{\alpha_i^*}\hat{\Lambda}_f(\vec{\alpha},\vec{\beta}) = \partial_{\beta_i}\hat{\Lambda}_f(\vec{\alpha},\vec{\beta}) = 0. \tag{47}$$

This is fulfilled if f is analytic. Thus, we can obtain the following stochastic equations:

$$\dot{\alpha}_i = -i\sum_j H_{ij}\alpha_j + if'\alpha_i\sum_j V_{ij}\alpha_j\beta_j^* + \alpha_i\sum_j Z_{ij}\xi_j^{(1)}, \tag{48}$$

$$\dot{\beta}_i = -i\sum_j H_{ij}\beta_j + if'\beta_i\sum_j V_{ij}\beta_j\alpha_j^* + \beta_i\sum_j Z_{ij}\xi_j^{(2)}. \tag{49}$$

A further generalization of Eqs. (45) and (46) is the following:

$$\hat{\rho} = \int \mathcal{D}\alpha\mathcal{D}\beta d\Omega\,\hat{\Lambda}_{g,f}(\Omega,\vec{\alpha},\vec{\beta})P_{g,f}(\Omega,\vec{\alpha},\vec{\beta}), \tag{50}$$

where

$$\hat{\Lambda}_{g,f}(\vec{\alpha},\vec{\beta}) \equiv \Omega\exp[f(\vec{\beta}^*\cdot\vec{\alpha})]|\,|\vec{\alpha}\rangle\langle\vec{\beta}\,|| = \Omega\hat{\Lambda}_f(\vec{\alpha},\vec{\beta}). \tag{51}$$

It includes, as a particular case, the positive-P, the gauge-P, and the Bargmann representations.

It is evident that the representations (50) and (51) can be always reduced to the case $f=0$ with the variable transformation $\Omega\rightarrow\exp(-f)\Omega$. Without loss in generality, from now on we consider this representation and call it ''Bargamm gauge-P representation.'' It is related to the gauge-P representation by means of the transformation $\Omega \rightarrow \exp(-\vec{\alpha}\cdot\vec{\beta}^*)\Omega$ to have nondiverging trajectories. Note that for $f=0$ it is not necessary to introduce the variable Ω to have nondiverging trajectories. However, also in this case the boundary terms are not negligible, unless the number of particle is well-defined. For an N-particle system, the representation becomes

$$\hat{\rho} = \int \mathcal{D}\alpha\mathcal{D}\beta d\Omega\,\hat{\Lambda}_g^B(\Omega,\vec{\alpha},\vec{\beta})P_g^B(\Omega,\vec{\alpha},\vec{\beta}), \tag{52}$$

where

$$\hat{\Lambda}_g^B(\Omega,\vec{\alpha},\vec{\beta}) \equiv \Omega|N{:}\vec{\alpha}\rangle\langle N{:}\vec{\beta}|. \tag{53}$$

For $\Omega\equiv 1$, we recover the representation of Ref. [9]. With Ω constant the dynamical equations are the same as in the Bargmann representation, i.e. [see Eqs. (48) and (49)],

$$\dot{\alpha}_i = -i\sum_j H_{ij}\alpha_j + \alpha_i\sum_j Z_{ij}\xi_j^{(1)},$$

$$\dot{\beta}_i = -i\sum_j H_{ij}\beta_j + \beta_i\sum_j Z_{ij}\xi_j^{(2)}. \tag{54}$$

As in the gauge-P representation, it is possible to add suitable diffusion and drift terms to the Fokker-Planck equation without modifying the dynamics of the density operator. We have the following stochastic equations:

$$\dot{\alpha}_i = -i\sum_j H_{ij}\alpha_j + \alpha_i \sum_j Z_{ij}\xi_j^{(1)} - \sum_k \alpha_i Z_{ik} g_{a,k},$$

$$\dot{\beta}_i = -i\sum_j H_{ij}\beta_j + \beta_i \sum_j Z_{ij}\xi_j^{(2)} - \sum_k \beta_i Z_{ik} g_{b,k},$$

$$\dot{\Omega} = \Omega \sum_k [g_{a,k}\xi_k^{(1)} + g_{b,k}^* \xi_k^{(2)}]. \tag{55}$$

For

$$g_{a,k} = -N\sum_j \frac{|\alpha_j|^2}{|\alpha|^2} Z_{jk},$$

$$g_{b,k} = -N\sum_j \frac{|\beta_j|^2}{|\beta|^2} Z_{jk}, \tag{56}$$

the variation $\delta \ln|\hat{\Lambda}_g^B|$ is zero at the order $(\delta t)^{1/2}$. Equations (55) become

$$\dot{\alpha}_i = -i\sum_j \left[H_{ij}\alpha_j + \alpha_i Z_{ij}\xi_j^{(1)} - iN\alpha_i \frac{|\alpha_j|^2}{|\alpha|^2} V_{ij} \right],$$

$$\dot{\beta}_i = -i\sum_j \left[H_{ij}\beta_j + \beta_i Z_{ij}\xi_j^{(2)} - iN\beta_i \frac{|\beta_j|^2}{|\beta|^2} V_{ij} \right],$$

$$\dot{\Omega} = -N\Omega \sum_{kj} \left[\frac{|\alpha_j|^2}{|\alpha|^2} Z_{jk}\xi_k^{(1)} + \frac{|\beta_j|^2}{|\beta|^2} Z_{jk}^* \xi_k^{(2)} \right]. \tag{57}$$

The variation of $\ln|\hat{\Lambda}_g^B|$ at the order δt is equal to $\delta \ln|\hat{\Lambda}_g^N|$ of Eq. (35). This is evident, since the gauge-P and the Bargmann gauge-P representations differ by a transformation of Ω.

Note that $\hat{\Lambda}_g^B(\Omega, \vec{\alpha}, \vec{\beta})$ satisfies the following property:

$$\hat{\Lambda}_g^B(\Omega, \vec{\alpha}, \vec{\beta}) = \hat{\Lambda}_g^B(1, \Omega^{N/2}\vec{\alpha}, \Omega^{N/2}\vec{\beta}). \tag{58}$$

Thus, in a N-particle system the Bargmann gauge-P representation is equivalent to the Bargmann representation, whose variables $\vec{\alpha}$ and $\vec{\beta}$ are replaced by $\vec{\alpha}' = \Omega^{N/2}\vec{\alpha}$ and $\vec{\beta}' = \Omega^{N/2}\vec{\beta}$. With a little of algebra, we find that the equations for $\vec{\alpha}'$ and $\vec{\beta}'$ are

$$\dot{\alpha}_i' = -i\sum_j H_{ij}\alpha_j' - i(N-1)\alpha_i' \sum_j V_{ij}|\alpha_j'|^2 + \frac{i}{2}(N-1)\alpha_i' \sum_{jk} V_{jk} \frac{|\alpha_j'|^2 |\alpha_k'|^2}{|\alpha'|^4} + \sum_k Q_{\alpha'}^{ik} \alpha_k' \sum_j Z_{kj}\xi_j^{(1)}, \tag{59}$$

$$\dot{\beta}_i' = -i\sum_j H_{ij}\beta_j' - i(N-1)\beta_i' \sum_j V_{ij}|\beta_j'|^2 + \frac{i}{2}(N-1)\beta_i' \sum_{jk} V_{jk} \frac{|\beta_j'|^2 |\beta_k'|^2}{|\beta'|^4} + \sum_k Q_{\beta'}^{ik} \beta_k' \sum_j Z_{kj}\xi_j^{(1)}, \tag{60}$$

where $\Sigma_k Q_\alpha^{ik} v_k$ projects the vector $\vec{v}$ orthogonally to $\vec{\alpha}$. These are an implementation of the stochastic approach of Refs. [8,9] (see, in particular, Ref. [8]). These equations can be obtained also without introducing the variable Ω. In the Bargmann representation, we have

$$\left(\sum_i \alpha_i \frac{\partial}{\partial \alpha_i} - N \right) \hat{\Lambda}^B = \left(\sum_i \beta_i^* \frac{\partial}{\partial \beta_i^*} - N \right) \hat{\Lambda}^B = 0. \tag{61}$$

They allow us to add the following terms to the Fokker-Planck equation associated with the stochastic Eqs. (54):

$$\sum_{ijl} \left\{ iV_{ij} \frac{|\alpha_i|^2}{|\alpha|^2} \alpha_j \left[\sum_k \alpha_k \frac{\partial}{\partial \alpha_k} - (N-1) \right] \frac{\partial}{\partial \alpha_j} - \frac{i}{2} V_{ij} \frac{|\alpha_i|^2 |\alpha_j|^2}{|\alpha|^4} \sum_l \alpha_l \left[\sum_k \alpha_k \frac{\partial}{\partial \alpha_k} - (N-1) \right] \frac{\partial}{\partial \alpha_l} + c.c. + \alpha \leftrightarrow \beta \right\} \hat{\Lambda}^B. \tag{62}$$

With suitable choice of terms for the derivatives $\partial_{\alpha_i}\partial_{\alpha_j^*}$ and $\partial_{\beta_i}\partial_{\beta_j^*}$ we obtain a positive definite Fokker-Planck equation, whose associated stochastic equations are Eqs. (59) and (60).

VI. CONCLUSION

We have shown that the gauge-P representation is not able to eliminate boundary term problems, unless the number of atoms is definite. We have found in this representation a set of optimized stochastic equations that considerably reduce the statistical errors, as compared to previous equations. We have analyzed the possibility to reduce the statistical errors with appropriate decompositions of the diffusion matrix and we have found that a single-step optimization is obtained with the standard decomposition. We have also studied the relation between the gauge-P representation, the Bargmann representation, and the one used in Refs. [8,9], whose results are recovered.

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